DIBORON-MEDIATED REDUCTIVE COUPLING OF IMINES: DIVERGENT DIASTEREOCONTROL AND ACTIVATION OF TETRAALKOXYDIBORONS

By

Ryan M. Fornwald

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ABSTRACT

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Diborons are a paradox: despite featuring a highly electron deficient boron-boron bond, they are powerful reducers. The steric and electronic properties of their substituents have an enormous influence on the reactivity of the boron-boron bond, offering the potential to control diastereoselectivity, regioselectivity, chemoselectivity, and absolute stereochemistry of diboron-mediated reactions.

Recently, *N*-borylpyridinyl radicals were reported to form via homolytic cleavage of dicoordinate bis-pyridine-diboron complexes. These species reductively dearomatize pyrazines, aromatize *p*-quinones, and deoxygenate sulfoxides. Additionally, they undergo dimerization reactions that suffer from poor regioselectivity and diastereoselectivity. However, more recently, dicoordinate bis-isoquinoline-diboron complexes were reported to undergo highly diastereoselective carbon-carbon bond forming [3,3]-sigmatropic rearrangements. Impressively, this work was expanded to include enantioselective reductive imine couplings.

However, these reactions can only selectively access thermodynamic diastereomers, and a preference for *kinetic* diastereomers has never been reported. This limitation extends to all reductive imine coupling reactions that use different reagents, conditions, or mechanisms. We sought to develop reactions that would overcome this limitation, and to understand the factors that influence diastereoselectivity in diboron-mediated reductive coupling reactions of imines. We found that varying the steric and electronic properties of

the diolate ligands on the diboron, and the solvent, enabled the stereodivergent synthesis of all diastereomers of 2,3-diaryltetrahydroquinoxalines. Additionally, we developed unique conditions for the activation of tetraalkoxydiborons, resulting in greatly increased reactivity and kinetic diastereoselectivity. We then explored the mechanism of these reactions computationally to aid in our understanding of how to proceed with further optimization. Finally, we developed a simple, fast protocol for the synthesis of tetraalkoxydiborons and diboron diolates to enable us to rapidly explore the effects of the structure of the diboron on reactivity and selectivity.

For my grandfather, who returned my mother from panic while I erased my innocence with confident claims that the gas evolved from a pile of nails deposited in hydrogen peroxide would inflate a thermonuclear Hindenberg for which Ivy Mike was no rival. However, our home survived its whimpers, and my career in chemistry continued.

Inadvisably.

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I thank Dr. Melanie Sanford (University of Michigan) for giving me my first opportunity to work in a research lab, and Dr. John Wolfe, who sparked my ever-lasting love for organic chemistry. My experiences at UM are why I knew graduate school is what I needed to do next in my life. My thanks also go out to my labmates in the Smith and Maleczka groups for their friendship – especially for the conversations with Tim (about hypercanes), conversations with Cash (about ergospheres), adventurous bowling trips with Alex, and for Yu-Ling, who is greatly missed.

I give thanks to my family: my parents, who tolerated my ill-advised science experiments at a young age (without their relentless and unwavering support, there is no way I would've lived long enough to make it into a Ph.D. program); and my sister Natalie, who makes me laugh at all hours of the day.

Finally, I acknowledge (a) my partner, Dr. Maris Cinelli, for being incredibly supportive throughout my graduate school experience, I look forward to our lifetime together in chemistry and otherwise; and (b) our favorite little kitty-cat, Nitro, who never failed to extend his claws to remind me that he still existed while I wrote this thesis.

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KEY TO ABBREVIATIONS

4-*t*Bu-cat	4-*tert*-Butylcatecholato
AcCl	Acetyl chloride
All	Allyl
B-B	Boron-boron bond
$B(OMe)_3$	Trimethyl borate
B_2cat_2	Bis(catecholato)diboron
B_2eg_2	Bis(ethyleneglycolato)diboron
B_2pin_2	Bis(pinacolato)diboron
$B_2(NMe_2)_4$	Tetrakis(dimethylamino)diboron
$B_2(OEt)_4$	Tetraethoxydiboron
$B_2(OMe)_4$	Tetramethoxydiboron
$B_3O_3(OMe)_3$	Trimethoxyboroxine
Bn	Benzyl
C-C	Carbon-carbon bond
*c*Pr	Cyclopropyl
cat	Catecholato
$CDCl_3$	Deuterated chloroform
CD_3CN	Deuterated acetonitrile
$CH(OEt)_3$	Triethyl orthoformate
$CH(OMe)_3$	Trimethyl orthoformate
cod	1,5-Cyclooctadiene
d	Doublet (NMR)

dan	1,8-Diaminonaphthalene
dba	Dibenzylideneacetone
DCM	Dichloromethane
DMF	*N*,*N*-Dimethylformamide
DFT	Density Functional Theory
dtbpy	4,4'-Di-*tert*-butyl-2,2'-bipyridine
eg	Ethylene glycolate or glycolato
Et	Ethyl
EtO	Ethoxyl
Et_2O	Diethyl ether
Et_3N	Triethylamine
Equiv	Equivalents
GC-MS	Gas Chromatography-Mass Spectrometry
HCl	Hydrochloric acid
hmp	*o*-2-(Hydroxymethyl)phenylato
Hz	Hertz
*i*Pr	Isopropyl
kcal	Kilocalorie
m	Multiplet (NMR)
M	Molar (concentration)
Me	Methyl
MeCN	Acetonitrile
MeO	Methoxyl

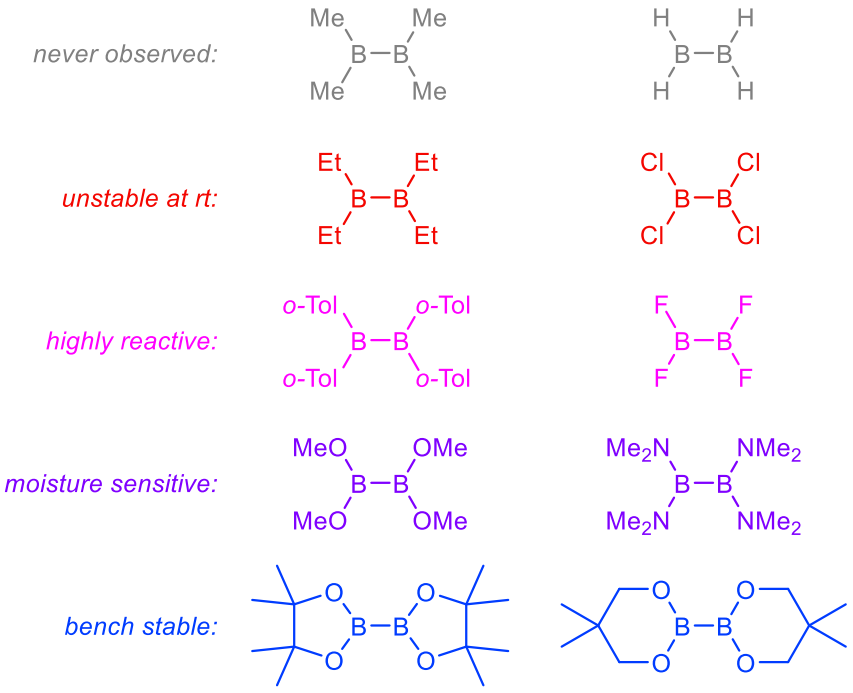
MeOH	Methanol
MHz	Megahertz
mol	Mole
mp	Melting point
*n*Pr	*n*-Propyl
neop	Neopentylglycolate
NMR	Nuclear magnetic resonance
o-Tol	*ortho*-Tolyl
Ph	Phenyl
pin	Pinacolato
PPh_3	Triphenylphosphine
PTFE	Polytetrafluoroethylene
rt	Room temperature
THF	Tetrahydrofuran
TFA	Trifluoroacetic acid
TFAA	Trifluoroacetic anhydride
s	Singlet (NMR)
SMD	Solvent Model based on Density
t	Triplet (NMR)
*t*Bu	*tert*-Butyl

Chapter 1. Introduction to the Chemistry of Diborons and Vicinal Diamines

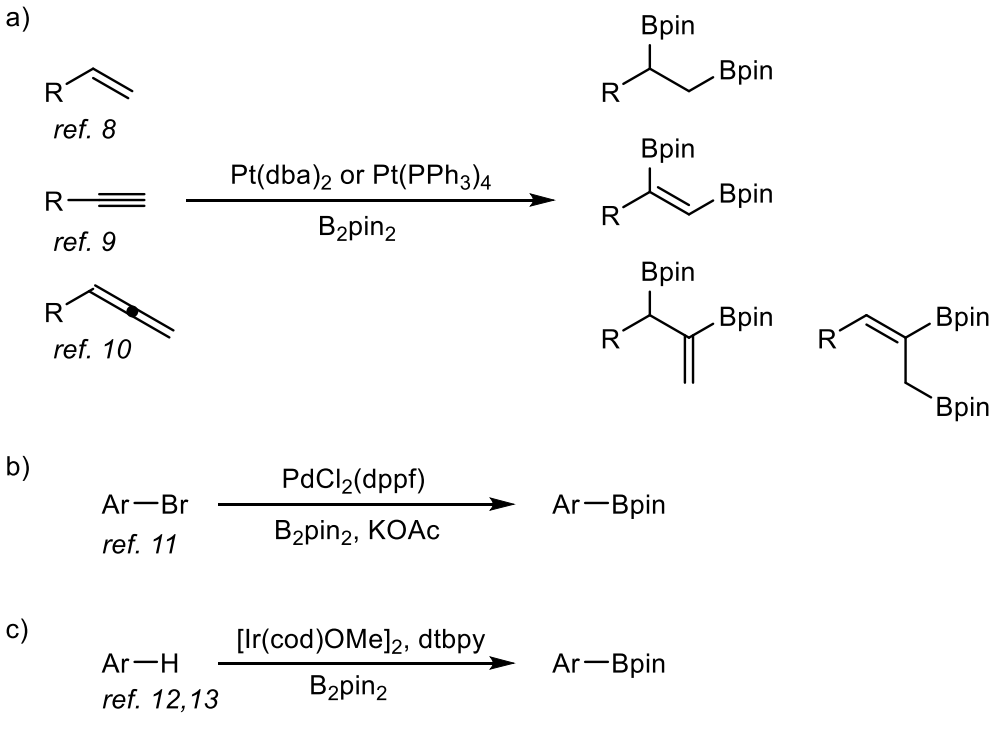
Although diborons ($Y_2B^{II}–B^{II}Y_2$) possess a pair of adjacent, empty p-orbitals in their extremely electron deficient (and paradoxically, powerfully reducing) B-B bond, they can be stabilized via judicious choice of substituents to allow convenient use and for their reactivity to be controlled (Figure 1.1).[1] Diborons with hydrogen or alkyl substituents are generally very unstable, and only sterically bulky tetraalkyldiborons have been characterized – for example, while B_2Et_4[2] has been synthesized, B_2Me_4 and B_2H_4 are unknown compounds. Halogen substituents can somewhat stabilize the B-B bond via π-donation, and B_2F_4, featuring excellent orbital overlap between boron and fluorine atoms, is stable at room temperature.[3] Less favorable orbital overlap between boron and the other halogens results in diminished stability for B_2Cl_4 and B_2Br_4, which spontaneously disproportionate (in the absence of solvent) into boron trihalides and polyhedral boron halides $(BX)_n$ (X = Cl, Br) at room temperature.[4] Nitrogen and oxygen are much stronger π-donors than the halogens, and so diborons with dialkylamino substituents are vastly more stable,[5] and those derived from diolate ligands are even bench stable.[1]

Interest in the reactivity of diborons has increased dramatically in the last few decades, beginning with their use as reagents (boron donors) in metal-catalyzed transformations (Scheme 1.1), such as alkyne, allene, and alkene diborylations,[8-10] Miyuara borylations,[11] and C-H borylation of arenes.[12-13]

Figure 1.1. Relative stability and reactivity of various common diborons.[1-7]



Scheme 1.1. Several metal-catalyzed reactions of diborons.[8-13]



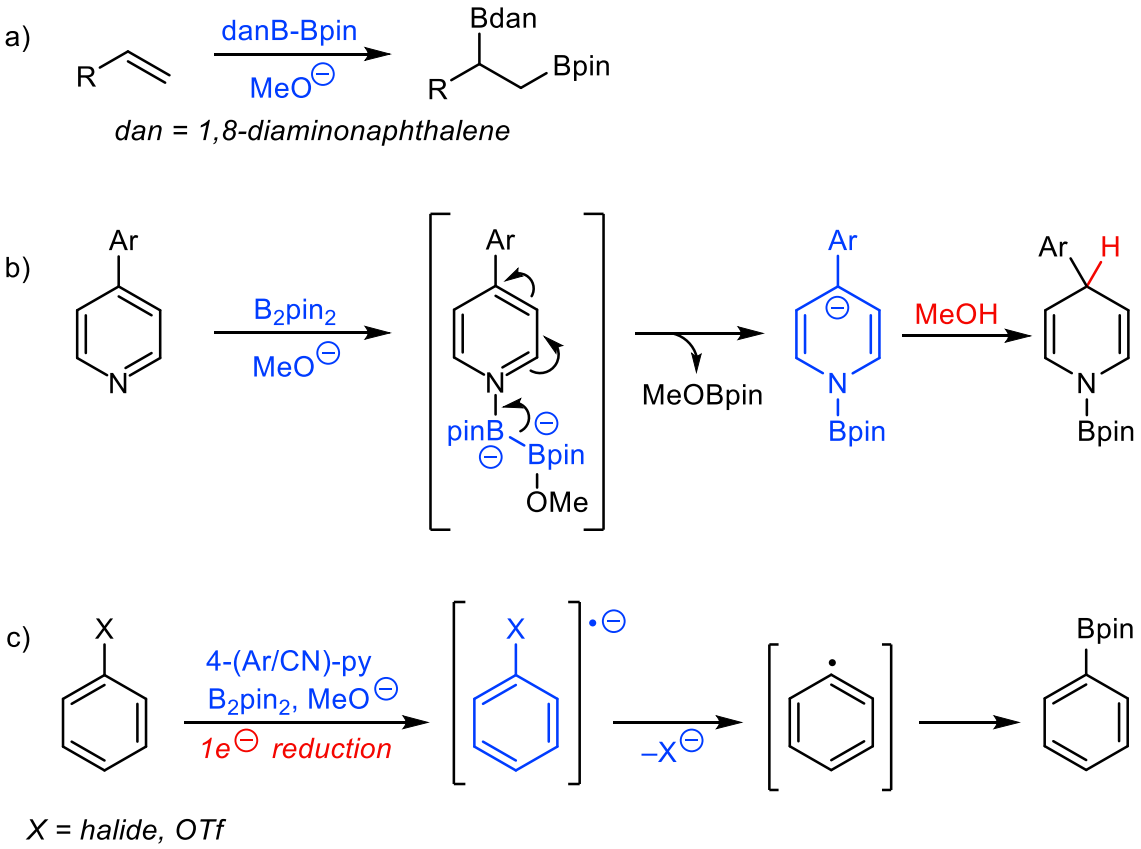
More recently, interest in metal-free transformations has surged. Many transition metal-catalyzed transformations have been replicated without metals, such as the aforementioned diborylation reactions, and a variety of related new transformations, such as diborations of alkenes.[14] Critically, there are a few specific classes of metal-free reactions of diborons that have been explored in great depth that are relevant to the topic of this thesis:

1. *Ionic reactions:* Those catalyzed or mediated by strong nucleophiles (alkoxide bases, NHCs, and amines), sometimes employing pyridines as catalysts or substrates.
2. *Non-photochemical radical reactions:* Those catalyzed or mediated by pyridines, generating a reactive *N*-borylpyridinyl radical intermediate.
3. *Sigmatropic reactions:* Those that proceed through [3,3]-sigmatropic rearrangements of diboron complexes, such as those derived from allylic alcohols or imines – having closed transition states, they offer high levels of stereocontrol.

Ionic Reactions.

Ionic diboron reactions can be divided into three fundamental types (Scheme 1.2), where a diboron complex is either: (a) The reactive intermediate (Scheme 1.2a); or (b) a precursor to a reactive intermediate, generated by B-B bond heterolysis (Scheme 1.2b); or (c) a powerful single-electron reductant, or a precursor to a powerful single-electron reductant (Scheme 1.2c).

Scheme 1.2. Examples of three fundamental ionic diboron reaction types.[a,15-17]



[a] Three possible intermediates for reaction (c) are shown in Scheme 1.3 (highlighted in blue).

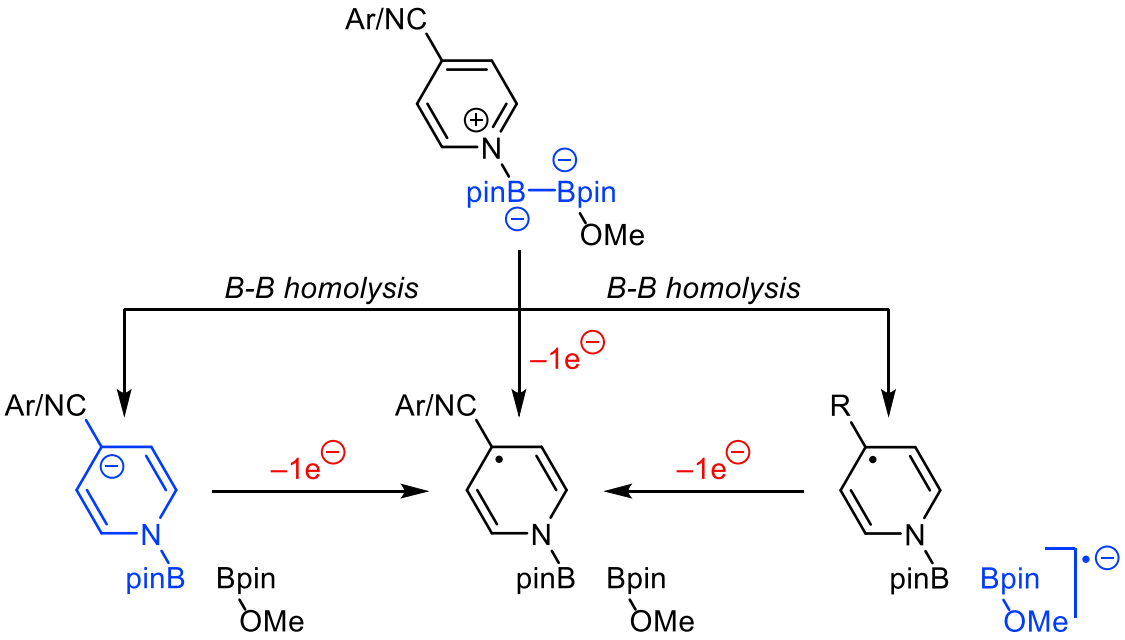
Alkenes can be diborylated by diborons in the presence of a nucleophilic catalyst, such as alkoxide[15] or amine[18] bases (Scheme 1.2a). These reactions have been proposed to proceed directly from an anionic diboron-alkoxide or diboron-NHC complex.[19] Chiral versions have been developed using B_2neop_2 (neop = neopentylglycolato) as the stoichiometric diboron source and a variety of chiral 1,2-diols as catalysts.[20] Borylation of imines,[21] and α,β-unsaturated carbonyl compounds,[22-23] can also be accomplished by these complexes, and vinylepoxides and vinylaziridines undergo borylative ring opening.[24]

Studies into the nature of the reductant generated by the reaction of 4-phenylpyridine with KOMe and B_2pin_2 revealed that heterolysis of the B-B bond occurred to form a

dearomatized anionic complex – when treated with methanol, the 1,4-hydropyridine was generated (Scheme 1.2b).[16]

Aryl halides can be borylated in the presence of pyridines and alkoxide bases (effectively a metal-free Miyaura borylation)[17] (Scheme 1.2c). While the nature of the reducing species is unclear[25] (possibilities are shown in Scheme 1.3), single electron reduction of aryl halides occurs under these conditions. These aryl halide radical anions fragment to afford aryl radicals, which rapidly react with the diboron (or a diboron complex) to yield aryl boronic esters.

Scheme 1.3. Postulated single-electron reductants in reactions with diborons, base, and pyridines.[25]

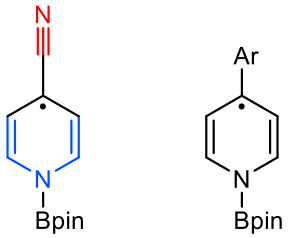


Radical Reactions.

Naked boryl radicals themselves are exceedingly unstable due to their electron deficient nature.[26] However, *N*-borylpyridinyl radicals are far more stable – not only is their electron deficiency greatly attenuated, but spin is also delocalized by the pyridine,

and 4-arylpyridines are able to further delocalize spin. Pyridines with electron withdrawing substituents at the *para*-position are particularly effective, due to captodative stabilization.[28] Both 4-arylpyridines and 4-cyanopyridines have found numerous applications as catalysts for organic reactions of diborons.[29]

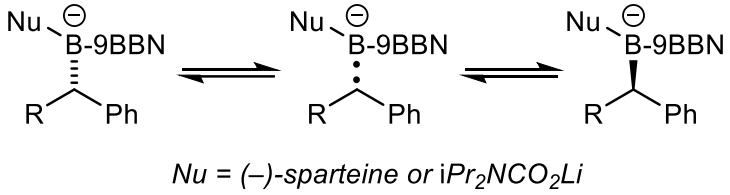
Scheme 1.4. Captodative stabilization vs. spin delocalization in *N*-borylpyridinyl radicals.[a,27-28]



[a] Captodative effects illustrated by blue (electron donating) and red (electron withdrawing) moieties.

The ability of the pyridine ligand to accept an electron via a π-bond is critical: Examples of trialkylamine-stabilized boryl radicals are relatively few. Although (–)-sparteine was proposed to stabilize a boryl radical (as an explanation for an undesired racemization process), another nucleophile was present in the reaction, and the active species was not determined (Scheme 1.5).[3]

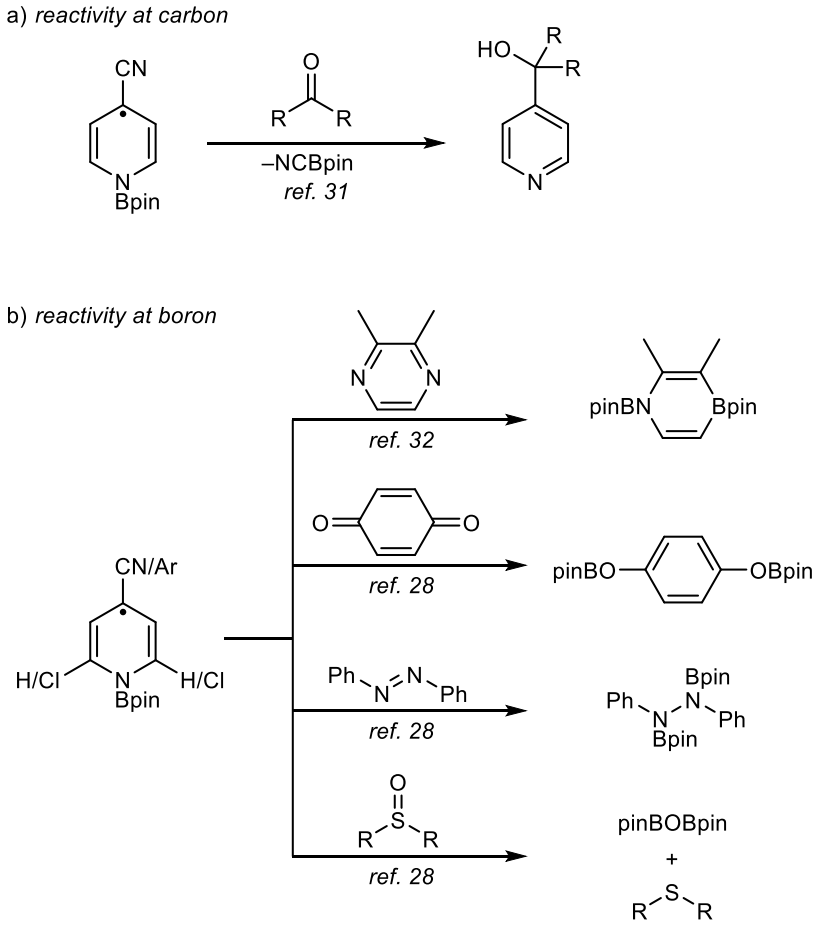
Scheme 1.5. Racemization of organoboranes induced by nucleophiles.[a,30]



[a] Both (–)-sparteine and *i*Pr_2NCO_2Li were present, and it was not determined which caused racemization.

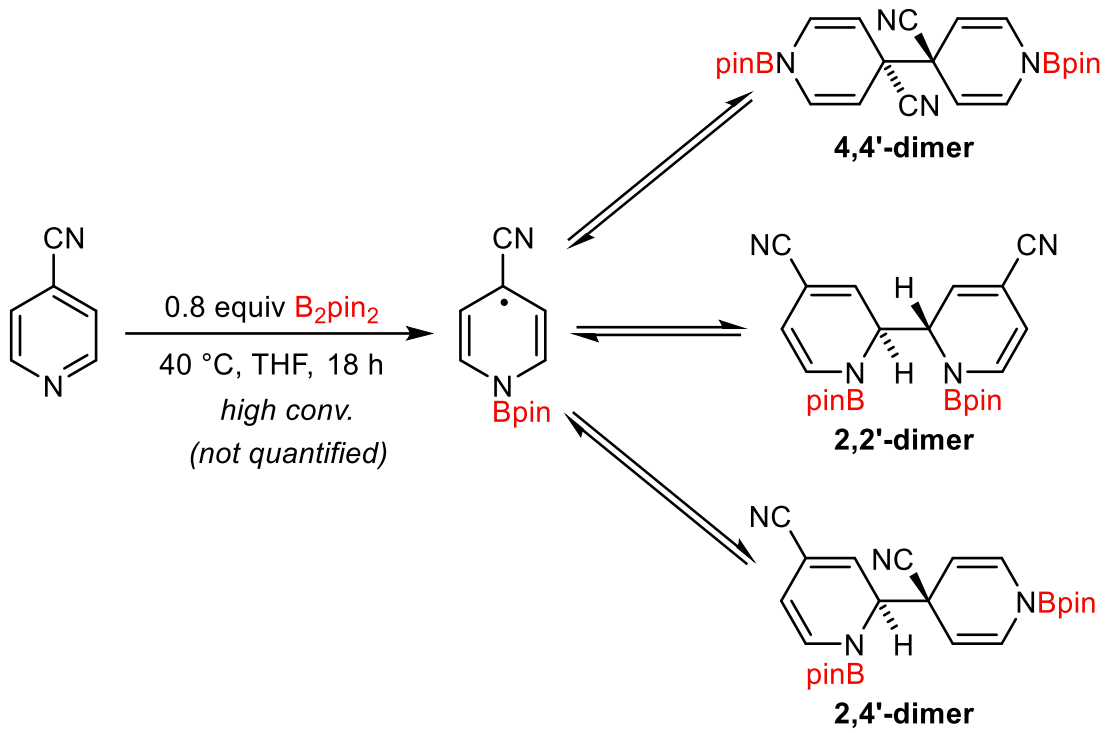
N-Borylpyridinyl radicals retain much of the reducing ability of diborons. Using these radicals, a wide variety of compounds can be reductively dearomatized (pyrazines),[32] aromatized (quinones),[28] diborylated (diazenes),[28] or deoxygenated (sulfoxides)[28] (Scheme 1.6).

Scheme 1.6. Reactions of *N*-borylpyridinyl radicals.[28,31,32]



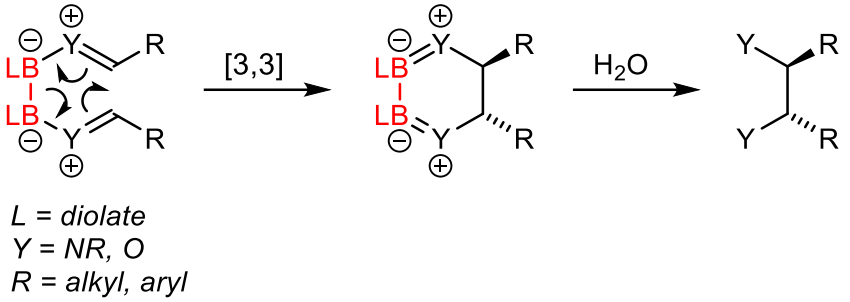
Another recent example describes 4-cyanopyridine-catalyzed reactions with B_2pin_2, which are proposed to proceed via *N*-borylpyridinyl radical intermediates.[17,28,31] Spectroscopic evidence was provided for transient populations of regiochemically and stereochemically undefined *N*-boryl pyridinyl radical dimers[31] – their presence is consistent with the mechanistic hypothesis (Scheme 1.7).

Scheme 1.7. *N*-Borylpyridinyl radicals and reversible dimerization via radical recombination.[31]



Formation of pyridinyl radical dimers has generally only been previously observed previously with metal-mediated reductions (typically alkali metals) of pyridinium cations (with rare exceptions, such as a dithionite-mediated reduction of *N*-methyl-4-cyanopyridinium cations).[33]

Scheme 1.8. Concerted [3,3]-sigmatropic reaction mechanism from a diboron complex.[34,35,36]

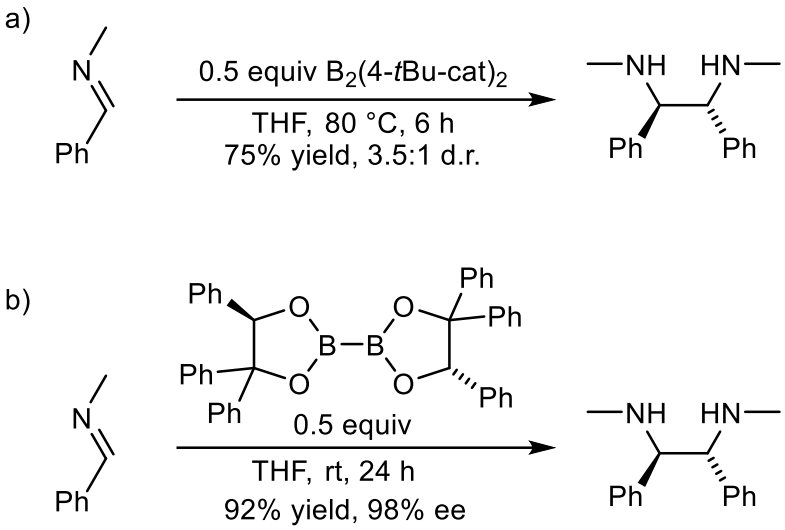


Sigmatropic Reactions.

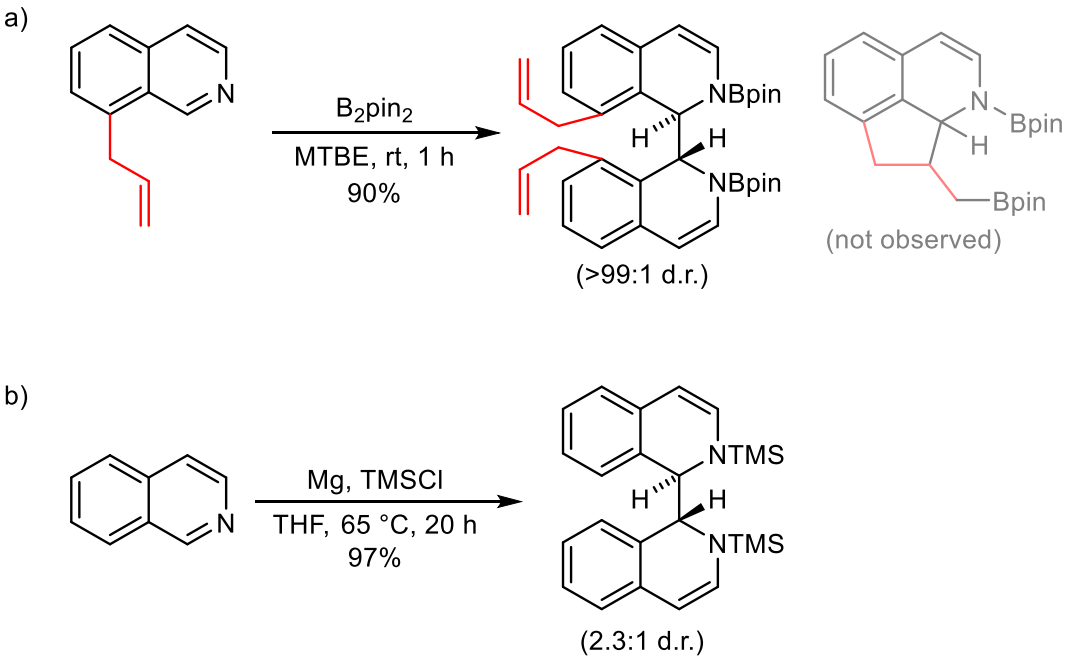
Concerted, diboron-mediated sigmatropic reactions (Scheme 1.8) are relatively uncommon. These reactions are attractive targets for investigation, as they proceed through closed transition states that often offer greater levels of stereocontrol than other reaction types, such as those with open transition states or radical mechanisms. Deoxygenative borylations of allylic alcohols by diborons in the presence of catalytic base are proposed to proceed through a [3,3]-sigmatropic rearrangement and are highly stereoselective.[34] A reductive imine coupling using B_2(4-*t*-Bu-cat)$_2$, reported initially by Baker and Wescott (Scheme 1.9a), was also proposed to proceed through a [3,3]-sigmatropic rearrangement. Aldehydes were also found to be reactive, and underwent a pinacol rearrangement after the reductive coupling.[35]

Much later, diastereoselective B_2pin_2-mediated reductive dimerizations of isoquinolines and 3,4-dihydroisoquinolines were also reported (Scheme 1.10a),[36] and only one diastereomer was generated, in stark contrast to the low diastereoselectivity observed with metal-mediated reactions (Scheme 1.10b)[37] Also noteworthy is that cyclization onto the allyl tether was not observed, providing evidence against a radical mechanism (Scheme 1.10a).

Scheme 1.9. Diboron-mediated reductive couplings of imines.[35,38]



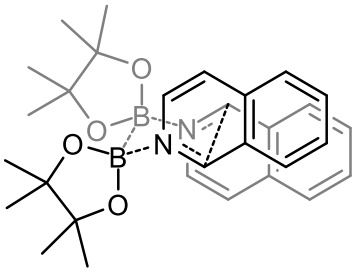
Scheme 1.10. Reductive couplings of isoquinolines with (a) diborons vs. (b) metals.[36,37]



This transformation was also highly enantioselective when chiral diboron reagents were employed. This work was expanded to the enantioselective reductive coupling of imines to afford vicinal diamines (Scheme 1.9b).[38] While the scope of the substituent on

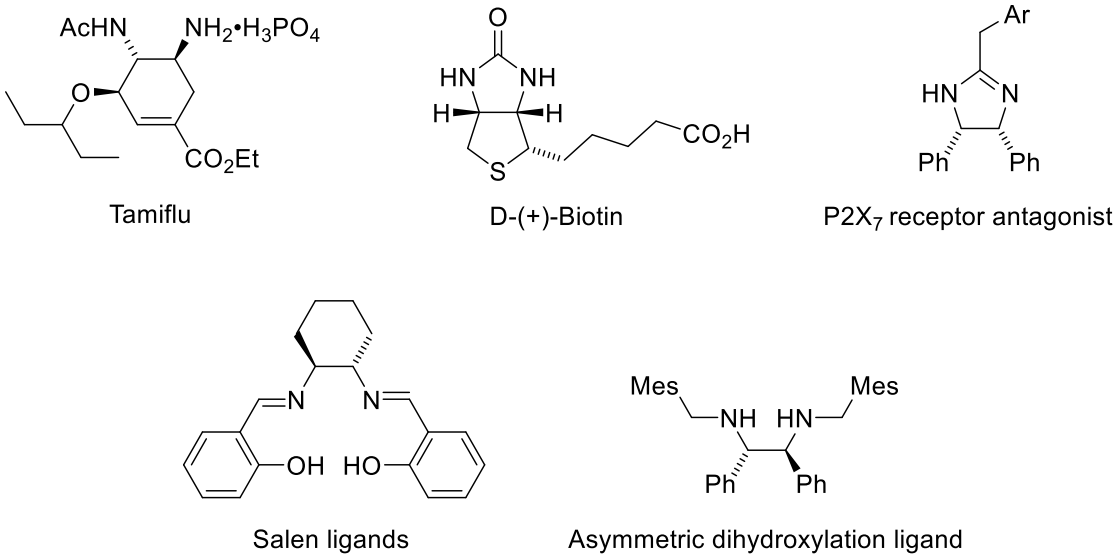
the imino carbon was expansive, the *N*-substituents were limited to *N*-Me and *N*-H. These reactions were highly selective for the thermodynamic diastereomer. However, selectivity for the *kinetic* product has yet to be observed. In fact, to the best of our knowledge, this challenge has not been overcome for reductive imine couplings using any known set of reductants (including transition metals, photoredox chemistry, and other methods).

Scheme 1.11. Reductive coupling transition state from a B_2pin_2•2(isoquinoline) complex.[36]



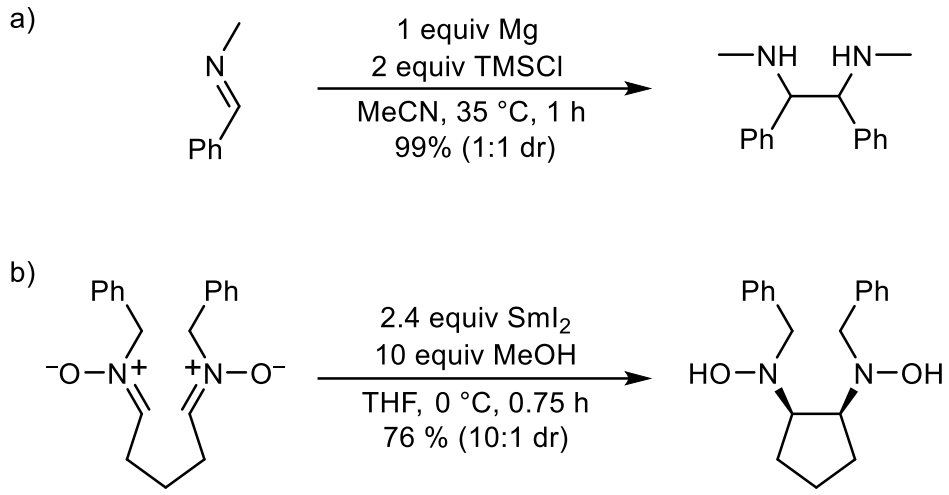
This limitation is an opportunity for the development of new reductive coupling reactions, as vicinal diamines (1,2-diamino compounds) are a common part of numerous significant and stereochemically complex molecules. Vicinal diamines are found in approved drugs, drug candidates, and various ligands for synthetic procedures (Figure 1.2).[39] Some promising antiviral drug candidates containing vicinal diamine motifs are unfortunately difficult to synthesize in useful quantities, and the routes to these compounds are frequently not amenable to analog synthesis. Many of these are natural products and their derivatives, notorious for the substantial challenges they typically offer to the inspired or enterprising chemist. Alas, Nature does not design molecules with synthetic feasibility in mind.

Figure 1.2. Significant molecules containing the vicinal diamine motif.[39]



Hence, new methods of synthesizing vicinal diamines to form complex ring structures, or to exploit pseudosymmetry buried deep within a retrosynthesis, are of great interest. Inspired by the pinacol coupling reaction, reductive imine coupling reactions were developed as a means to synthesize vicinal diamines. Reports of progress in this area have surfaced periodically over the last few decades, but many of these reactions are hampered by harsh conditions, limited scope and/or poor functional group tolerance, and requirements for stoichiometric quantities of metal reductants (Scheme 1.12a) or expensive reagents such as samarium (II) iodide (Scheme 1.12b).[40-44]

Scheme 1.12. A metal-mediated aza-pinacol coupling.[40,41]



Photoredox pinacol and aza-pinacol reactions also generate copious amounts of organic waste that can sometimes be difficult to separate from the product.[45,46] Additionally, imines, aldehydes, and ketones react under identical conditions, and so to avoid undesired reactions with a ketone or aldehyde present elsewhere in the molecule, one would have to add a protection and deprotection step to the overall sequence.

Inspired by the chemistry of diboron diolates (including the pyridine radical and isoquinoline and imine dimerization examples), their versatile applications in reductive chemistry,[1] and the utility of vicinal diamines as a target, we sought to develop a new, operationally simple, highly chemoselective aza-pinacol reaction, employing only reagents known to degrade into non-toxic materials under aqueous workup conditions. Many diboron diolates tolerate exposure to air, and so their ease of use is alluring to synthetic chemists. They are easily degraded into boric acid and thus removed via aqueous workup, making these attractive reactions for preparations of pharmaceuticals or their intermediates.[1] The main focus of this work is developing reductive imine coupling

reactions that, unlike previous reports, favor the kinetic product (offering kinetic control over diastereoselectivity). The development and scope of this reaction, and computational modeling of proposed mechanisms are described in Chapters 2-4. Additionally, we have developed a versatile preparation of different diboron diolates and tetrahydroxydiborons (Chapter 5), which are useful reagents both for imine chemistry and many other processes.

REFERENCES

REFERENCES

(1) Neeve, E. C.; Geier, S. J.; Mkhalid, I. A. I.; Westcott, S. A.; Marder, T. B. Chem. Rev. Diboron(4) Compounds: From Structural Curiosity to Synthetic Workhorse. *Chem. Rev*. **2016**, *116*, 9091–9161.

(2) Nöth, H.; Pommerening, H. Beiträge zur Chemie des Bors, 120. Tetraorganyldiborane(4): Darstellung und Stabilität. *Chem. Ber*. **1981**, *114*, 3044–3055.

(3) Finch, A.; Schlesinger, H. I. Diboron Tetrafluoride. *J. Am. Chem. Soc.* **1958**, *80*, 3573–3574.

(4) Ahmed, L.; Castillo, J.; Saulys, D. A.; Morrison, J. A. Reactivity of the Diboron Tetrahalides. Diboration of Ethylene with Diboron Tetrabromide and Thermal Decomposition and Ligand Exchanges of Diboron Tetrabromide and Diboron Tetrachloride in Carbon Tetrabromide and Carbon Tetrachloride. *Inorg. Chem.* **1992**, *31*, 706–710.

(5) Malhotra, S. C. The Chemistry of Tetrakis(dimethylamino)diboron. *Inorg. Chem.* **1964**, *3*, 862–865.

(6) Tsukahara, N.; Asakawa, H.; Lee, K.-H.; Lin, Z.; Yamashita, M. Cleaving Dihydrogen with Tetra(o-tolyl)diborane(4). *J. Am. Chem. Soc.* **2017**, *139*, 2593–2596.

(7) Brotherton, R. J.; McCloskey, A. L.; Boone, J. L.; Manasevit, H. M. The Preparation and Properties of Some Tetraalkoxydiborons. *J. Am. Chem. Soc.* **1960**, *82*, 6245–6248.

(8) Ishiyama, T.; Matsuda, N.; Murata, M.; Ozawa, F.; Suzuki, A.; Miyaura, N. Platinum(0)-Catalyzed Diboration of Alkynes with Tetrakis(alkoxo)diborons: An Efficient and Convenient Approach to cis-Bis(boryl)alkenes. *Organometallics* **1996,** *15*, 713–720.

(9) Ishiyama, T.; Kitano, T.; Miyaura, N. Platinum(0)-Catalyzed Diboration of Allenes with Bis(pinacolato)diboron. *Tetrahedron Lett.* **1998**, *39*, 2357–2360.

(10) Ishiyama, T.; Yamamoto, M.; Miyaura, N. Diboration of alkenes with bis(pinacolato)diboron catalysed by a platinum(0) complex. *Chem. Commun.* **1997**, 689–690.

(11) Ishiyama, T.; Murata, M.; Miyaura, N. Palladium(0)-Catalyzed Cross-Coupling Reaction of Alkoxydiboron with Haloarenes: A Direct Procedure for Arylboronic Esters. *J. Org. Chem.* **1995**, *60*, 7508–7510.

(12) Iverson, C. N.; Smith, M. R., III. Stoichiometric and Catalytic B−C Bond Formation from Unactivated Hydrocarbons and Boranes. *J. Am. Chem. Soc.* **1999**, *121*, 7696–7697.

(13) Liskey, C. W.; Wei, C. S.; Pahls, D. R.; Hartwig, J. F. Pronounced effects of substituents on the iridium-catalyzed borylation of aryl C–H bonds. *Chem. Commun.* **2009**, 5603–5605.

(14) Cuenca, A. B.; Shishido, R.; Ito, H.; Fernández, E. Transition-metal-free B–B and B–interelement reactions with organic molecules. *Chem. Soc. Rev.* **2017**, *46*, 415–430.

(15) Miralles, N.; Cid, J.; Cuenca, A. B.; Carbó, J. J.; Fernández, E. Mixed diboration of alkenes in a metal-free context.

(16) Yang, H.; Zhang, L.; Zhou, F.-Y.; Jiao, L. An umpolung approach to the hydroboration of pyridines: a novel and efficient synthesis of N-H 1,4-dihydropyridines. *Chem. Sci.* **2020**, *11*, 742–747.

(17) Zhang, L.; Jiao, L. Pyridine-Catalyzed Radical Borylation of Aryl Halides. *J. Am. Chem. Soc.* **2017**, *139*, 607–610.

(18) Farre, A.; Soares, K.; Briggs, R. A.; Balanta, A.; Benoit, D. M.; Bonet, A. Amine Catalysis for the Organocatalytic Diboration of Challenging Alkenes. *Chem. Eur. J.* **2016**, *22*, 17552–17556.

(19) Bonet, A.; Pubill-Ulldemolins, C.; Bo, C.; Gulyás, H.; Fernández, E. Transition-Metal-Free Diboration Reaction by Activation of Diboron Compounds with Simple Lewis Bases. *Angew. Chem. Int. Ed.* **2011**, *50*, 7158–7161.

(20) Fang, L.; Yan, L.; Haeffner, F.; Morken, J. P. Carbohydrate-Catalyzed Enantioselective Alkene Diboration: Enhanced Reactivity of 1,2-Bonded Diboron Complexes. *J. Am. Chem. Soc.* **2016**, *138*, 2508−2511.

(21) Solé, C.; Gulyása, H. Fernández, E. Asymmetric synthesis of α-amino boronate esters via organocatalytic pinacolboryl addition to tosylaldimines. *Chem. Commun.* **2012**, *48*, 3769–3771.

(22) Lee, K.-S.; Zhugralin, A. R.; Hoveyda, A. H. Efficient C−B Bond Formation Promoted by N-Heterocyclic Carbenes: Synthesis of Tertiary and Quaternary B-Substituted Carbons through Metal-Free Catalytic Boron Conjugate Additions to Cyclic and Acyclic α,β-Unsaturated Carbonyls. *J. Am. Chem. Soc.* **2009**, *131*, 7253–7255.

(23) Wen, K.; Chen, J.; Gao, F.; Bhadury, P. S.; Fan, E.; Sun, Z. Metal free catalytic hydroboration of multiple bonds in methanol using N-heterocyclic carbenes under open atmosphere. *Org. Biomol. Chem.* **2013**, *11*, 6350–6356.

(24) Sanz, X.; Lee, G. M.; Pubill-Ulldemolins, C.; Bonet, A.; Gulyás, H.; Westcott, S. A.; Bo, C.; Fernández, E. Metal-free borylative ring-opening of vinyl epoxides and aziridines. *Org. Biomol. Chem.* **2013**, *11*, 7004–7010.

(25) Zhang, L.; Jiao, L. Super electron donors derived from diboron. *Chem. Sci.* **2018**, *9*, 2711–2722.

(26) Wu, C.; Hou, X.; Zheng, Y.; Li, P.; Lu, D. Electrophilicity and Nucleophilicity of Boryl Radicals. *J. Org. Chem.* **2017**, *82*, 2898−2905.

(27) Cao, J.; Wang, G.; Gao, L.; Cheng, X.; Li, S. Organocatalytic reductive coupling of aldehydes with 1,1-diarylethylenes using an in situ generated pyridine-boryl radical. *Chem. Sci.* **2018**, *9*, 3664–3671.

(28) Wang, G.; Zhang, H.; Zhao, J.; Li, W.; Cao, J.; Zhu, C.; Li, S. Homolytic Cleavage of a B-B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. *Angew. Chem. Int. Ed.* **2016**, *55*, 5985–5989.

(29) Misal Castro, L. C.; Sultan, I.; Tsurugi, H.; Mashima, K. Pyridine-Mediated B–B Bond Activation of $(RO)_2B–B(OR)_2$ for Generating Borylpyridine Anions and Pyridine-Stabilized Boryl Radicals as Useful Boryl Reagents in Organic Synthesis. *Synthesis* **2021**, *53*, A–P.

(30) Stymiest, J. L.; Dutheuil, G.; Mahmood, A.; Aggarwal, V. K. Lithiated Carbamates: Chiral Carbenoids for Iterative Homologation of Boranes and Boronic Esters. *Angew. Chem. Int. Ed.* **2007**, *46*, 7491–7494.

(31) Wang, G.; Cao, J.; Gao, L.; Chen, W.; Huang, W.; Cheng, X.; Li, S. Metal-Free Synthesis of C-4 Substituted Pyridine Derivatives Using Pyridine-boryl Radicals via a Radical Addition/Coupling Mechanism: A Combined Computational and Experimental Study. *J. Am. Chem. Soc.* **2017**, *139*, 3904–3910.

(32) Gao, L.; Zhang, H.; Liu, X.; Wang, G.; Li, S. Mechanistic insights into the dearomative diborylation of pyrazines: a radical or non-radical process? *Dalton Trans.* **2021**, *50*, 6982–6990.

(33) Kosower, E. M.; Cotter, J. L. Stable Free Radicals. II. The Reduction of 1-Methyl-4-cyanopyridinium Ion to Methylviologen Cation Radical. *J. Am. Chem. Soc.* **1964**, *86*, 5524–5527.

(34) Miralles, N.; Alman, R.; Szabó, K.; Fernández, E. Transition-Metal-Free Borylation of Allylic and Propargylic Alcohols. *Angew. Chem. Int. Ed.* **2016**, *55*, 4303–4307.

(35) Carter, C. A. G.; John, K. D.; Mann, G.; Martin, R. L.; Cameron, T. M.; Baker, R. T.; Bishop, K. L.; Broene, R. D.; Wescott, S. A. Bifunctional Lewis Acid Reactivity of Diol-Derived Diboron Reagents. *ACS Symposium Series: Group 13 Chemistry* **2002**, *822*, 70–87.

(36) Chen, D.; Xu, G.; Zhou, Q.; Chung, L. W.; Tang, W. Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. *J. Am. Chem. Soc.* **2017**, *139*, 9767–9770.

(37) Grignon-Dubois, M.; Fialeix, M.; Leger, J. Silylation de l'isoquinoléine: influence des conditions opératoires sur l'obtention de nouveaux hétérocycles siliciés. *Canadian Journal of Chemistry*, **1993**, *71*, 754–762.

(38) Zhou, M.; Li, K.; Chen, D.; Xu, R.; Xu, G.; Tang, W. Enantioselective Reductive Coupling of Imines Templated by Chiral Diboron. *J. Am. Chem. Soc.* **2020**, *142*, 10337–10342.

(39) Kotti, S. R. S. S.; Timmons, C.; Li, G. Vicinal Diamino Functionalities as Privileged Structural Elements in Biologically Active Compounds and Exploitation of their Synthetic Chemistry. *Chem. Biol. Drug. Des.* **2006**, *67*, 101–114.

(40) Alexakis, A.; Aujard, I.; Mangeney, P. Practical and Efficient Synthesis of C_2 Symmetrical Diamines with Zn/Me_3SiCl. *Synlett* **1998**, *8*, 873–874.

(41) Ebran, J.-P.; Hazell, R. G.; Skrydstrup, T. Samarium diiodide-induced intramolecular pinacol coupling of dinitrones: synthesis of cyclic cis-vicinal diamines. *Chem. Commun.* **2005**, 5402–5404.

(42) Yamamoto, Y.; Hattori, R.; Itoh, K. Highly *trans*-selective intramolecular pinacol coupling of dials catalyzed by bulky Cp_2TiPh. *Chem. Commun.* **1999**, *0*, 825–826.

(43) Taniguchi, N.; Hata, T.; Uemura, M. Enantiomerically Pure Cyclic *trans*-1,2-Diols, Diamines, and Amino Alcohols by Intramolecular Pinacol Coupling of Planar Chiral Mono-$Cr(CO)_3$ Complexes of Biaryls. *Angew. Chem. Int. Ed.* **1999**, *38*, 1232–1235.

(44) Khan, N. H.; Zuberi, R. K.; Siddiqui, A. A. Reduction of Schiff's Bases and Phenylhydrazones by Zinc Dust. *Synth. Commun.* **1980**, *10*, 363–371.

(45) Nakajima, M.; Fava, E.; Loescher, S.; Jiang, Z.; Rueping, M. Photoredox-Catalyzed Reductive Coupling of Aldehydes, Ketones, and Imines with Visible Light. *Angew. Chem. Int. Ed.* **2015**, *54*, 8828–8832.

(46) Prier, C. K.; Rankic, D. A.; MacMillan, D. W. C. Visible Light Photoredox Catalysis with Transition Metal Complexes: Applications in Organic Synthesis. *Chem. Rev.* **2013**, *113*, 5322–5363.

Chapter 2. Diboron-Mediated Stereodivergent Synthesis of All Diastereomers of 2,3-Diaryltetrahydroquinoxalines via Reductive Cyclization of Diimines

Introduction.

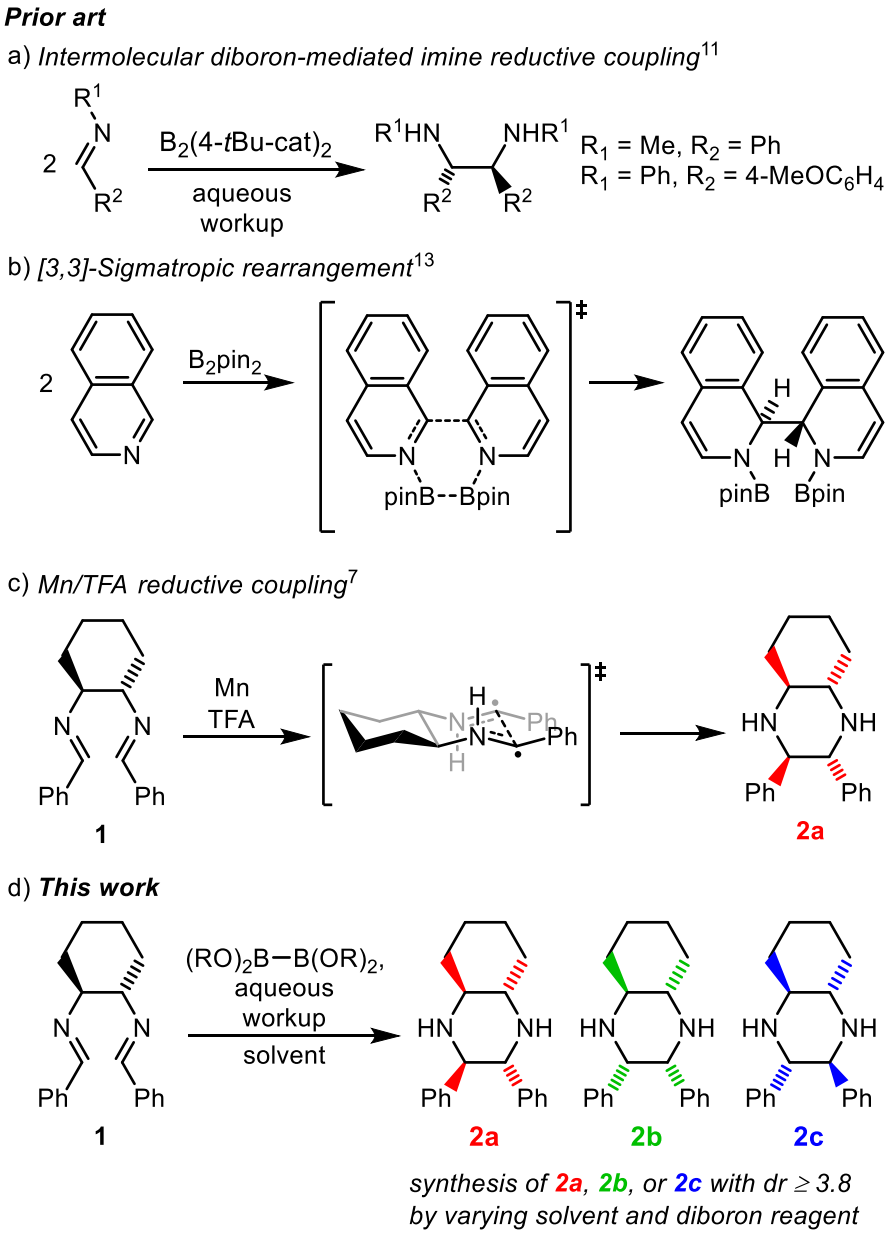
Vicinal diamines (1,2-diamino compounds) have versatile applications ranging from chiral ligands in catalysis[1-3] to important motifs in druglike molecules.[4] Many methods have been developed for their synthesis, including the reductive coupling of imines. Reductive coupling processes typically use metal-based reductants and proceed through diradical intermediates.[5-10] Kinetic control over diastereoselectivity is rarely observed, and diastereomeric ratios of the obtained diamines are typically low for intermolecular reactions.

In 2002, Baker, Broene, and Wescott reported the serendipitous discovery of diboron reagents as alternative reductants for intermolecular reductive imine coupling reactions, with moderate to high diastereoselectivity for the *trans*-diamine.[11] As shown in Scheme 2.1a, reactions for imines and B_2(4-*t*Bu-cat)$_2$ (4-*t*Bu-cat = 4-*tert*-butylcatecholato) in THF afforded vicinal diamines upon aqueous workup. Electron-rich aromatic imines were found to be most reactive, while longer reaction times and lower yields were reported for electron-deficient or bulky imines, limiting its scope (and practical use).

More recently (2020), Xu and Tang reported an enantioselective reductive coupling of sterically unhindered imines (HN=CHR or MeN=CHR) using chiral diborons.[12] This work followed their previous report of enantioselective and diastereoselective B_2pin_2-mediated reductive dimerizations of isoquinolines and 3,4-dihydroisoquinolines (Scheme 2.1b).[13] For both reactions, a concerted, [3,3]-sigmatropic rearrangement mechanism was

proposed.[11,13] The high diastereoselectivity (>99:1 dr) of the isoquinoline coupling reaction contrasts the low diastereoselectivities for most metal-mediated reductive couplings of isoquinolines.[14]

Scheme 2.1. Imine and isoquinoline reductive couplings related to this work.

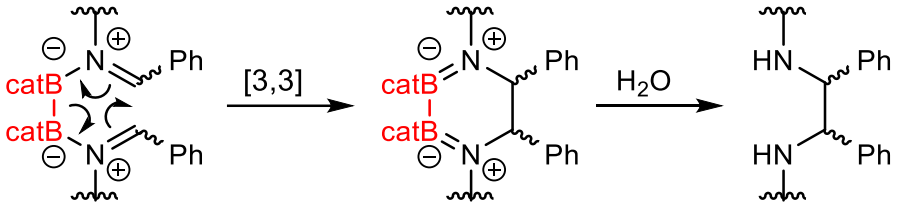


Highly diastereoselective intramolecular imine couplings can also be achieved with Mn/TFA, as shown in the work of Mercer and Sigman.[7] The reduction of benzaldehyde-derived diimine **1** yielded **2a** as the sole product (Scheme 2.1c). An intramolecular diradical combination mechanism (resulting from $1e^-$ reduction of protonated iminium ions) is proposed to proceed through a chair-like transition state, consistent with the observed diastereoselectivity. Although effective, the outcome of this reaction is limited to one diastereomer only.

In this chapter, we describe the intramolecular reductive cyclizations of diimine **1** mediated by diborons, where all three possible diastereomers (**2a**-**2c**) can be made selectively by simply varying the solvent and the structure of the diboron reagent (Scheme 2.1d). This is the first report of diastereocontrol enforced by solvent or the ligands on a boron reagent (including related reactions, such as allylborations[15]).

Discussion of a Potential Mechanism.

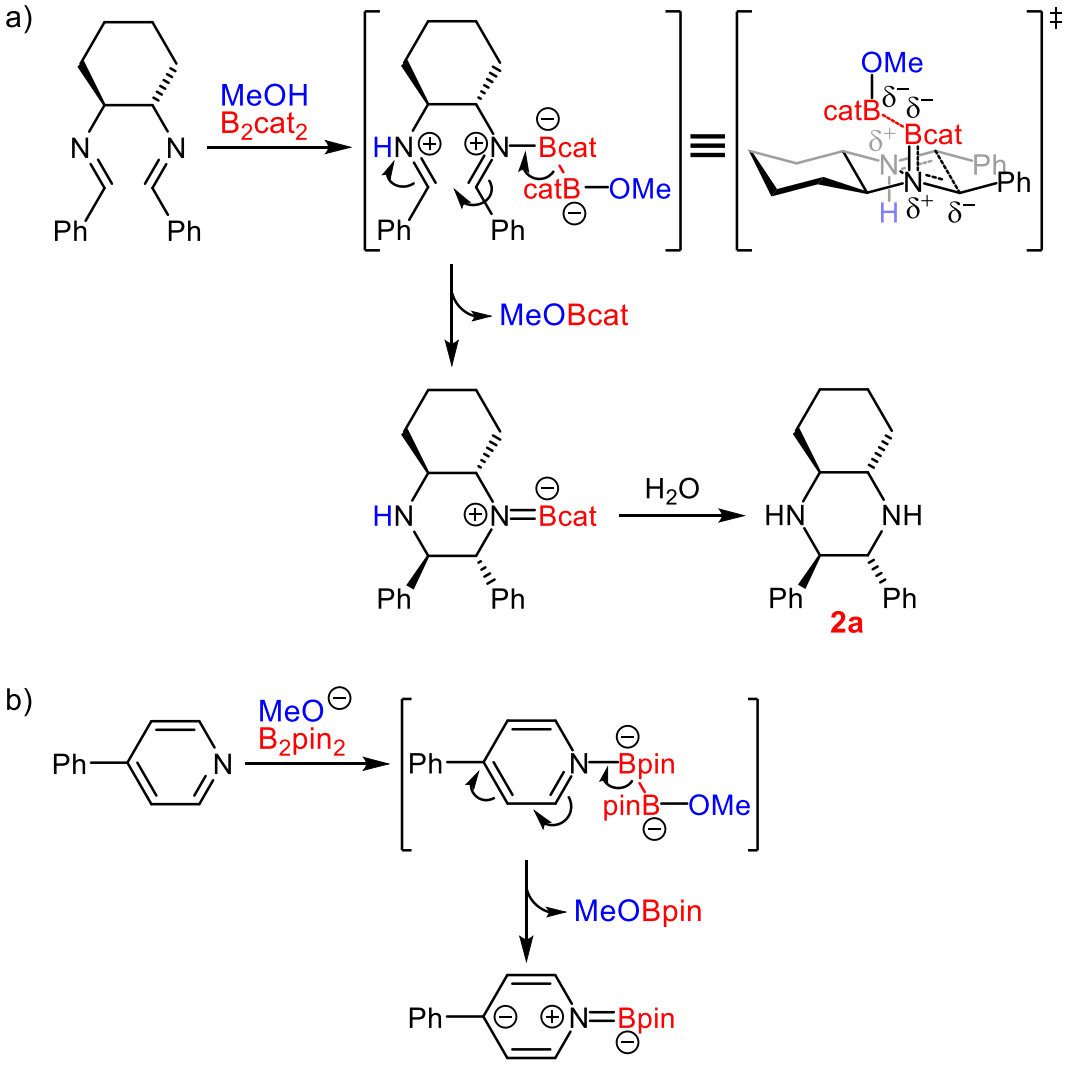
Scheme 2.2. Reductive [3,3]-sigmatropic rearrangement of a diimine-diboron complex.



It is proposed that two mechanisms may be operative depending on the solvent. The first mechanism, favored in aprotic solvents (DMF or DCM), is a [3,3]-sigmatropic rearrangement (Scheme 2.2) that can afford two different kinetic diastereomers depending on both a) the relative rate of *E*/*Z* imine isomerization vs. reductive cyclization, and b) competing $A^{1,3}$ strain between the imine and the cyclohexane ring vs. the imine and the

diboron. The second mechanism (Scheme 2.3a), favored in protic solvents (MeOH), is an ionic pathway that proceeds through an open transition state that affords the thermodynamic diastereomer **2a** (Scheme 2.3).

Scheme 2.3. Proposed mechanism for formation of **2a** and heterolytic cleavage of pyridine diboron alkoxide complexes.[16]



The reaction of **1** with B_2cat_2 in MeOH gives 2,3-diaryltetrahydroquinoxaline **2a** with high diastereoselectivity (>99% **2a**) in 79% yield (Scheme 2.4). The [3,3]-sigmatropic rearrangement transition state requires *E*/*Z* imine isomerization (Scheme 2.5) to give the

relative stereochemistry for **2a**. Attempts to model a transition state involving **1**-(*Z*,*E*) and B_2cat_2 led to severe steric clashes ($A^{1,3}$ strain) between the *Z*-imine and the cyclohexane ring. Thus, the ionic mechanism (Scheme 2.3a) is a more plausible pathway for the selective formation of **2a** under the conditions in Scheme 2.4. Given the report that heterolytic B–B bond cleavage readily generates *N*-boryl pyridyl anions from pyridine diboron alkoxide complexes[16] (Scheme 2.3b), it is proposed that monocoordinate diimine diboron alkoxide complexes may undergo a similar process, driving nucleophilic cyclization onto a tethered iminium moiety via accumulation of negative charge on the *N*-borylimino carbon (Scheme 2.3a).

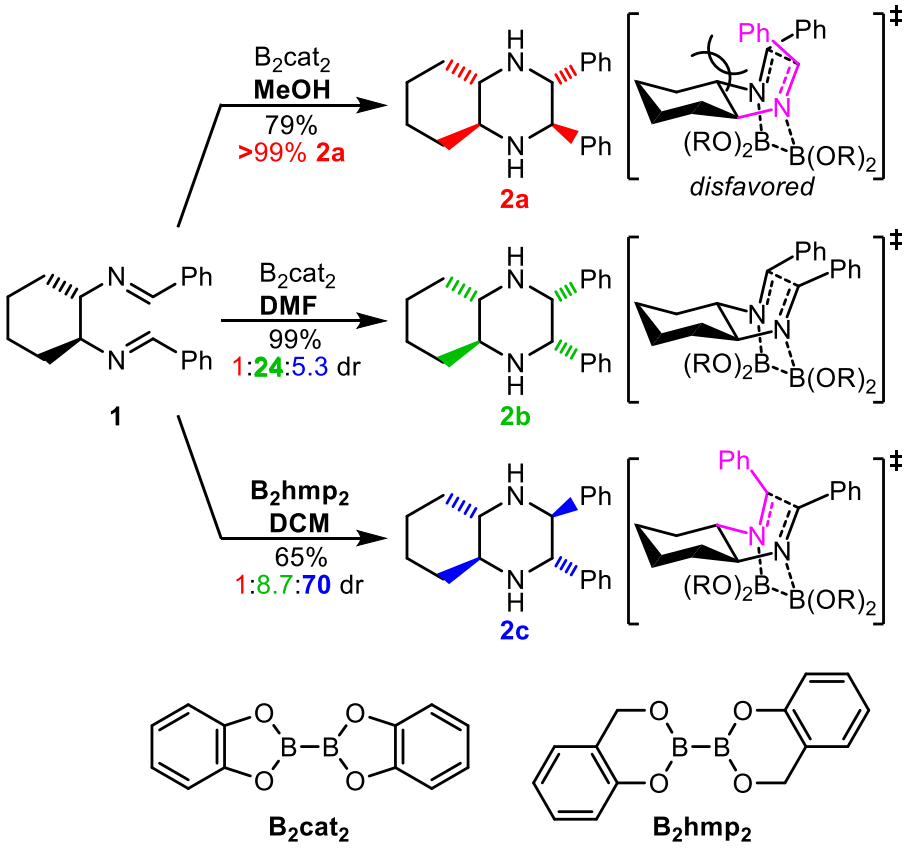
In contrast, the reaction of **1** with B_2cat_2 in DMF affords the *cis*-product **2b** as the major component (**24**:5.3:1, **2b:2c:2a**) in a diastereomeric mixture also containing **2a** and **2c** (99% yield). Models of a putative [3,3]-sigmatropic transition state for B_2cat_2 and **1**-(*E*,*E*) leading to **2b** do not reveal steric problems like those encountered for **2a**. The observed stereoselectivity can be explained by a concerted [3,3]-sigmatropic rearrangement of a *E*,*E*-diimine-diboron complex that proceeds through the boat-like transition state shown in Scheme 2.4.

The reaction of **1** with B_2hmp_2 in DCM affords **2c** as the major component (**70**:8.7:1, **2c**:**2b**:**2a**) in a diastereomeric mixture also containing **2a** and **2b**. (Selectivity with B_2cat_2 in DCM was lower: **17**:9.3:1, **2c**:**2b**:**2a**). In this case, isomerization of **1**-(*E*,*E*) to **1**-(*E*,*Z*) is required for the reaction to proceed through the [3,3]-sigmatropic rearrangement transition state shown in Scheme 2.4.

E/*Z* imine isomerization has been observed at room temperature in the presence of Lewis acids such as triarylboranes[17] and triarylboroxines[15] (Scheme 2.5). The exact

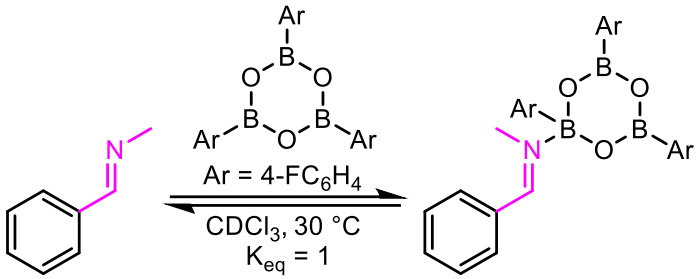
mechanism for this process is unclear, though it is likely that reversible nucleophilic attack (by solvent, the imine, or traces of water or amines) on iminium ions facilitates isomerization via C–N bond rotation in the intermediate complex (aminal, hemiaminal, etc.).[18] Given that the barrier to unimolecular isomerization is known to be high (~30 kcal/mol),[19] it is clear that Lewis acids dramatically accelerate this process.

Scheme 2.4. Reaction conditions for diastereoselective synthesis of **2a-2c** along with putative transition states corresponding to the formation of each major isomer via a [3,3]-sigmatropic pathway.[a]



[a] *Z*-imines in proposed transition states are highlighted in magenta for clarity.

Scheme 2.5. *E*/*Z* Isomerization of imines in the presence of boroxines.[a,15]



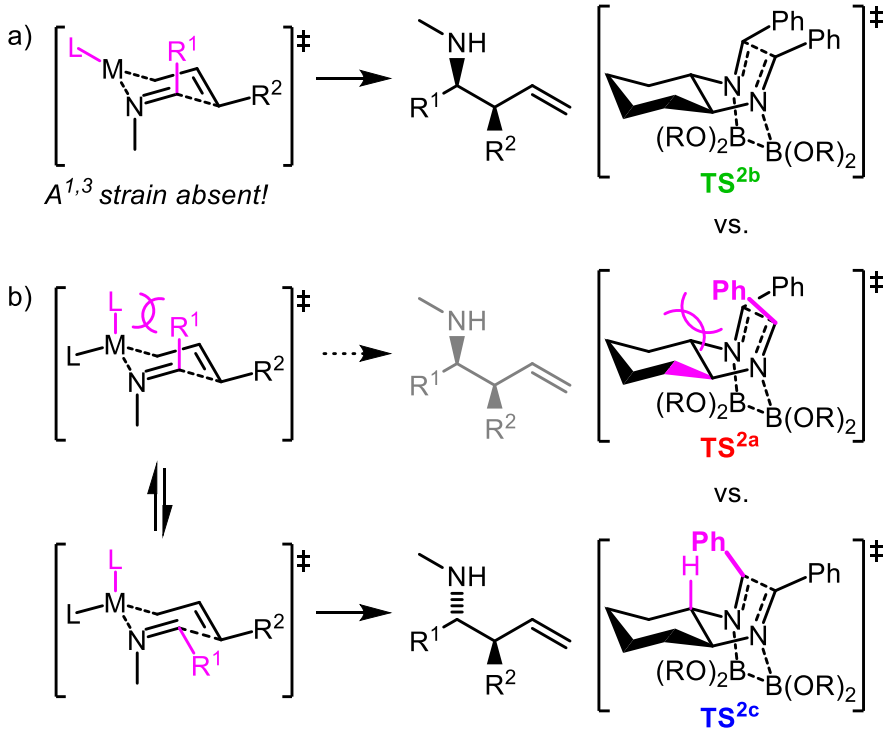
[a] *E*/*Z* imine stereoisomers are highlighted in magenta for clarity.

This isomerization process is featured in *anti*-selective imine allylborations that also proceed through a [3,3]-sigmatropic rearrangement mechanism, where reaction with the Z-imine is favored due to significant $A^{1,3}$ strain between substituents on the borane and the *E*-imine (Scheme 2.6b).[15] In contrast, if the metal(loid) lacks axial substituents in the chair-like transition state,[20] such as with some Cu-catalyzed allylations,[21] the reaction proceeds from the *E*-imine and diastereoselectivity is complementary (Scheme 2.6a). However, to the best of our knowledge, diastereoselectivity for these reactions is always subject to substrate control, and solvent control has not been reported for any of these systems.

We propose that a Curtin-Hammett scenario may explain the shift in diastereoselectivity with conditions for **2c** vs. **2b**. In a polar aprotic solvent (DMF), reductive cyclization of the *E*,*E*-diimine is faster than either *E*/*Z* imine isomerization or reductive cyclization of the *E*,*Z*-diimine, and so the reaction is selective for **2b**. Stabilization of partial charges in the transition state could account for this effect. However, in a less polar solvent (DCM) and with a bulkier diboron (B_2hmp_2), reductive cyclization of the *E*,*E*-diimine is slower than both *E*/*Z* imine isomerization and reductive cyclization of the *E*,*Z*-diimine, and so the reaction is selective for **2c**.

In less polar solvents, formation of polar diimine diboron complexes likely becomes more endothermic, and given that *Z*-imine triarylboroxine complexes are more stable than their *E*-imine counterparts, this may favor pathways that proceed through a *Z*-imine. The attenuated electrophilicity of B_2hmp_2 and increased $A^{1,3}$ strain between the *E*-imine and the larger diboron diolate ligands could strengthen this effect. This dynamic kinetic resolution pathway for reductive cyclization of the diimine bears some resemblance to that proposed for anti-selective imine allylborations.[15]

Scheme 2.6. Role of $A^{1,3}$ strain in controlling diastereoselectivity in Scheme 2.2.[a,20,21]



[a] Important $A^{1,3}$ interactions are highlighted in magenta for clarity.

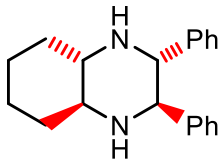
Conclusions.

We have discovered a new reductive coupling of diimines where control over relative stereochemistry can be influenced by both the solvent and structure of the diboron reagent used. This reaction was used to prepare all three possible diastereomers of 2,3-

diaryltetrahydroquinoxalines. It is proposed that the diboron-mediated reductive dynamic kinetic resolution of diimine **1** in aprotic solvents (DMF, DCM) proceeds via *E*/*Z* imine isomerization and [3,3]-sigmatropic rearrangement of a diimine-diboron complex, while in protic solvents (MeOH), an ionic mechanism is operative. This is the first report of solvent control over the relative stereochemistry of a reaction where the product-determining step is preceded by *E/Z* imine isomerization. Chapter 3 describes investigations of the scope of this chemistry, while Chapter 4 describes computational exploration of the two mechanisms discussed above, and Chapter 5 describes improved preparation of diboron reagents that could be useful in this chemistry.

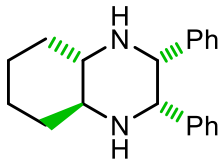
Experimental Section.

General. All reactions were carried out under a nitrogen atmosphere unless otherwise noted. All reagents were obtained from commercial sources and were used as obtained without further purification unless otherwise specified. Additionally, dichloromethane, dimethylformamide, methanol, and anhydrous diethyl ether were obtained from commercial sources and used without further purification. Yields refer to isolated yields of compounds estimated to be ≥95% pure as determined by ^{1}H NMR analysis unless otherwise noted. The yields reported in the manuscript and supporting information describe the result of a single experiment. Compound **1** was prepared by literature procedures.[22]



2a

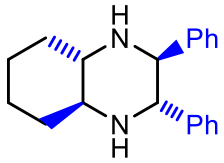
(±)-(2*S*,3*S*,4a*R*,8a*R*)-2,3-Diphenyldecahydroquinoxaline (2a). B_2cat_2[24] (118.9 mg, 0.5 mmol) was added to a 4 mL vial, followed by a stir bar and 0.5 mL MeOH. (±)-(1*E*,1*E′*)-*N*,*N′*-((1*R*,2*R*)-Cyclohexane-1,2-diyl)bis(1-phenylmethanimine) (**1**)[22] (72.6 mg, 0.25 mmol) was added and the vial flushed with N_2 before sealing with a PTFE cap. After stirring the reaction mixture for 3 hours, solvent was removed in vacuo. The residue was quenched with 1 mL 1 M HCl and extracted 3x with 2 mL Et_2O (discarding the organic layer), and then basified with 1 mL 6 M NaOH. The aqueous layer was then extracted 3x with 2 mL Et_2O. The combined organic extracts were dried with NaCl/Na_2SO_4, filtered, and then the solvent removed in vacuo to afford **2a** (57.8 mg, 79%) as an off-white solid. Spectral data were consistent with literature values.[23]



2b

(±)-(2*R*,3*S*,4a*R*,8a*R*)-2,3-Diphenyldecahydroquinoxaline (2b). B_2cat_2[24] (118.9 mg, 0.5 mmol) was added to a 4 mL vial, followed by a stir bar and 0.5 mL DMF. Diimine **1** (72.6 mg, 0.25 mmol) was added and the vial flushed with N_2 before sealing with a PTFE cap. After stirring the reaction mixture for 1 hour, solvent was removed in vacuo. The residue was quenched with 1 mL 1 M HCl and extracted 3x with 2 mL Et_2O (discarding

the organic layer), and then basified with 1 mL 6 M NaOH. The aqueous layer was then extracted 3x with 2 mL Et_2O. The combined organic extracts were dried with $NaCl/Na_2SO_4$, filtered, and then the solvent removed in vacuo to afford **2b** as the major component (24:5.3:1, **2b**:**2c**:**2a**) in a diastereomeric mixture also containing **2a** and **2c** (73.0 mg, 99%) as a pale-yellow oil. Spectral values for [H-**2b**+][$HB(C_6F_5)_3$] have previously been reported.[25] For **2b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68–7.63 (m, 2H), 7.32–7.26 (m, 2H), 7.21–7.11 (m, 5H), 7.09–7.04 (m, 1H), 4.64 (d, *J* = 4.0 Hz, 1H), 4.20 (d, *J* = 4.0 Hz, 1H), 2.92–2.86 (m, 1H), 2.69 (ddd, *J* = 11.0, 9.0, 3.5 Hz, 1H), 1.88–1.17 (m, 10H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 141.9, 141.6, 130.1, 127.9, 127.5, 127.0, 126.6, 126.6, 64.1, 63.1, 63.1, 53.5, 32.2, 32.2, 24.9, 24.9.



2c

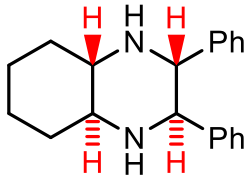
(±)-(2*R*,3*R*,4a*R*,8a*R*)-2,3-Diphenyldecahydroquinoxaline (2c). B_2hmp_2[26] (66.5 mg, 0.25 mmol) was added to a 4 mL vial, followed by a stir bar and 0.25 mL DCM. Diimine **1** (36.3 mg, 0.125 mmol) was added and the vial flushed with N_2 before sealing with a PTFE cap. After stirring for 24 hours, solvent was removed in vacuo. The residue was quenched with 1 mL 1 M HCl and extracted 3x with 2 mL Et_2O (discarding the organic layer), and then basified with 1 mL 6 M NaOH. The aqueous layer was then extracted 3x with 2 mL Et_2O. The combined organic extracts were dried with $NaCl/Na_2SO_4$, filtered, and then the solvent removed in vacuo to afford **2c** as the major component (**70**:8.7:1, **2c**:**2b**:**2a**) in a diastereomeric mixture also containing **2a** and **2b** (23.8 mg, 65%) as a pale-

yellow oil. Diastereomeric ratios were determined via spectral deconvolution using the line fitting protocol in MNova 14.2.0 (Mestrelab Research, S.L.; Santiago de Compostela, Spain) using Gaussian/Lorentzian peak shapes and simulated annealing. Relative stereochemistry was assigned by 1D NOESY experiments. For **2c**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (ddd, *J* = 8.1, 1.2, 1.2 Hz, 4H), 7.39 (dd, *J* = 7.7, 7.7 Hz, 4H), 7.34–7.22 (m, 2H), 4.53 (s, 2H), 2.74–2.57 (m, 2H), 1.77–1.63 (m, 4H), 1.59 (ddd, *J* = 12.7, 2.3, 2.3 Hz, 2H), 1.35–1.09 (m, 4H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 144.5, 128.3, 127.7, 126.6, 58.5, 54.8, 32.3, 25.0.

APPENDIX

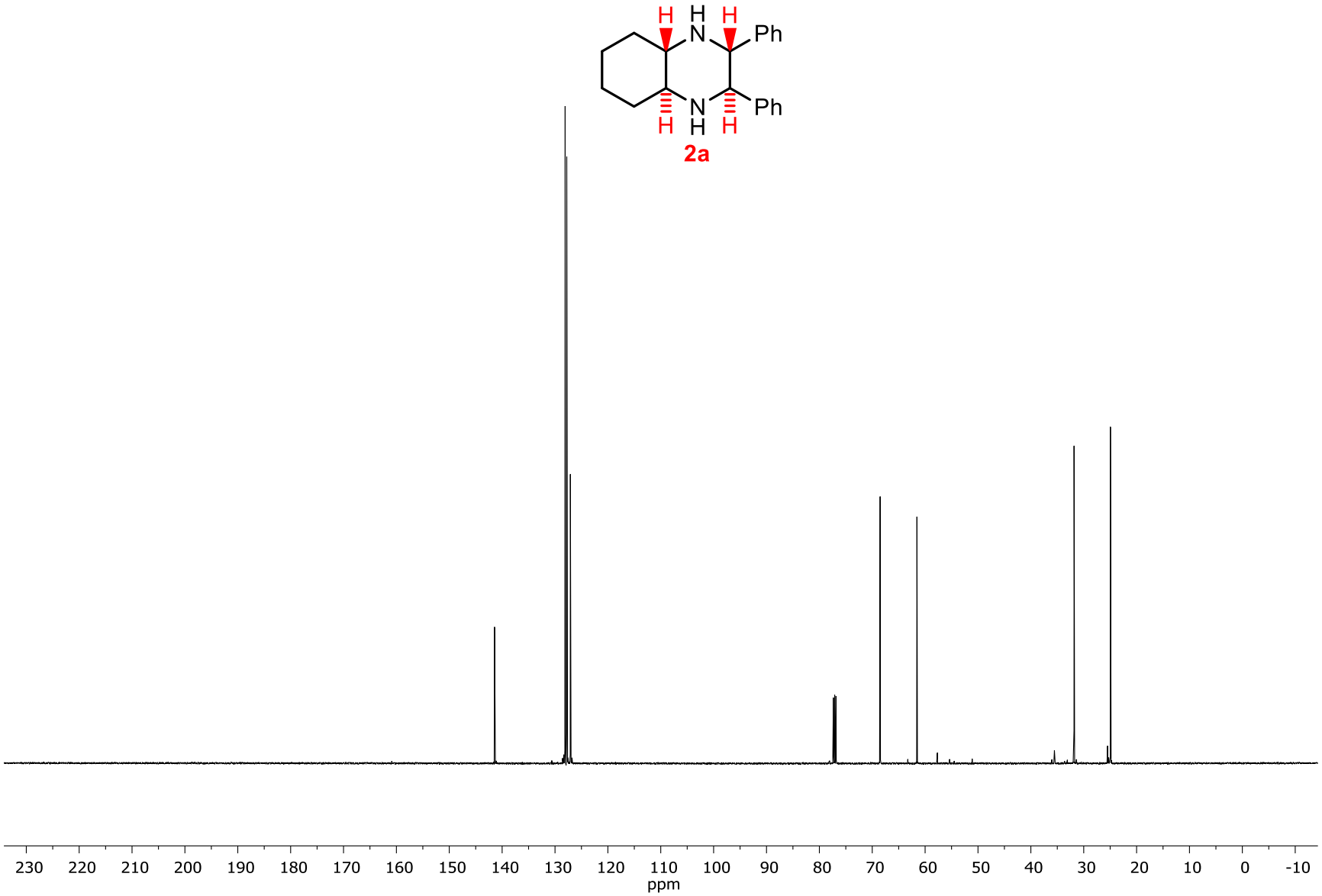
Spectral Data

^{1}H 500 MHz, $CDCl_3$

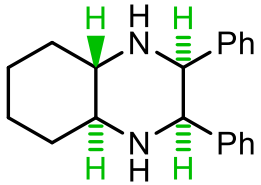


2a

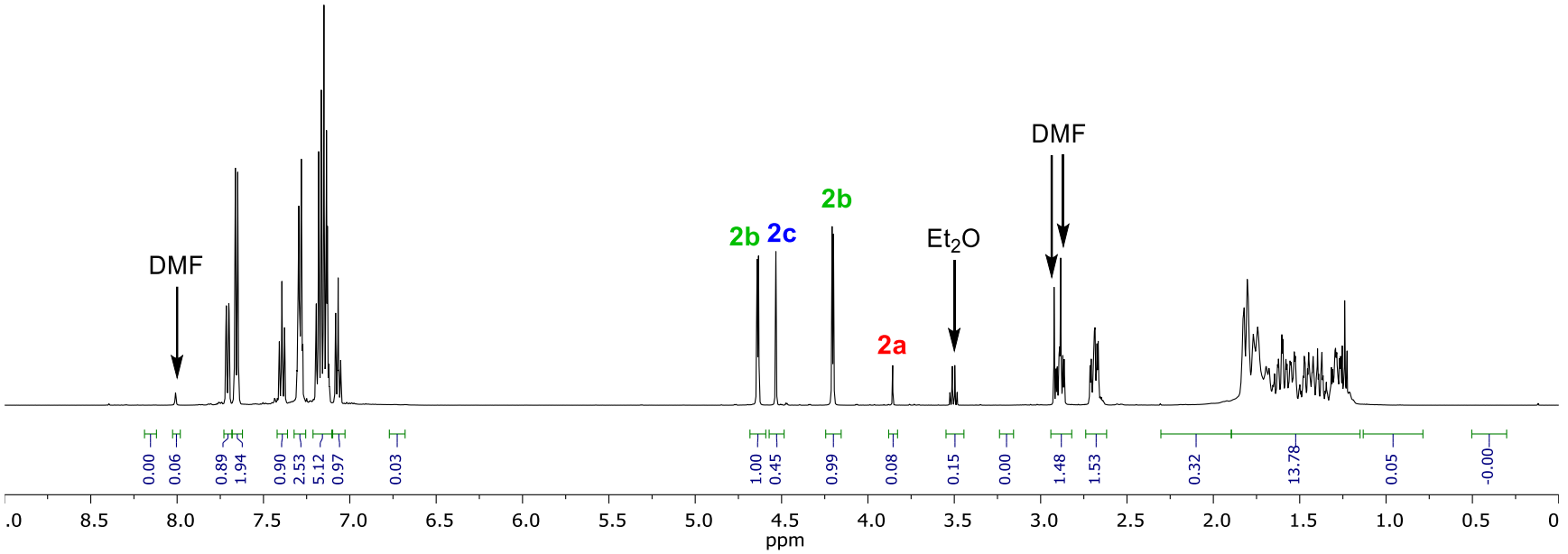
^{13}C 126 MHz, $CDCl_3$



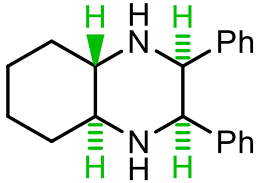
^{1}H 500 MHz, $CDCl_3$



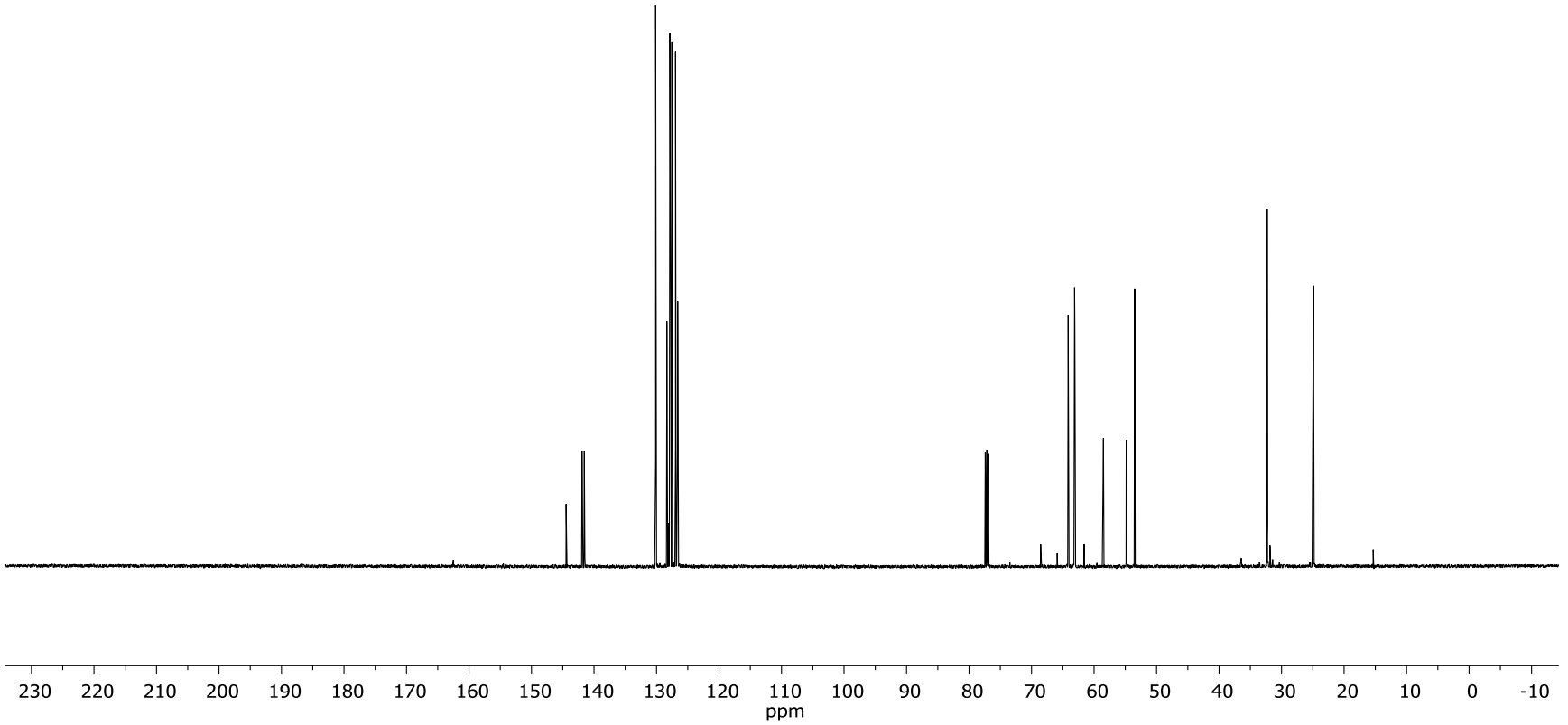
2b



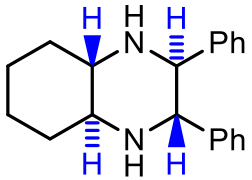
^{13}C 126 MHz, $CDCl_3$



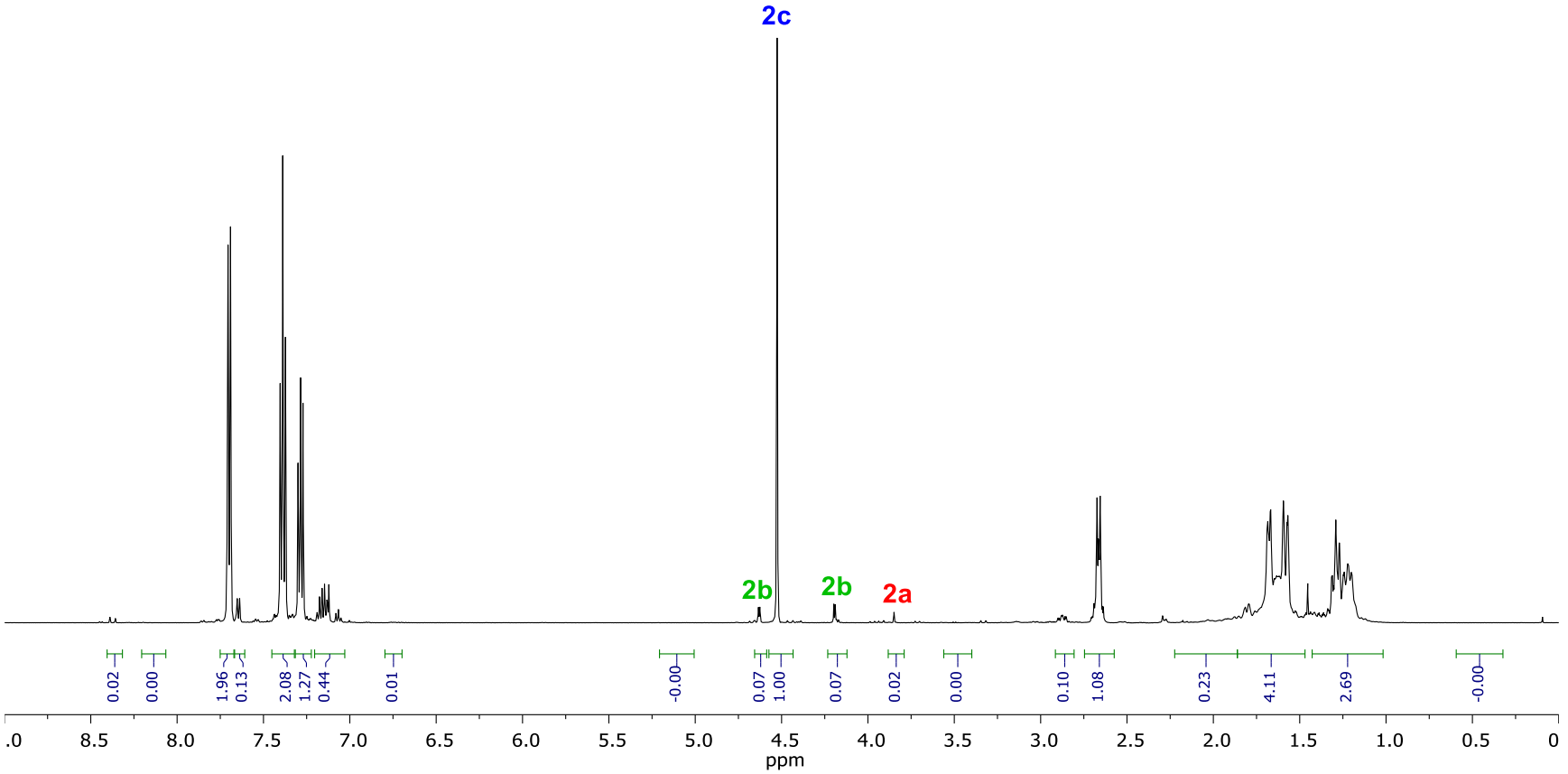
2b



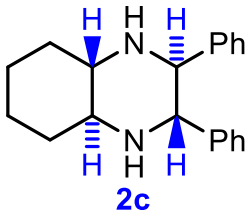
^{1}H 500 MHz, $CDCl_3$



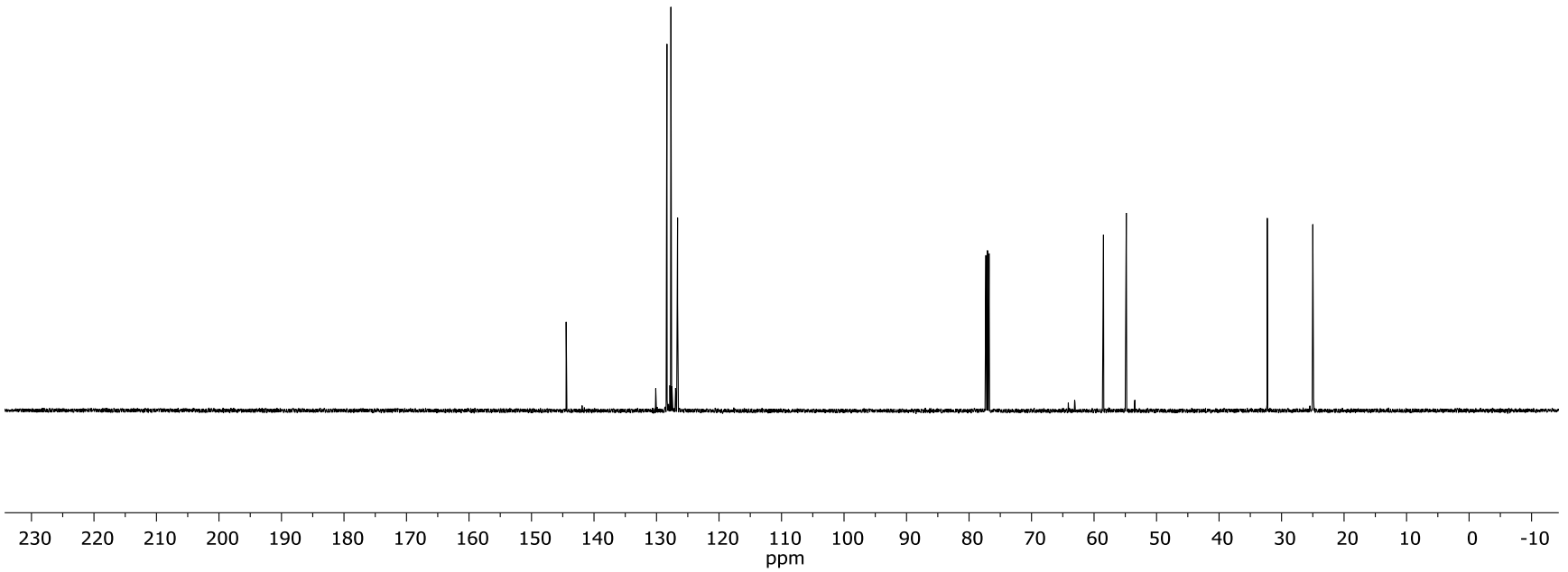
2c



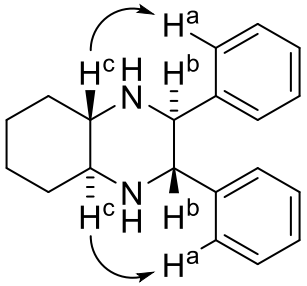
^{13}C 126 MHz, $CDCl_3$



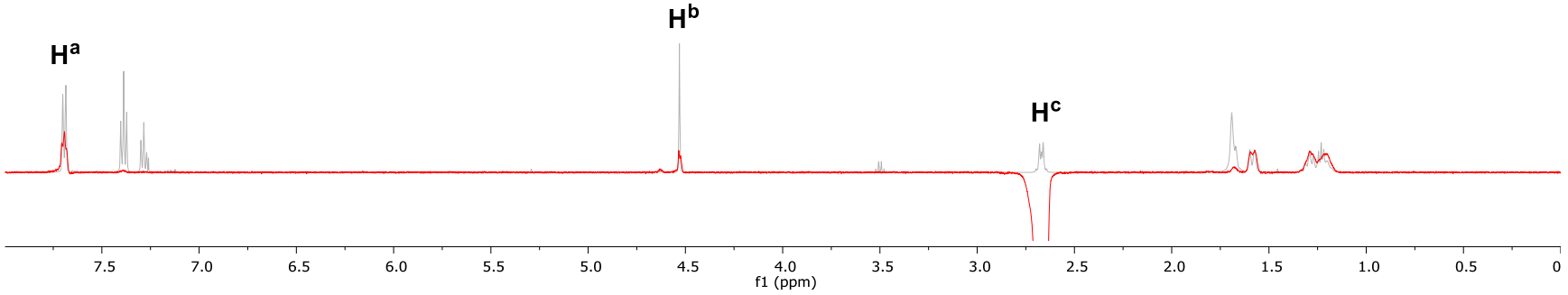
2c

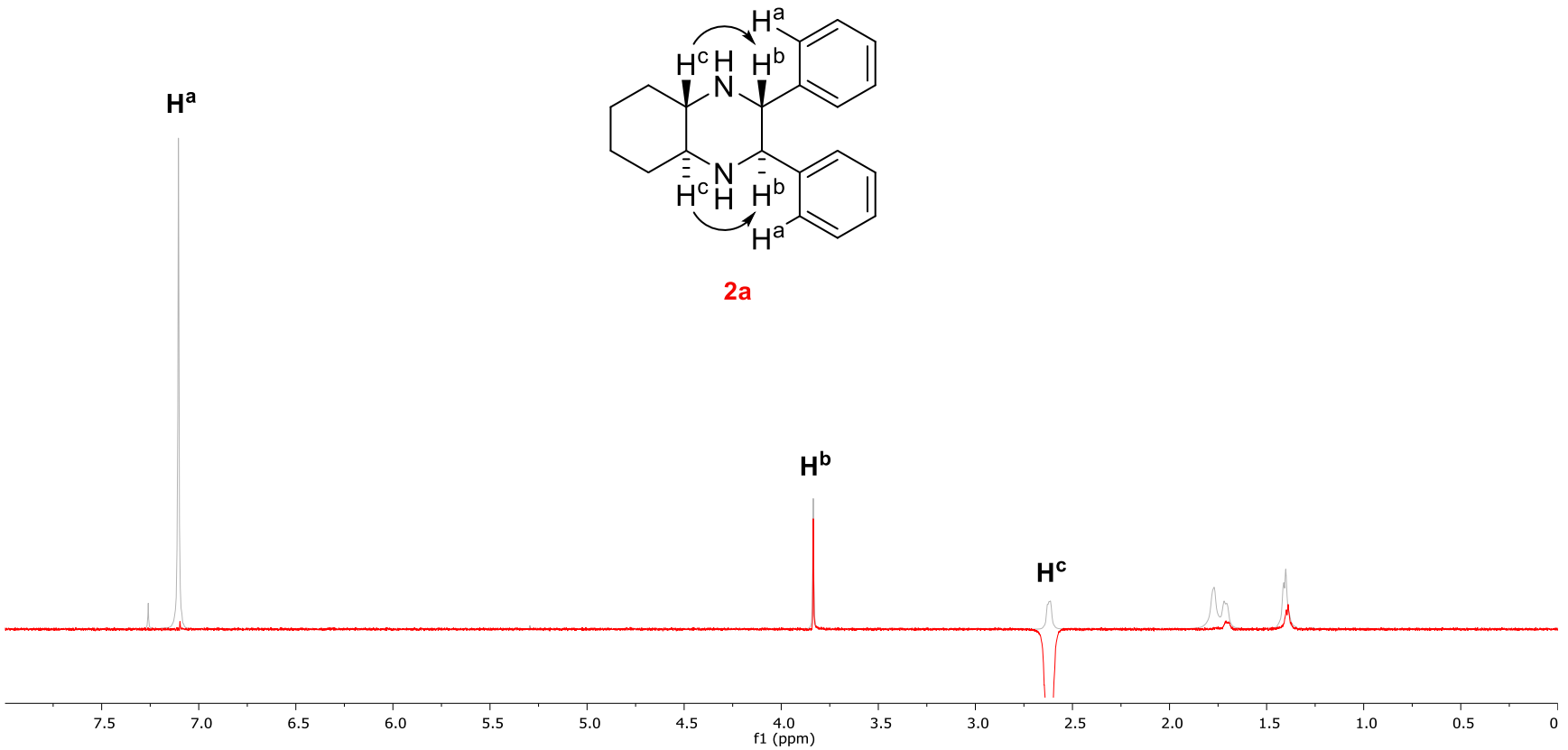


^{1}H 500 MHz, $CDCl_3$



2c




Ha
Hc H Hb
N
N
Hc H Hb
Ha
2a
Ha
Hb
Hc
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

REFERENCES

REFERENCES

(1) Zhang, W.; Loebach, J. L.; Wilson, S. R.; Jacobsen, E. N. Enantioselective epoxidation of unfunctionalized olefins catalyzed by salen manganese complexes. *J. Am. Chem. Soc.* **1990**, *112*, 2801–2803.

(2) Bennani, Y. L.; Hanessian, S. *Trans*-1,2-Diaminocyclohexane Derivatives as Chiral Reagents, Scaffolds, and Ligands for Catalysis: Applications in Asymmetric Synthesis and Molecular Recognition. *Chem. Rev.* **1997**, *97*, 3161–3196.

(3) Li, Z.; Yamamoto, H. Zirconium(IV)- and Hafnium(IV)-Catalyzed Highly Enantioselective Epoxidation of Homoallylic and Bishomoallylic Alcohols. *J. Am. Chem. Soc.* **2010**, *132*, 7878–7880.

(4) Saibabu Kotti, S. R. S.; Timmons, C.; Li, G. Vicinal diamino functionalities as privileged structural elements in biologically active compounds and exploitation of their synthetic chemistry. *Chem. Biol. Drug Des.* **2006**, *67*, 101–114.

(5) Talukdar, S.; Banerji, A. Low Valent Titanium Mediated Imino−Pinacol Coupling: An Improved and Expeditious Route to Vicinal Diamino-Based Ligands. *J. Org. Chem.* **1998**, *63*, 3468–3470.

(6) Hirao, T.; Hatano, B.; Imamoto, Y.; Ogawa, A. A Catalytic System Consisting of Vanadium, Chlorosilane, and Aluminum Metal in the Stereoselective Pinacol Coupling Reaction of Benzaldehyde Derivatives. *J. Org. Chem.* **1999**, *64*, 7665–7667.

(7) Mercer, G. J.; Sigman, M. S. Diastereoselective synthesis of piperazines by manganese-mediated reductive cyclization. *Org. Lett.* **2003**, *5*, 1591–1594.

(8) Arai, S.; Takita, S.; Nishida, A. A Facile Synthesis of Vicinal Diamines Promoted by Low-Valent Niobium: Preparation of Chiral Octahydrobiisoquinolines and Their Application to Catalytic Asymmetric Synthesis. *Eur. J. Org. Chem*. **2005**, *24*, 5262–5267.

(9) Vairaprakash, P.; Periasamy, M. A Simple Method of Synthesis of (±)-2,3-Diarylpiperazines and a Novel Method of Resolution of (±)-2,3-Diphenylpiperazine. *J. Org. Chem.* **2006**, *71*, 3636–3638.

(10) Aspinall, H. C.; Greeves, N.; Hin, S. L. F. A new Yb^{3+}-catalyzed pinacol and imine-coupling reaction. *Tetrahedron Lett*. **2010**, *51*, 1558–1561.

(11) Carter, C. A. G.; John, K. D.; Mann, G.; Martin, R. L.; Cameron, T. M.; Baker, R. T.; Bishop, K. L.; Broene, R. D.; Wescott, S. A. Bifunctional Lewis Acid Reactivity of Diol-Derived Diboron Reagents. *ACS Symposium Series: Group 13 Chemistry* **2002**, *822*, 70–87.

(12) Zhou, M.; Li, K.; Chen, D.; Xu, R.; Xu, G.; Tang, W. Enantioselective Reductive Coupling of Imines Templated by Chiral Diboron. *J. Am. Chem. Soc.* **2020**, *142*, 10337–10342.

(13) Chen, D.; Xu, G.; Zhou, Q.; Chung, L. W.; Tang, W. Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. *J. Am. Chem. Soc.* **2017**, *139*, 9767–9770.

(14) Grignon-Dubois, M.; Fialeix, M.; Leger, J.-M. Silylation de l'isoquinoléine: influence des conditions opératoires sur l'obtention de nouveaux hétérocycles siliciés. *Can. J. Chem.* **1993**, *71*, 754–761.

(15) Alam, R.; Das, A.; Huang, G.; Eriksson, L.; Himo, F.; Szabó, K. J. Stereoselective allylboration of imines and indoles under mild conditions. An *in situ E*/*Z* isomerization of imines by allylboroxines. *Chem. Sci.* **2014**, *5*, 2732–2738.

(16) Zhang, L.; Jiao, L. Super electron donors derived from diboron. *Chem. Sci.* **2018**, *9*, 2711–2722.

(17) Blackwell, J. M.; Piers, W. E.; Parvez, M.; McDonald, R. Solution and Solid-State Characteristics of Imine Adducts with Tris(pentafluorophenyl)borane. *Organometallics* **2002**, *21*, 1400–1407.

(18) Johnson, J. E.; Morales, N. M.; Gorczyca, A. M.; Dolliver, D. D.; McAllister, M. A. Mechanisms of Acid-Catalyzed *Z*/*E* Isomerization of Imines. *J. Org. Chem.* **2001**, *66*, 7979–7985.

(19) McCarty, C. G. *syn-anti* Isomerizations and rearrangements. *Carbon-Nitrogen Double Bonds* Patai, S. (Ed.) **1970**, 363–464.

(20) Mejuch, T.; Gilboa, N.; Gayon, E.; Wang, H.; Houk, K. N.; Marek, I. Axial Preferences in Allylation Reactions via the Zimmerman–Traxler Transition State. *Acc. Chem. Res.* **2013**, *46*, 1659–1669.

(21) Liu, R. Y.; Yang, Y.; Buchwald, S. L. Regiodivergent and Diastereoselective CuH-Catalyzed Allylation of Imines with Terminal Allenes. *Angew. Chem. Int. Ed.* **2016**, *55*, 14077–14080.

(22) Staab, H. A.; Vögtle, F. Untersuchungen über Schiffsche Basen, II: Darstellung von 1.2-Diamino-cyclopropanen und von Schiffschen Basen dieser Diamine. *Chem. Ber.* **1965**, *98*, 2691–2700.

(23) Arai, S.; Takita, S.; Nishida, A. A Facile Synthesis of Vicinal Diamines Promoted by Low-Valent Niobium: Preparation of Chiral Octahydrobiisoquinolines and Their Application to Catalytic Asymmetric Synthesis. *Chem. Eur. J.* **2005**, *2005*, 5262–5267.

(24) Lawlor, F. J.; Norman, N. C.; Pickett, N. L.; Robins, E. G.; Nguyen, P.; Lesley, G.; Marder, T. B.; Ashmore, J. A.; Green, J. C. Bis-Catecholate, Bis-Dithiocatecholate, and Tetraalkoxy Diborane(4) Compounds: Aspects of Synthesis and Electronic Structure. *Inorg. Chem.* **1998**, *37*, 5282–5288.

(25) Mahdi, T.; del Castillo, J. N.; Stephan, D. W. Metal-Free Hydrogenation of N-Based Heterocycles. *Organometallics* **2013**, *32*, 1971–1978.

(26) The Commonwealth of Australia Commonwealth Scientific and Industrial Research Organization US6346639, **2002**, B1.

Chapter 3. Activation of Tetraalkoxydiborons by B_2O_3: Scope and Reactivity

Introduction.

Previously (Chapter 2) we reported diimine reductive coupling reactions using diboron diolates where relative stereochemistry could be controlled by choice of solvent and influenced by the ligands on the diboron (catecholate vs. 2-hydroxybenzyl alcoholate). Herein we discuss new methods to alter the reactivity and selectivity of tetraalkoxydiborons via a unique activation strategy employing B_2O_3 or $B_3O_3(OMe)_3$ (trimethoxyboroxine). Modification of the reactivity of a diboron employed in synthetic organic reactions without changing the ligand or solvent has not previously been reported. Additionally, preliminary studies as to the nature of the active intermediate are discussed.

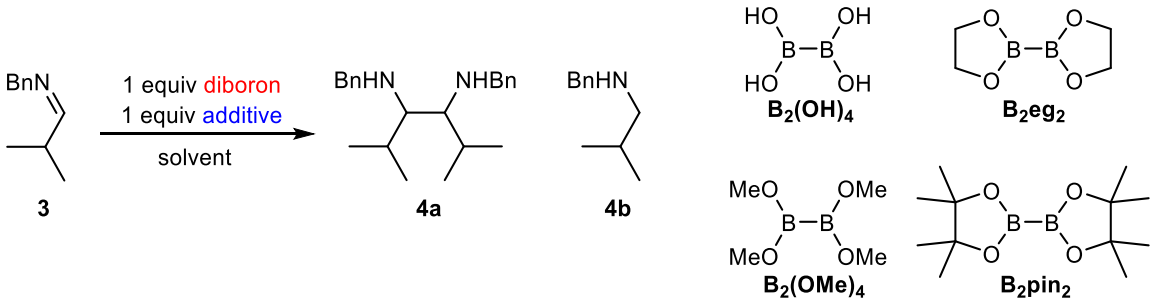
Scope of the Diboron and Additives.

Initial investigations of the scope of the diboron used isobutyraldehyde-derived imine **3** as the coupling substrate, with a variety of diborons (Table 3.1). Unfortunately, no reaction occurred with B_2pin_2 (Entry 13) or the relatively sterically unhindered diborons B_2eg_2 (Entry 5) and $B_2(OMe)_4$ (Entry 9). However, full conversion occurred within 48 hours with $B_2(OH)_4$ in DMF at 80 °C, affording a 1:1 mixture of the monoamine $2e^-$ reduction product (the isobutylbenzylamine) **4b** and the desired dimer **4a** (Entry 1).

Aromatic heterocycles, aldimines, ketones, and aldehydes are known to be reduced by diborons such as $B_2(OH)_4$ in the presence of H_2O,[1-3] and in this case, this pathway produces the amine **4b** as an unwanted side-product. This reduction can even break aromaticity (see Scheme 3.1 for an example from the literature[1]), highlighting the power of wet $B_2(OH)_4$ as a reductant. However, $B_2(OH)_4$ exists in solution in equilibrium with

H_2O and its anhydride $B_4O_2(OH)_4$ (Scheme 3.2),[4] so suppressing the unwanted $2e^-$ reduction pathway by removing H_2O proved challenging.

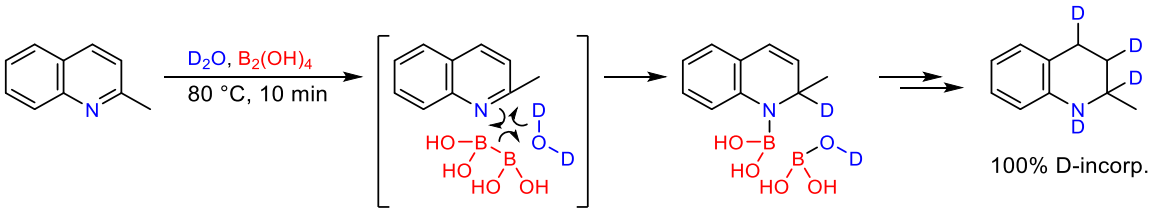
Table 3.1. Screen of diborons and additives for reductive coupling of imine **3**.[a]



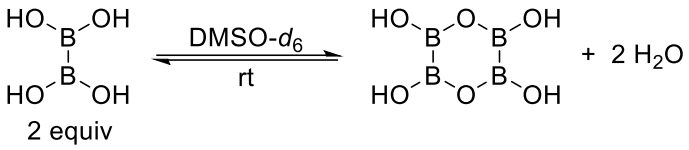
Entry	Solvent	Diboron	Additive	Temp (˚C)	Time (h)	Conv. (~%)	4a:4b	d.r.
1	DMF	$B_2(OH)_4$		80	48	100	1:1	-
2	DMF	$B_2(OH)_4$		25	1	40	1:1	-
3	DMF	$B_2(OH)_4$	B_2O_2	25	1	60	1:1	-
4	DMF	$B_2(OH)_4$	B_2O_3	25	8	90	10:1	1.2:1
5	MeCN	B_2eg_2		25	24	0	-	-
6	MeCN	B_2eg_2	B_2O_3	25	24	trace	-	-
7	MeCN	B_2eg_2	$B_3O_3(OMe)_3$	25	24	60	10:0	-
8	MeCN	B_2eg_2	$B_3O_3Me_3$	25	1	50	10:0	-
9	MeCN	$B_2(OMe)_4$		25	1	0	-	-
10a	MeCN	$B_2(OMe)_4$	B_2O_3	25	0.2	90	10:0	-
10b	MeCN	$B_2(OMe)_4$	B_2O_3	25	1	100	10:0	1.2:1
11a	MeCN	$B_2(OMe)_4$	$B_3O_3(OMe)_3$	25	0.2	90	10:0	-
11b	MeCN	$B_2(OMe)_4$	$B_3O_3(OMe)_3$	25	1	100	10:0	1.3:1
12	MeCN	$B_2(OMe)_4$	$B_3O_3Me_3$	25	1	100	10:0	-
13	MeCN	B_2pin_2		60	72	0	-	-

[a] Conversion to **4a** and **4b** was estimated by GC-MS analysis. Diastereomeric ratios were determined by ^1H NMR analysis.

Scheme 3.1. Wet $B_2(OH)_4$ as an aromaticity-breaking reductant.[1]



Scheme 3.2. Equilibrium between $B_2(OH)_4$ and its anhydride.[4]



The ratio of **4a** to **4b** was unaffected by using dry DMF or adding desiccants such as Na_2SO_4 or $MgSO_4$ (not shown in Table 3.1). Similarly, addition of boron monoxide[5] (B_2O_2) had no apparent effect on selectivity (Entry 3 – self-condensation of **3** accounts for a third of conversion). However, addition of boric anhydride (B_2O_3) dramatically improved selectivity for **4a** (Entry 4). Unfortunately, diastereoselectivity was poor (ratios estimated by ^{1}H NMR analysis). (Notably, the reaction also became *very* warm – failure to carefully control large scale reactions could result in violent exotherms.)

Only trace conversion to the dimer occurred with B_2eg_2 in MeCN (preferable to DMF for practical reasons) even with addition of B_2O_3 (Entry 6), but trimethoxyboroxine ($B_3O_3(OMe)_3$) resulted in partial conversion (Entry 7), and trimethylboroxine ($B_3O_3Me_3$) triggered a drastic increase in the reaction rate (Entry 8 – monoamine side product **4b** was not detected). Similarly, no reaction occurred with $B_2(OMe)_4$ (Entry 9), but addition of B_2O_3, $B_3O_3(OMe)_3$, or $B_3O_3Me_3$ resulted in high conversion in minutes without external heating (Entries 10-12). Unfortunately, diastereoselectivity was poor, like the previous reaction with $B_2(OH)_4$/B_2O_3 in DMF.

We elected to use $B_2(OMe)_4$ for further exploration of the scope of this chemistry, as it allowed us to avoid the tedious extraction protocols required when DMF is employed as the solvent (as $B_2(OH)_4$ is insoluble in MeCN), and to avoid the high cost of $B_3O_3Me_3$ (needed for rapid conversion with B_2eg_2). In addition to its enhanced solubility and easier

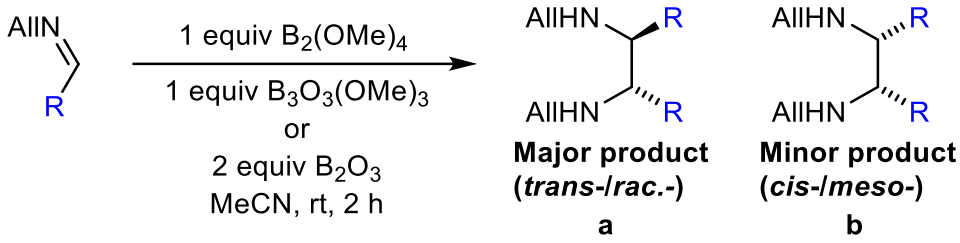
workup, the boron byproducts derived from reductive coupling of imines using $B_2(OMe)_4$ are easily removed by azeotropic distillation with methanol. Little difference in conversion, chemoselectivity, and diastereoselectivity was noted between conditions employing B_2O_3 or $B_3O_3(OMe)_3$ (Entries 10-11).

Scope of the Imine Substrate.

Next, the scope of the reaction with respect to imine substrate was explored (Table 3.2). Aromatic vicinal *N*,*N*'-diallyldiamines **6**, **8**, and **10** were afforded in good yield, but low diastereoselectivity, from imines **5**, **7**, and **9**, respectively (Entries 1-3). In some cases $B_3O_3(OMe)_3$ was used for operational simplicity (no waiting for an hour for B_2O_3 to dissolve). As mentioned above, its performance is nearly identical to B_2O_3.

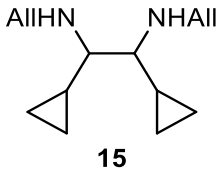
The reaction appears to be tolerant of different substituents on the 4-position of the phenyl ring of the imine substrate (Entries 1-3, imines **5**, **7**, and **9**). Linear *N*-allylaldimine **11** (Entry 4) and α,β-unsaturated aldimine **17** (Entry 8) afforded complex mixtures, while the bulky aliphatic aldimine **16** was unreactive (Entry 7). Interestingly, no ring-opened products were observed with imine **14** (Entry 6). This example provided crucial mechanistic information, as the formation of **15** is inconsistent with a radical mechanism for the reductive coupling.

Table 3.2. Scope of imine coupling partners.



Entry (imine)	R	Additive	Yield (%)	d.r. (major:minor)
1 (5)	*p*-$MeOC_6H_4$	B_2O_3	64	1.2:1 (**6a:6b**)
2 (7)	Ph	B_2O_3	51	1.1:1 (**8a:8b**)
3 (9)	*p*-BrC_6H_4	B_2O_3	65	1:1.4 (**10a:10b**)
4 (11)	*n*-Pr	B_2O_3	Complex mixture	-
5 (12)	*i*-Pr	$B_3O_3(OMe)_3$	73	1.7:1[a] (**13**)
6 (14)	*c*-Pr	$B_3O_3(OMe)_3$	65	1.5:1[a] (**15**)
7 (16)	*t*-Bu	$B_3O_3(OMe)_3$	No reaction	-
8 (17)	*E*-styryl	-	Complex mixture	-

[a] The relative stereochemistry for the major diastereomer has not been resolutely assigned.

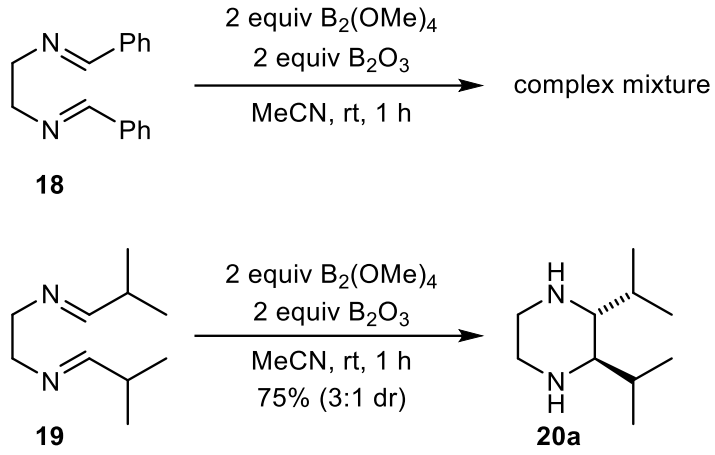


15

No ring-opened products observed!

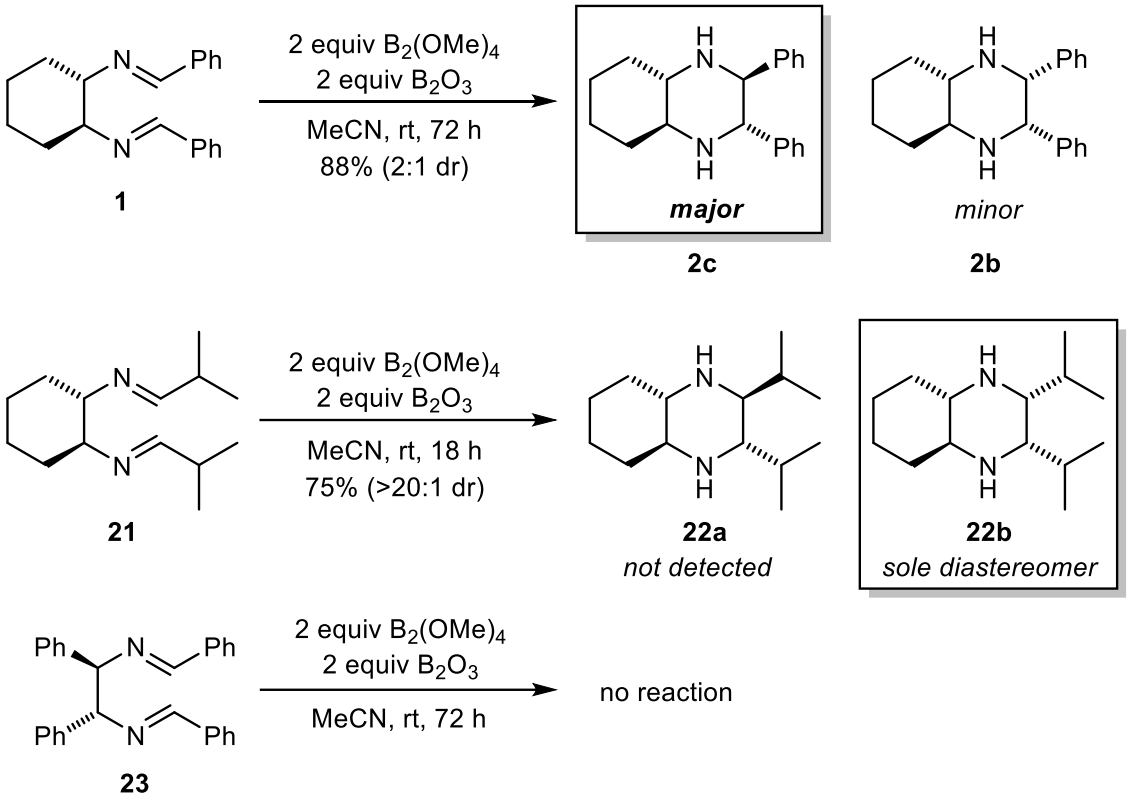
This reaction can also be used to construct heterocyclic structures, such as piperazines and diazepanes. While attempts to reductively couple aromatic diimine **18** (Scheme 3.3) only afforded complex mixtures (instead of the *trans*-diphenylpiperazine), the reductive intramolecular coupling of aliphatic diimine **19** afforded the *trans*-diisopropylpiperazine **20a** in good yield and 3:1 (**20a:20b**) diastereomeric ratio.

Scheme 3.3. Construction of piperazines, I.



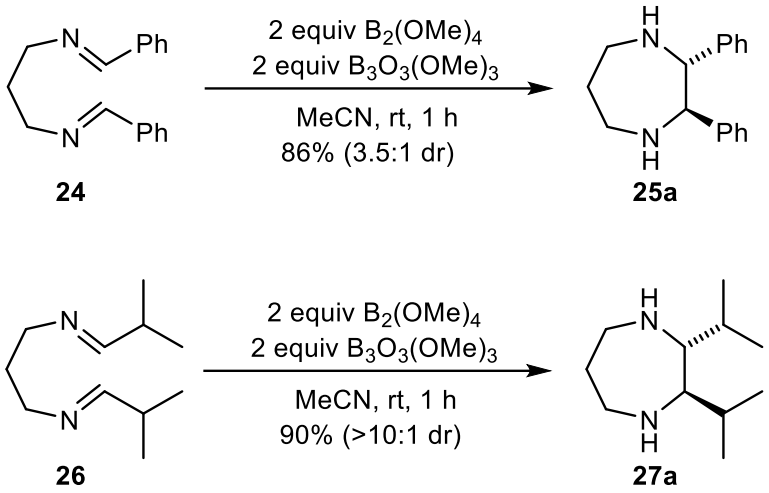
Aromatic diimine **2** (a ring fused analog of **18**) (Scheme 3.4, see Chapter 2) cyclized to afford the highly strained *trans*-diastereomer **2c** and the *cis*-diastereomer **2b** in a 2:1 ratio. When diimine **21** was utilized, in contrast with Scheme 3.3, no trace of *trans*-**22** (**22a**) was detected, the product of reported diastereoselective metal-mediated reductions[6] and our prior report of the reaction of diimine **1** with B_2cat_2 in methanol. The *cis*-diastereomer **22b** was obtained exclusively, a surprising result given the steric interactions between *cis*-1,2 orientations of isopropyl groups in six-membered rings. Diimine **23** (Scheme 3.4) was unreactive, possibly because of steric hindrance.

Scheme 3.4. Construction of piperazines, II.



Trans-1,4-diazepanes could also be synthesized by this method (Scheme 3.5). Diimines **24** and **26** were reductively coupled to afford diphenyl (**25a**) and di-isopropyl-1,4-diazepanes (**27**) in good yield and diastereoselectivity, respectively. The relative stereochemistry of **25a** was determined by comparison to its *cis*-diasteromer (**25b**, prepared by literature methods).[6] The relative stereochemistry of **25b** was established by adding a large excess of benzaldehyde to a $CDCl_3$ solution of this diastereomer. NMR analysis of the aminal derivative and its symmetry revealed the literature product to be the *cis*-diastereomer **25b** which was distinct from **25a** (see Experimental Section for further details).

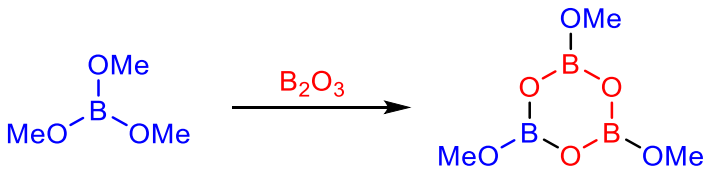
Scheme 3.5. Construction of 1,4-diazepanes by diboron-mediated reductive coupling of imines.[a]



[a] These substrates were added slowly to a rapidly stirred solution of the diboron to avoid erosion of yield via formation of aminal side products.

Inspired by the novelty of this chemistry and the scope of the reaction, we next sought to investigate the composition of the active diboron intermediate. As B_2O_3 is known to react with $B(OMe)_3$ to form trimethoxyboroxine[7] (Scheme 3.6), it is possible a similar transformation is occurring in situ with $B_2(OMe)_4$ during this reaction to form borylboroxine **28** (Scheme 3.7, *insertion*). Boroxines are known to be more electrophilic than their parent boronic acids and esters, increasing the rate of many reactions, and could theoretically accelerate this transformation.[8]

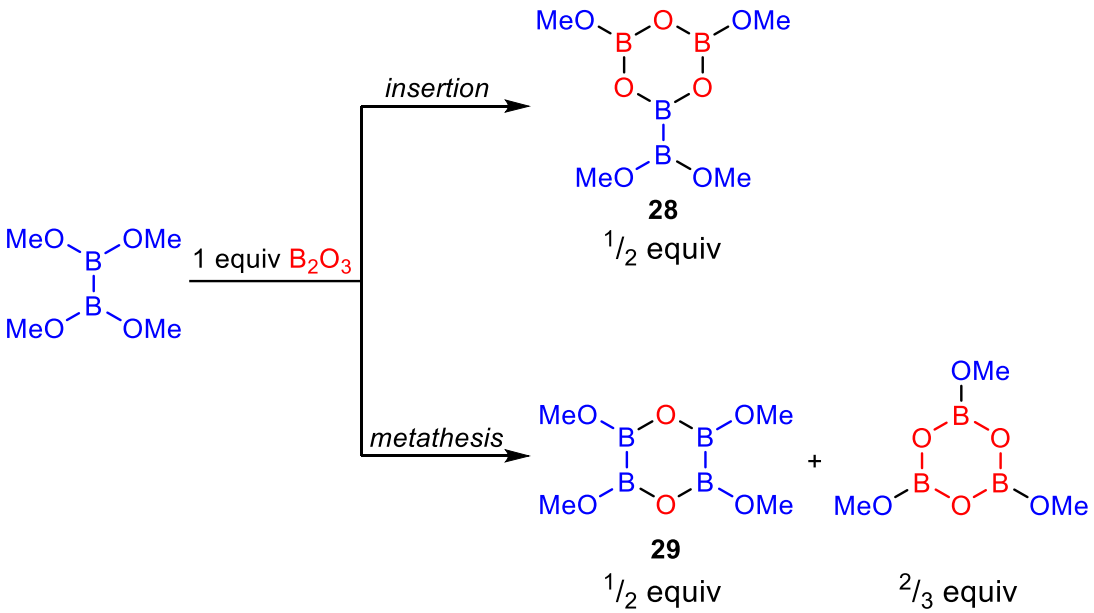
Scheme 3.6. Reported formation of trimethoxyboroxine.[7]



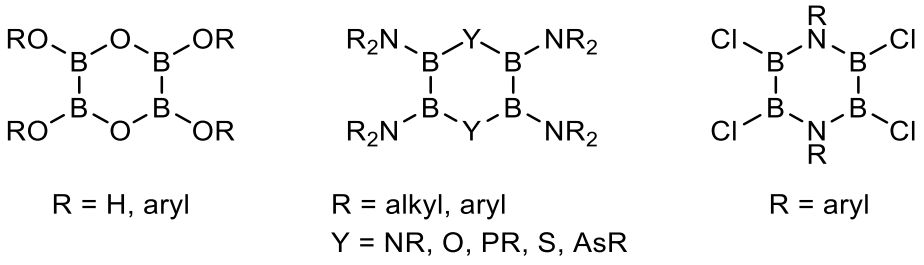
NMR analysis of the reaction of $B_2(OMe)_4$ with 1 equiv of B_2O_3 in CD_3CN revealed a new set of ^1H, ^{13}C, and ^{11}B resonances that were shifted slightly from those of $B_2(OMe)_4$,

as well as resonances consistent with formation of $B_3O_3(OMe)_3$. However, it was unclear whether B_2O_3 was being incorporated into the new product (the proposed active species), forming a borylboroxine (**28**, Scheme 3.7, *insertion*) whose resonances coincided with those of $B_3O_3(OMe)_3$, or if B_2O_3 was driving the formation of a "*bis*-pyrodiborate" derivative (**29**) of $B_2(OMe)_4$ (Scheme 3.7, *metathesis*). Notably, the latter structure is similar to $B_4O_2(OH)_4$ (Scheme 3.8) and numerous other known compounds.[9-16]

Scheme 3.7. Reaction of $B_2(OMe)_4$ with B_2O_3: insertion vs. metathesis.



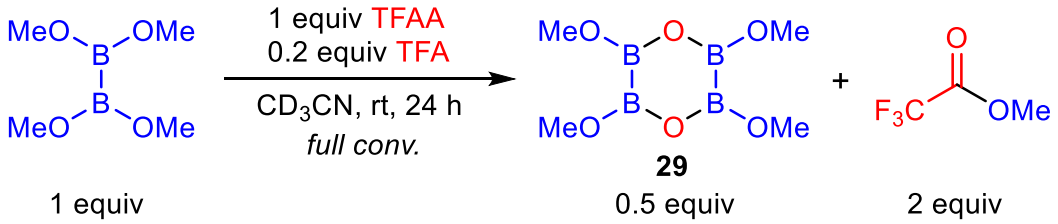
Scheme 3.8. Prior reports of bis-pyrodiborate structures and analogs.[9-16]



As such, we sought a boron-free reagent to perform the proposed metathesis reaction and try to generate the active boron intermediate. Gratifyingly, we found that the

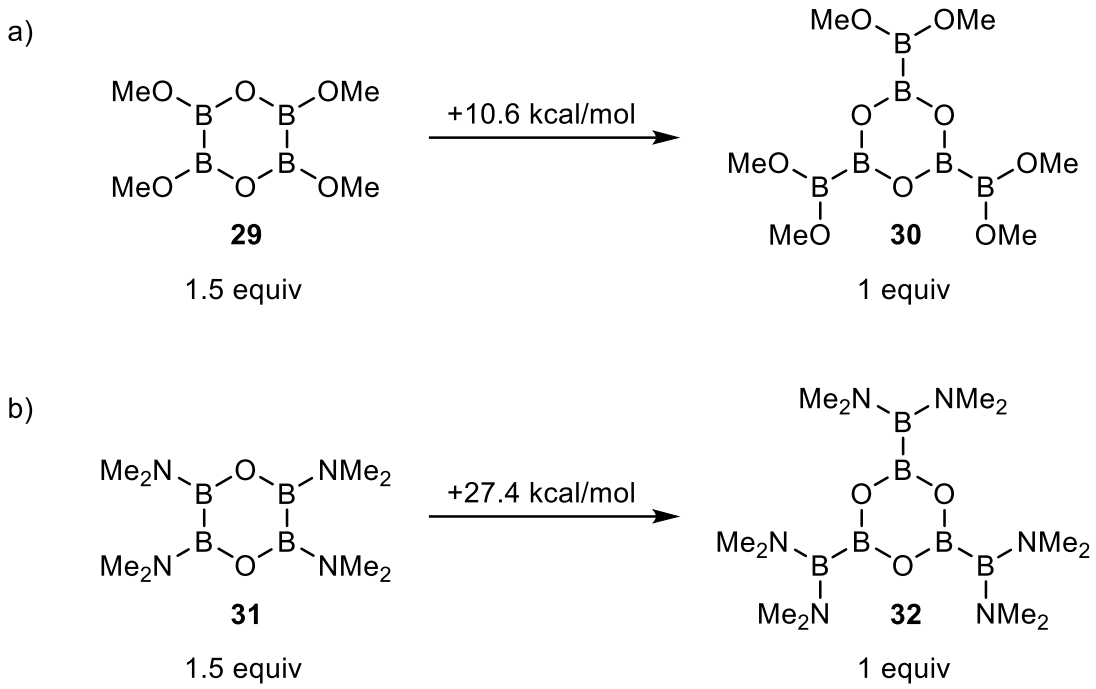
reaction of $B_2(OMe)_4$ with 1 equiv TFAA in CD_3CN at room temperature (Scheme 3.9) proceeded to full conversion, forming a single product whose ^1H-, ^{13}C-, and ^{11}B-NMR resonances were indistinguishable from the new resonances observed after the reaction of $B_2(OMe)_4$ with B_2O_3. Addition of imine **12** resulted in rapid reductive coupling, consistent with the formation of the active intermediate.

Scheme 3.9. Reaction of $B_2(OMe)_4$ with TFAA.



Although boroxines containing a B-B bond have never been reported, triborylboroxine **30** was considered as an alternative to the proposed bis-pyrodiborate structure **29** (Scheme 3.10a). The proportionate energy of the computational model for triborylboroxine **30** was 10.6 kcal/mol higher than that for the bis-pyrodiborate structure **29**, while the triborylboroxine derivative (**32**) of known compound **31**[17] (Scheme 3.10b) was 27.4 kcal/mol higher. However, it is possible the reaction is subject to kinetic control, and so the insights afforded here are limited. Further efforts to characterize the tentatively proposed bis-pyrodiborate will be necessary for its structure to be assigned.

Scheme 3.10. Relative energies of bis-pyrodiborates and analogs.[a]



[a] DFT quantum chemical calculations were carried out using the Gaussian 16 software package[18] for solution-phase optimizations and calculation of harmonic vibrational frequencies (at 298.15 ˚K) with the M06-2X functional[19-21] and the 6-31g(d,p) basis set. Frequency calculations were performed to ensure that one imaginary frequency exists for all transition states and no imaginary frequencies exist for all local minima. Solvation effects were included by performing optimizations and frequency calculations with the SMD model for acetonitrile.

Conclusions.

We have developed a new method for enhancing the reactivity of diborons without changing the ligands that enable reductive coupling reactions of a wide variety of imines that fail to react with diboron diolates such as B_2pin_2 or B_2eg_2. While diastereocontrol is poor for intermolecular reactions, unusual diastereochemical outcomes are often observed for intramolecular reactions, such as those that construct substituted piperazines and 1,4-diazepanes. Future work should include studies to determine the structure of the active intermediate under our conditions.

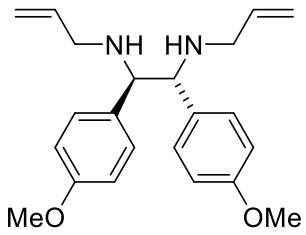
Experimental Section.

Computational Methods. DFT quantum chemical calculations were carried out using the Gaussian 16 software suite (Revision A.03)[18] using the M06-2X[19-21] functional and the 6-31G(d,p) basis set for all atoms. Structures were minimized until program default convergence limits were reached. Gaussian 16 was utilized for solution-phase optimizations and calculation of harmonic vibrational frequencies (at 298.15 ˚K). The frequency calculations were performed to ensure that one imaginary frequency for all transition states and no imaginary frequencies for all local minima. Solvation effects were included by performing optimizations and frequency calculations with the SMD model for acetonitrile.

General: All reactions were carried out under a nitrogen atmosphere in flame-dried glassware unless otherwise noted. All reagents, unless noted otherwise, were obtained from commercial sources and were used as obtained. THF was purified by distillation before use. Acetonitrile, dichloromethane, dimethylformamide, and anhydrous diethyl ether were obtained from commercial sources and used without further purification. Boron monoxide was prepared as previously described in the literature.[5] Yields refer to isolated yields of compounds estimated to be ≥95% pure as determined by ^{1}H NMR analysis unless otherwise noted. The yields reported in this chapter describe the result of a single experiment.

General Procedure: Reductive Dimerization of Imine Substrates with $B_2(OMe)_4$ and B_2O_3 A 1-dram vial was charged with a stir bar and $(B_2O_2)_n$ (27 mg, 1 mmol). MeOH (10 µL, 0.25 mmol) was added, followed by $CH(OMe)_3$ (120 µL, 1.1 mmol) and TFA (4 µL, 0.05 mmol). The vial was briefly flushed with nitrogen and capped, sealed

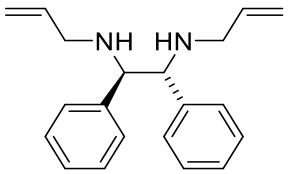
with Teflon tape, and stirred at 60 °C for 1-2 hours (until virtually all solid material had dissolved–the solution remained slightly cloudy). It was returned to room temperature, uncapped, and quickly B_2O_3 (35 mg, 0.5 mmol) was added, and then the mixture was briefly flushed with nitrogen and capped, sealed with Teflon tape and stirred at room temperature for 1 hour. (This solution can be stored on the bench for several days.) The vial was then uncapped, the mixture was quickly diluted with acetonitrile (0.25 mL), and the imine was added (0.5 mmol) with rapid stirring. The vial was then briefly flushed with nitrogen and capped. *(WARNING: THESE REACTIONS BECOME VERY WARM – FAILURE TO CONTROL LARGE SCALE REACTIONS COULD RESULT IN VIOLENT EXOTHERMS.)* After the reaction was complete, the mixture was diluted with MeOH (2 mL) and the solvent removed in vacuo. MeOH was then added, and the solvent removed in vacuo again. The residue was then dissolved in DCM, filtered through a small plug of basic alumina, and the solvent removed in vacuo to afford the title compound.



6a

(±)-(1*R*,2*R*)-*N*,*N*′-Diallyl-1,2-bis(4-methoxyphenyl)ethane-1,2-diamine (6a). The general procedure (reaction time: 48 h) was employed for the reductive dimerization of *N*-allyl-1-(4-methoxyphenyl)methanimine[22] (**5**) (88 mg, 0.5 mmol). The title compound was isolated by silica flash chromatography (56 mg, 64%) as a mixture of diastereomers (1.2:1 **6a:6b** d.r.), isolated as a clear colorless oil. Relative stereochemistry was assigned by comparison to spectral data reported for **8a**[23]. Spectral data is for the mixture of

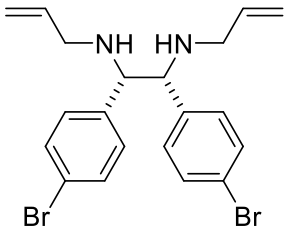
diastereomers (we were unable to fully and separately assign the spectral data for each diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26–7.22 (m, 4H), 6.95–6.91 (m, 4H), 6.90–6.86 (m, 4H), 6.71–6.67 (m, 4H), 5.86 (dddd, *J* = 16.9, 10.2, 6.5, 5.4 Hz, 2H), 5.65 (dddd, *J* = 17.1, 10.3, 6.8, 5.1 Hz, 2H), 5.12–5.01 (m, 4H), 4.99–4.88 (m, 4H), 3.81 (s, 6H), 3.74 (s, 2H), 3.73 (s, 6H), 3.64 (s, 2H), 3.12 (dddd, *J* = 14.1, 5.4, 1.6, 1.6 Hz, 2H), 3.01–2.93 (m, 4H), 2.80 (dddd, *J* = 14.4, 6.8, 1.3, 1.3 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 159.0, 158.3, 137.1, 136.8, 133.1, 132.7, 129.4, 128.9, 115.6, 115.6, 113.8, 113.3, 67.5, 66.9, 55.2, 55.1, 49.9, 49.5.



8a

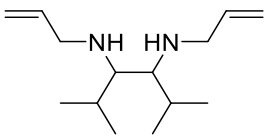
(±)-(1*R*,2*R*)-*N*,*N*′-Diallyl-1,2-diphenylethane-1,2-diamine (8a). The general procedure (reaction time: 2 h) was employed for the reductive dimerization of *N*-allyl-1-phenylmethanimine[24] (**7**) (73 mg, 0.5 mmol). The title compound was isolated by silica flash chromatography (37 mg, 51%) as a mixture of diastereomers (1.1:1 **8a:8b** d.r.), isolated as a clear colorless oil. Relative stereochemistry was assigned by comparison of spectral data to literature values.[23] Spectral data is for each diastereomer: **8a**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18–7.09 (m, 6H), 7.07–7.00 (m, 4H), 5.87 (dddd, *J* = 16.9, 10.2, 6.5, 5.4 Hz, 2H), 5.13–5.02 (m, 4H), 3.71 (s, 2H), 3.14 (dddd, *J* = 14.2, 5.4, 1.6, 1.6 Hz, 2H), 2.99 (dddd, *J* = 14.0, 6.6, 1.3, 1.3 Hz, 2H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 141.1, 137.1, 127.9, 127.9, 126.9, 115.7, 68.2, 50.0. **8b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37–7.24 (m, 10H), 5.67 (dddd, *J* = 17.1, 10.3, 6.7, 5.1 Hz, 2H), 5.00–4.88 (m, 4H), 3.84 (s, 2H), 3.00

(dddd, J = 14.4, 5.1, 1.6, 1.6 Hz, 2H), 2.83 (dddd, J = 14.4, 6.7, 1.3, 1.3 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.7, 136.7, 128.4, 128.3, 127.6, 115.6, 67.4, 49.6.



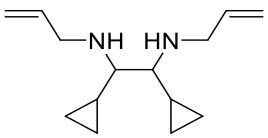
10b

(±)-(1*R*,2*S*)-*N*,*N′*-Diallyl-1,2-bis(4-bromophenyl)ethane-1,2-diamine (10b). The general procedure (reaction time: 2 h) was employed for the reductive dimerization of *N*-allyl-1-(4-bromophenyl)methanimine[25] (**9**) (112 mg, 0.5 mmol). The title compound was isolated by silica flash chromatography (73 mg, 65%) as a mixture of diastereomers (1.4:1 **10b:10a** d.r.), isolated as a clear colorless oil. Relative stereochemistry was assigned by comparison to spectral data reported for **8a**. Spectral data is for the mixture of diastereomers (we were unable to fully and separately assign the spectral data for each diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45–7.41 (m, 4H), 7.31–7.25 (m, 4H), 7.12–7.07 (m, 4H), 6.91–6.85 (m, 4H), 5.83 (dddd, J = 16.9, 10.2, 6.6, 5.4 Hz, 2H), 5.68 (dddd, J = 17.1, 10.3, 6.7, 5.1 Hz, 2H), 5.11–5.03 (m, 4H), 5.03–4.92 (m, 4H), 3.79 (s, 2H), 3.61 (s, 2H), 3.10 (dddd, J = 14.1, 5.4, 1.6, 1.6 Hz, 2H), 3.01 (dddd, J = 14.4, 5.2, 1.6, 1.6 Hz, 2H), 2.94 (dddd, J = 14.1, 6.6, 1.4, 1.4 Hz, 2H), 2.84 (dddd, J = 14.4, 6.8, 1.3, 1.3 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 140.0, 139.4, 136.7, 136.4, 131.4, 131.2, 130.1, 129.6, 121.4, 120.8, 116.0, 67.5, 66.5, 49.9, 49.5.



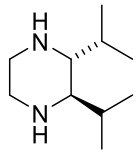
13

***N,N′*-Diallyl-2,5-dimethylhexane-3,4-diamine (13).** A 1-dram vial was charged with a stir bar, $B_2(OMe)_4$ (76 µL, 0.5 mmol), $B_3O_3(OMe)_3$ (73 µL, 0.5 mmol), and MeCN (0.5 mL). *N*-Allyl-2-methylpropan-1-imine[26] (**12**) (55.6 mg, 0.5 mmol) was added dropwise over 5 minutes with rapid stirring, and the vessel was then briefly flushed with nitrogen and capped. After stirring for 2 hours, solvent was removed in vacuo, and 5 mL Et_2O added (resulting in precipitation) and solvent removed in vacuo again. The solid residue was washed with Et_2O (3 x 2 mL). 0.4 mL MeOH was added followed by 4.0 mL Et_2O, and the solution then filtered through a basic alumina plug, flushing three times with Et_2O. Solvent was then removed in vacuo, the residue redissolved in Et_2O and filtered through a cotton plug, and solvent removed in vacuo again to afford the title compound (41 mg, 73%) as a mixture of diastereomers (1.7:1 d.r.), isolated as a clear colorless oil. Spectral data is for the mixture of diastereomers (we were unable to fully and separately assign the spectral data for each diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.94–5.84 (m, 4H), 5.19–5.00 (m, 8H), 3.32 (dddd, *J* = 13.8, 6.0, 1.4, 1.4 Hz, 2H), 3.25 (dddd, *J* = 7.1, 5.8, 1.5, 1.5 Hz, 4H), 3.20 (dddd, *J* = 13.7, 6.1, 1.5, 1.5 Hz, 2H), 2.30 (dd, *J* = 3.2, 1.3 Hz, 2H), 2.26–2.22 (m, 2H), 1.95–1.86 (m, 2H), 1.83–1.74 (m, 2H), 0.94 (d, *J* = 3.6 Hz, 6H), 0.93 (d, *J* = 3.7 Hz, 6H), 0.92 (d, *J* = 6.9 Hz, 6H), 0.90 (d, *J* = 6.9 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 137.7, 137.7, 115.3, 115.2, 63.8, 62.8, 53.2, 52.8, 31.2, 29.3, 21.7, 19.4, 18.9, 18.5.



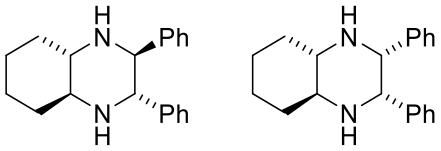
15

***N,N′*-Diallyl-1,2-dicyclopropylethane-1,2-diamine (15).** A 1-dram vial was charged with a stir bar, $B_2(OMe)_4$ (76 µL, 0.5 mmol), $B_3O_3(OMe)_3$ (73 µL, 0.5 mmol), and MeCN (0.5 mL). (*E*)-1-cyclopropyl-*N*-methylmethanimine[27] (**14**) (54.6 mg, 0.5 mmol) was added dropwise over 5 minutes with rapid stirring, and the vessel was then briefly flushed with nitrogen and capped. After stirring for 2 hours, solvent was removed in vacuo, and 5 mL Et_2O added (resulting in precipitation) and solvent removed in vacuo again. The solid residue was washed with Et_2O (3 x 2 mL). 0.4 mL MeOH was added followed by 4.0 mL Et_2O, and the solution then filtered through a basic alumina plug, flushing three times with Et_2O. Solvent was then removed in vacuo, the residue redissolved in Et_2O and filtered through a cotton plug, and solvent removed in vacuo again to afford the title compound (36 mg, 65%) as a mixture of diastereomers (1.6:1 d.r.), isolated as a clear colorless oil. Spectral data is for the mixture of diastereomers (we were unable to fully and separately assign the spectral data for each diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.94–5.81 (m, 4H), 5.19–5.01 (m, 8H), 3.46 (dddd, *J* = 14.1, 5.7, 1.6, 1.6 Hz, 2H), 3.34 (dddd, *J* = 14.2, 5.9, 1.5, 1.5 Hz, 2H), 3.27 (dddd, *J* = 14.1, 6.2, 1.5, 1.5 Hz, 2H), 3.17 (dddd, *J* = 14.1, 6.1, 1.5, 1.5 Hz, 2H), 1.88–1.84 (m, 2H), 1.84–1.80 (m, 2H), 1.03–0.93 (m, 2H), 0.82–0.73 (m, 2H), 0.61–0.51 (m, 4H), 0.51–0.40 (m, 4H), 0.31–0.21 (m, 4H), 0.21–0.08 (m, 4H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 137.8, 137.5, 115.5, 115.1, 66.0, 64.7, 50.6, 50.4, 14.2, 12.6, 4.6, 4.3, 2.6, 2.5.



20a

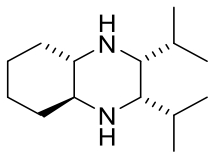
(±)-(2*R*,3*R*)-2,3-Diisopropylpiperazine (20a). The general procedure (reaction time: 1 h) was employed for the reductive dimerization of (1*E*,1*E*′)-*N*,*N*′-(ethane-1,2-diyl)bis(2-methylpropan-1-imine)[28] (**19**) (42.1 mg, 0.25 mmol). This procedure afforded the title compound (32 mg, 75%) as the major diastereomer (3:1 **20a:20b** d.r.), isolated as a clear yellow oil. Spectral data is for the mixture of diastereomers (we were unable to fully and separately assign the spectral data for each diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.97 (d, *J* = 8.1 Hz, 2H), 3.01–2.93 (m, 2H), 2.70 (d, *J* = 8.1 Hz, 2H), 2.75–2.67 (m, 2H), 2.55–2.48 (m, 2H), 2.34 (dd, *J* = 1.3, 1.3 Hz, 2H), 1.99–1.89 (m, 4H), 1.01 (d, *J* = 6.7 Hz, 6H), 0.96–0.92 (m, 6H), 0.95 (dd, *J* = 6.8, 1.3 Hz, 6H), 0.84 (d, *J* = 6.9 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 63.0, 62.9, 47.5, 45.2, 28.0, 27.0, 21.4, 20.9, 20.6, 15.2.



2c **2b**

(±)-(2*R*,3*R*,4a*R*,8a*R*)-2,3-Diphenyldecahydroquinoxaline (2c), and **(±)-(2*R*,3*S*,4a*R*,8a*R*)-2,3-Diphenyldecahydroquinoxaline (2b).** The general procedure (reaction time: 72 h) was employed, with a modified workup, for the reductive dimerization of (±)-(1*E*,1*E*′)-*N*,*N*′-((1*R*,2*R*)-cyclohexane-1,2-diyl)bis(1-phenylmethanimine)[29] **1** (72.6 mg, 0.25 mmol). The reaction was quenched with 0.5 M aq. HCl (2 mL). A large amount of white precipitate formed, which was removed via filtration, and basified with 1 M aq. NaOH (4 mL). NaCl was added until the solution became saturated, then extracted with

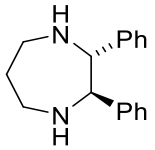
Et_2O (3 x 3 mL), the organic layers combined and dried with Na_2SO_4, and solvent removed in vacuo to afford **2c** (36 mg, 50%) as a single diastereomer, isolated as an white crystalline solid: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (ddd, *J* = 8.1, 1.2, 1.2 Hz, 4H), 7.39 (dd, *J* = 7.7, 7.7 Hz, 4H), 7.34–7.22 (m, 2H), 4.53 (s, 2H), 2.74–2.57 (m, 2H), 1.77–1.63 (m, 4H), 1.59 (ddd, *J* = 12.7, 2.3, 2.3 Hz, 2H), 1.35–1.09 (m, 4H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 144.4, 128.3, 127.7, 126.7, 58.5, 54.9, 32.3, 25.0. The filtrate was then basified with 1 M aq. NaOH (4 mL) and NaCl added until the solution became saturated. It was then extracted with Et_2O (3 x 3 mL), the organic layers combined and dried with Na_2SO_4, and solvent removed in vacuo to afford **2b** as the major component of a mixture with **2c** (28 mg, 38%, 3:1 dr), isolated as a pale yellow oil. For **2b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65–7.59 (m, 2H), 7.26 (dd, *J* = 5.8, 2.5 Hz, 2H), 7.19–7.10 (m, 5H), 7.08–7.01 (m, 1H), 4.61 (d, *J* = 4.0 Hz, 1H), 4.18 (d, *J* = 4.1 Hz, 1H), 2.86 (ddd, *J* = 10.6, 9.1, 3.8 Hz, 1H), 2.70–2.63 (m, 1H), 1.83–1.17 (m, 10H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 141.9, 141.5, 130.1, 127.8, 127.5, 126.9, 126.6, 126.6, 64.1, 63.1, 63.0, 53.5, 32.2, 32.1, 24.9, 24.9. The combined yield of diastereomers **2c** and **2b** was 64 mg (88% yield) with a 2:1 (**2c:2b**) overall dr.



22b

(±)-(2*R*,3*S*,4a*R*,8a*R*)-2,3-Diisopropyldecahydroquinoxaline (22b). The general procedure (reaction time: 18 h) was employed for the reductive dimerization of (1*E*,1*E*′)-*N*,*N*′-((1*R*,2*R*)-cyclohexane-1,2-diyl)bis(2-methylpropan-1-imine)[30] **21** (55.6 mg, 0.25 mmol). This procedure afforded the title compound (42 mg, 75%) as the sole diastereomer, isolated as an off-white oil: ^{1}H NMR (500 MHz, $CDCl_3$) 2.64 (ddd, *J* = 6.8, 3.2, 1.1 Hz,

1H), 2.61 (dd, *J* = 9.9, 2.0 Hz, 1H), 2.45–2.39 (m, 1H), 2.27–2.17 (m, 2H), 1.82–1.60 (m, 4H), 1.59–1.51 (m, 1H), 1.35–1.17 (m, 4H), 1.0 (dd, *J* = 17.6, 6.8 Hz, 6H), 0.9 (dd, *J* = 19.7, 6.5 Hz, 6H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 68.6, 63.3, 58.7, 55.6, 32.3, 32.0, 29.1, 26.5, 25.0, 24.9, 22.7, 21.2, 20.6, 20.3.



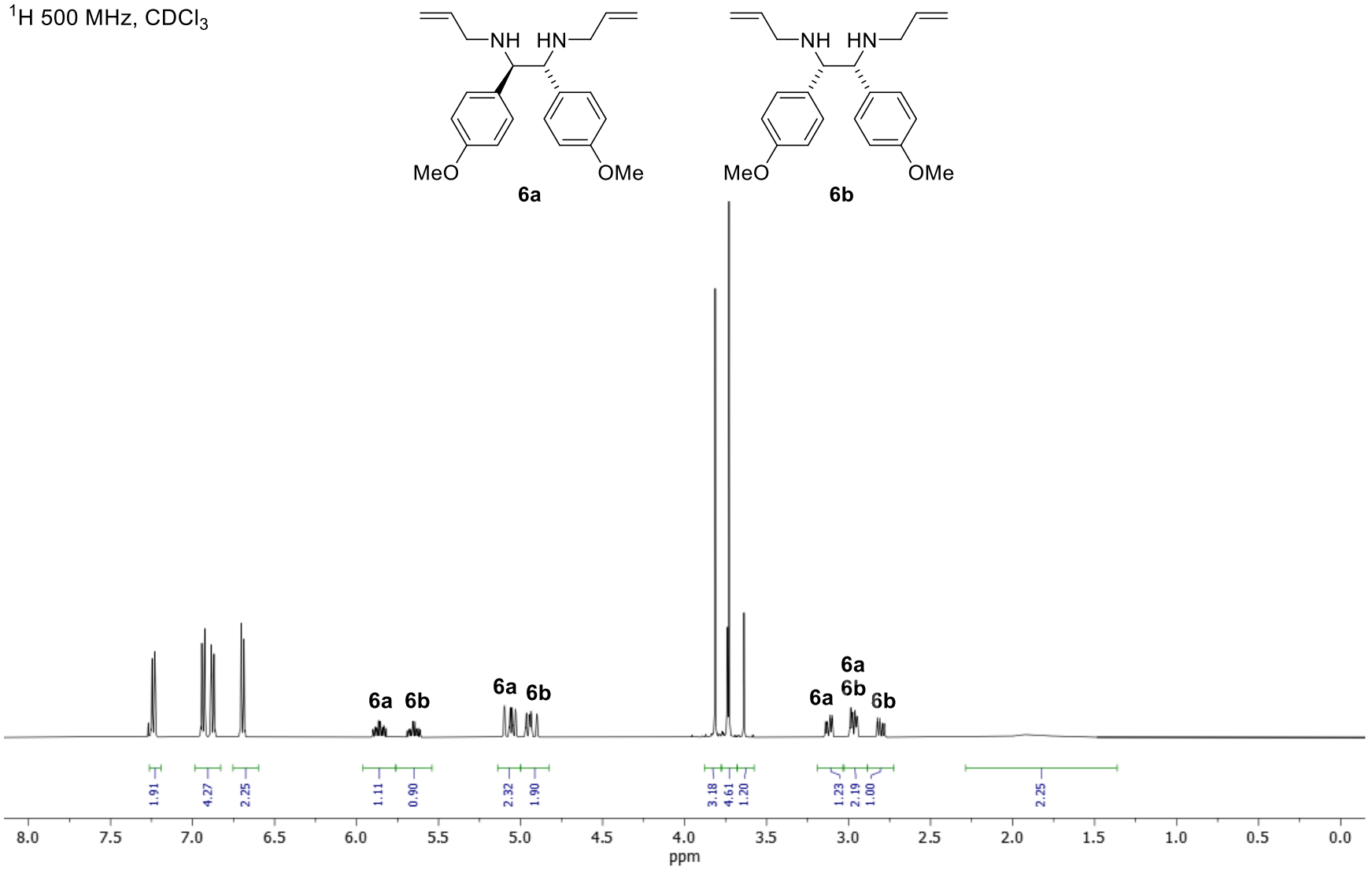
25a

(±)-(2*R*,3*R*)-2,3-Diphenyl-1,4-diazepane (25a). A 1 dram vial was charged with a stir bar, $B_2(OMe)_4$ (76 µL, 0.5 mmol), $B_3O_3(OMe)_3$ (73 µL, 0.5 mmol), and MeCN (0.5 mL). The imine (1*E*,1*E*′)-*N*,*N*′-(propane-1,3-diyl)bis(1-phenylmethanimine)[31] **24** (62.6 mg, 0.25 mmol) was added gradually, with rapid stirring, over a period of 30 minutes, and the vessel flushed with N_2 and capped after each addition. Stirring was then continued for another 30 minutes (total reaction time = 1 hour), and the reaction quenched with 1 M aq. HCl (1 mL). The solution was extracted with Et_2O (3 x 2 mL), and the organic layers discarded, and then basified with 6 M aq. NaOH (1 mL). After gas evolution subsided, the solution was extracted with Et_2O (3 x 2 mL), and the organic layer dried with NaCl and Na_2SO_4. Solvent was removed in vacuo to afford the title compound (54 mg, 86%) as a mixture of diastereomers (3.5:1), isolated as a yellow oil. Spectral data is for the major diastereomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.4–6.9 (m, 10H), 3.7 (s, 2H), 3.3 (ddd, *J* = 13.5, 4.8, 4.8 Hz, 2H), 3.2 (ddd, *J* = 13.5, 8.2, 8.2 Hz, 2H), 2.0–1.7 (m, 4H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 143.0, 127.9, 127.7, 127.0, 75.2, 47.4, 31.7.

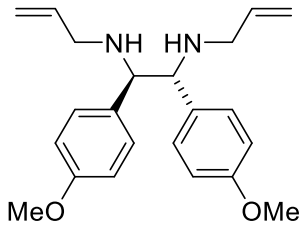
APPENDICES

APPENDIX A: Spectral Data

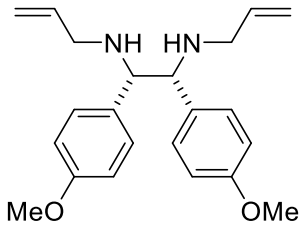
^{1}H 500 MHz, $CDCl_3$



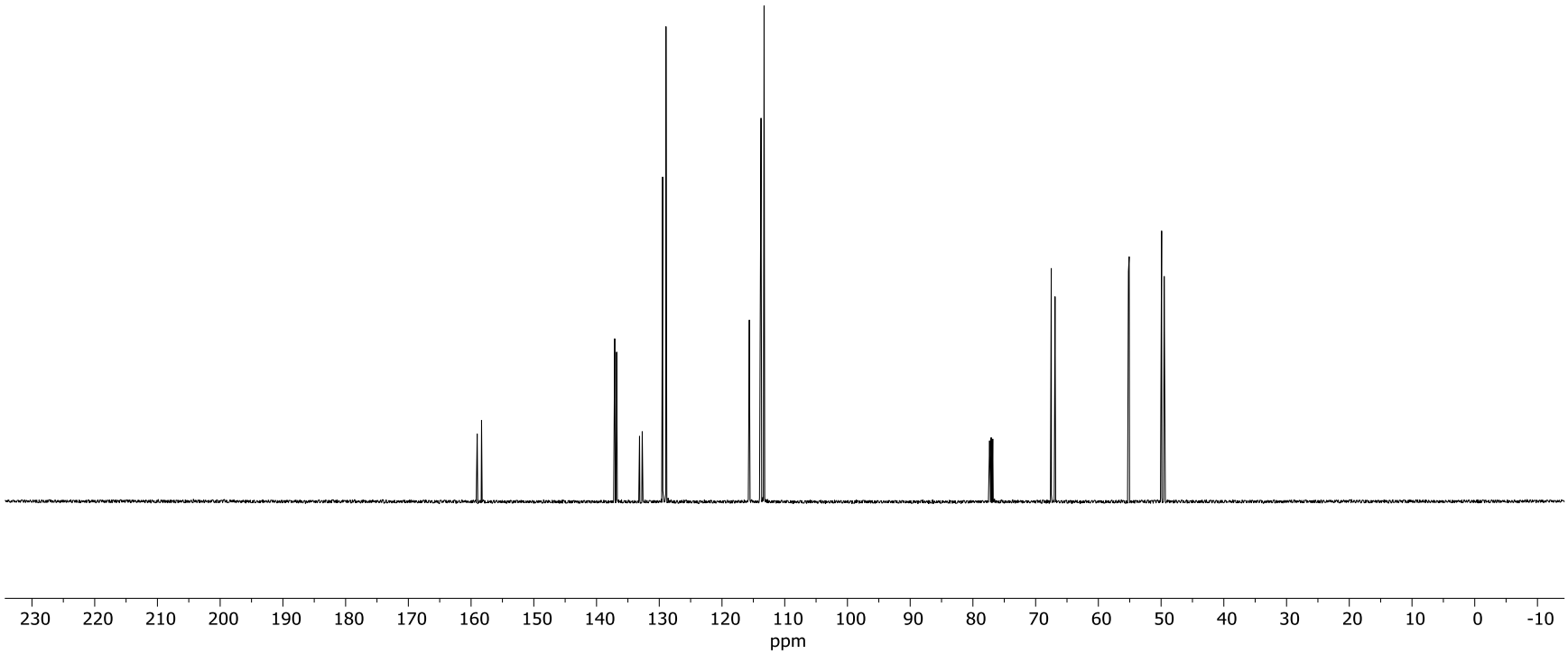
^{13}C 126 MHz, $CDCl_3$



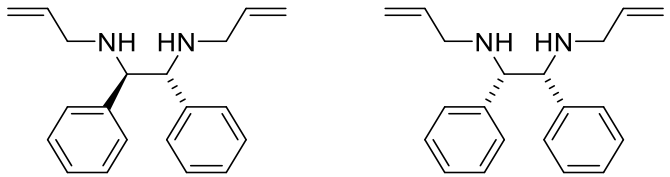
6a



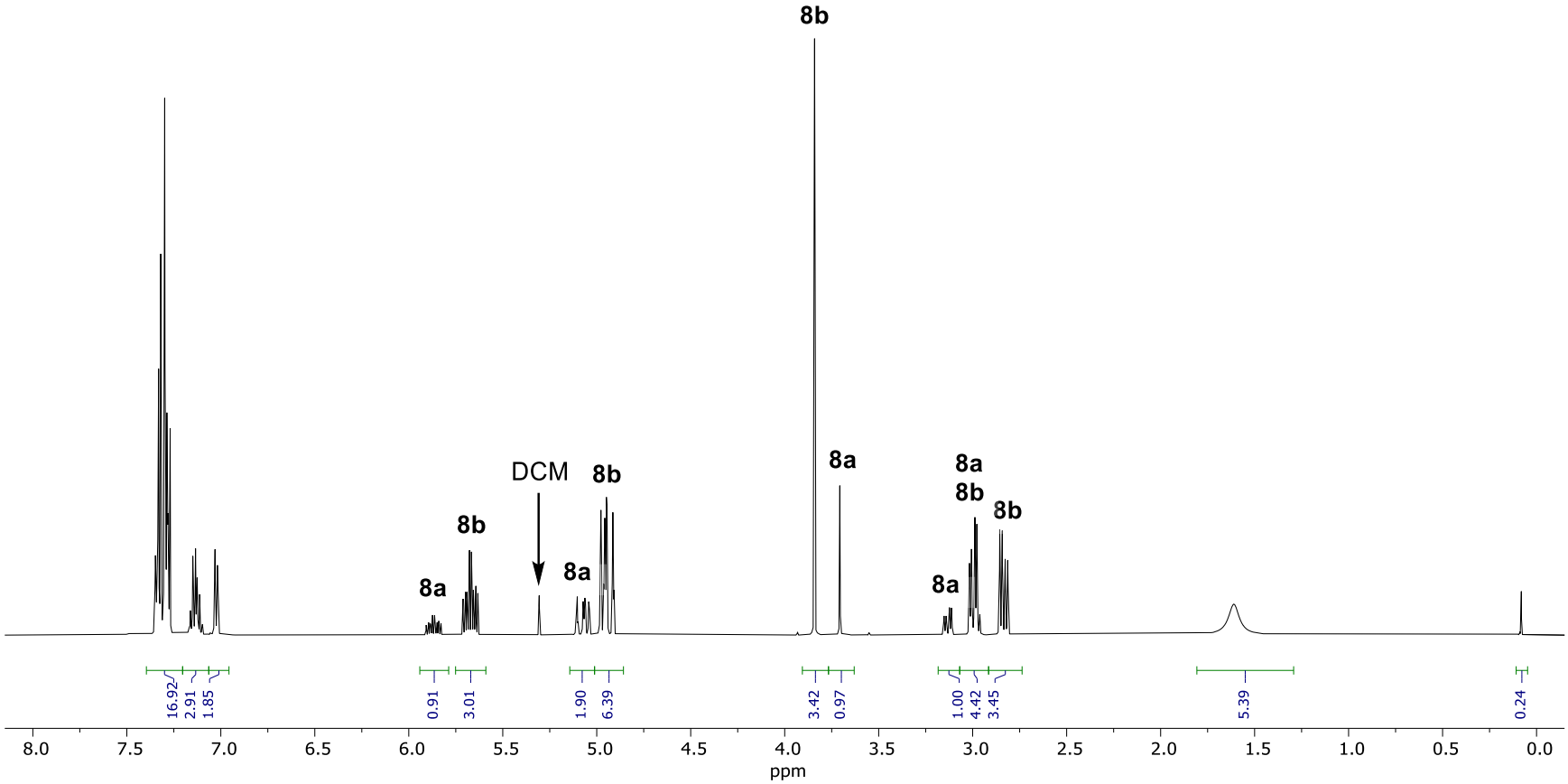
6b



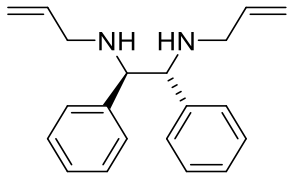
^{1}H 500 MHz, $CDCl_3$



8a **8b**



^{13}C 126 MHz, $CDCl_3$



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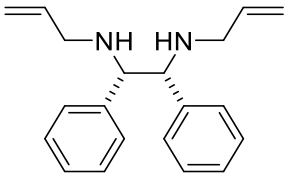

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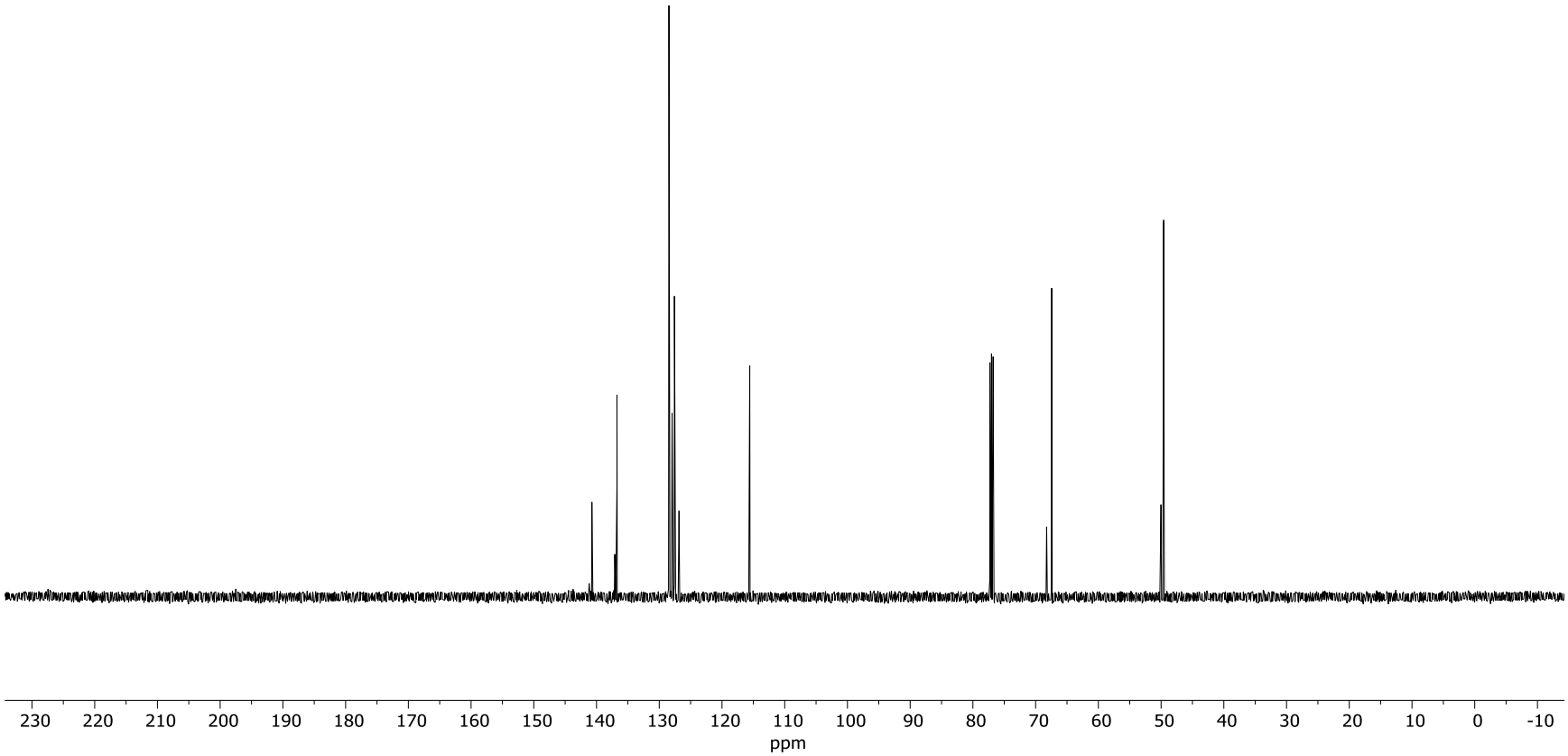

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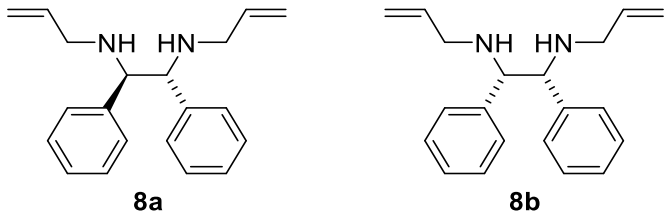

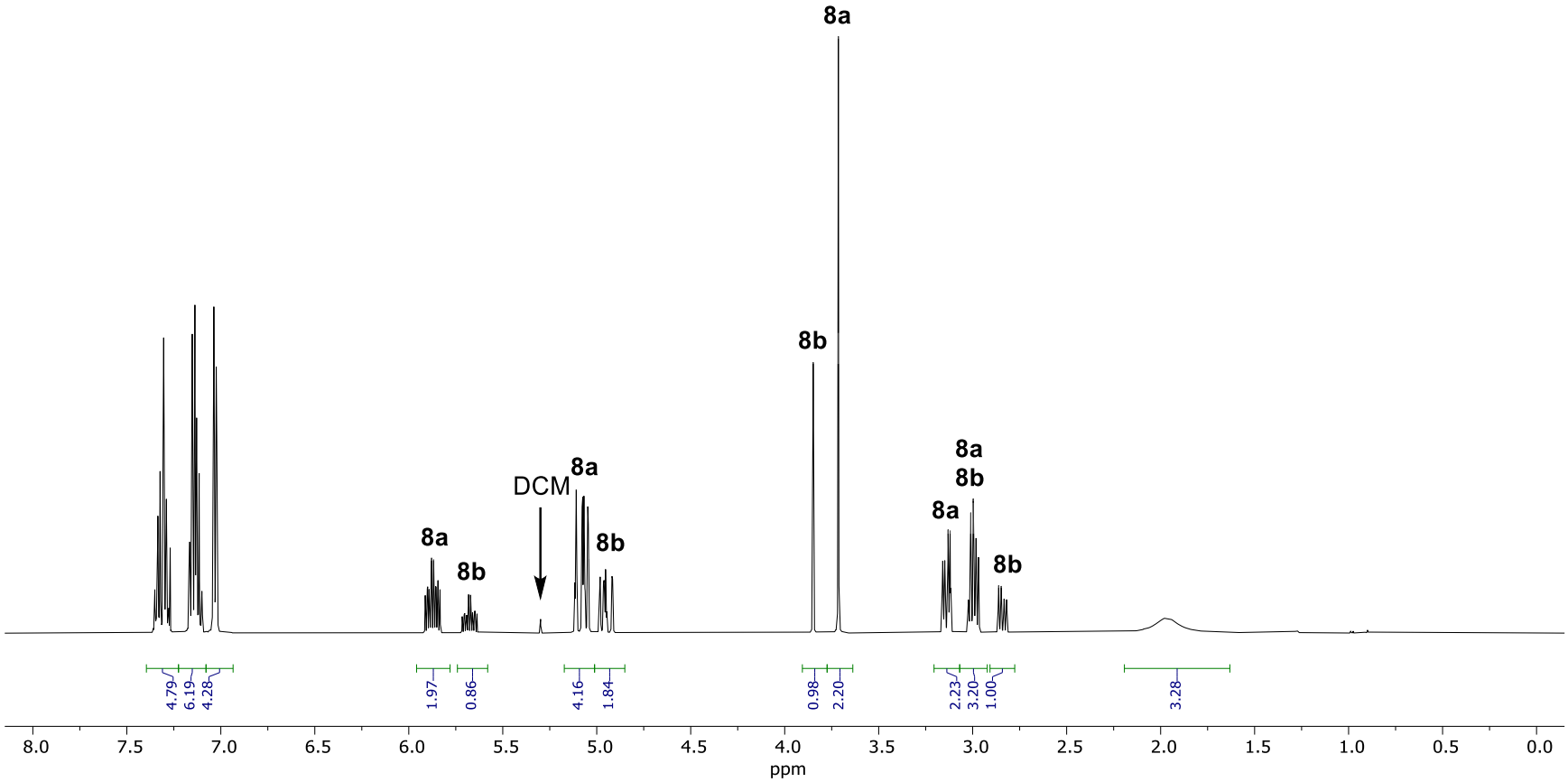

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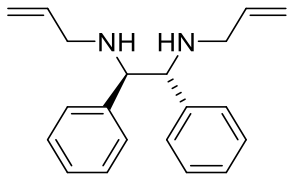

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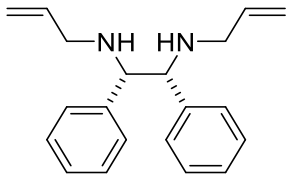

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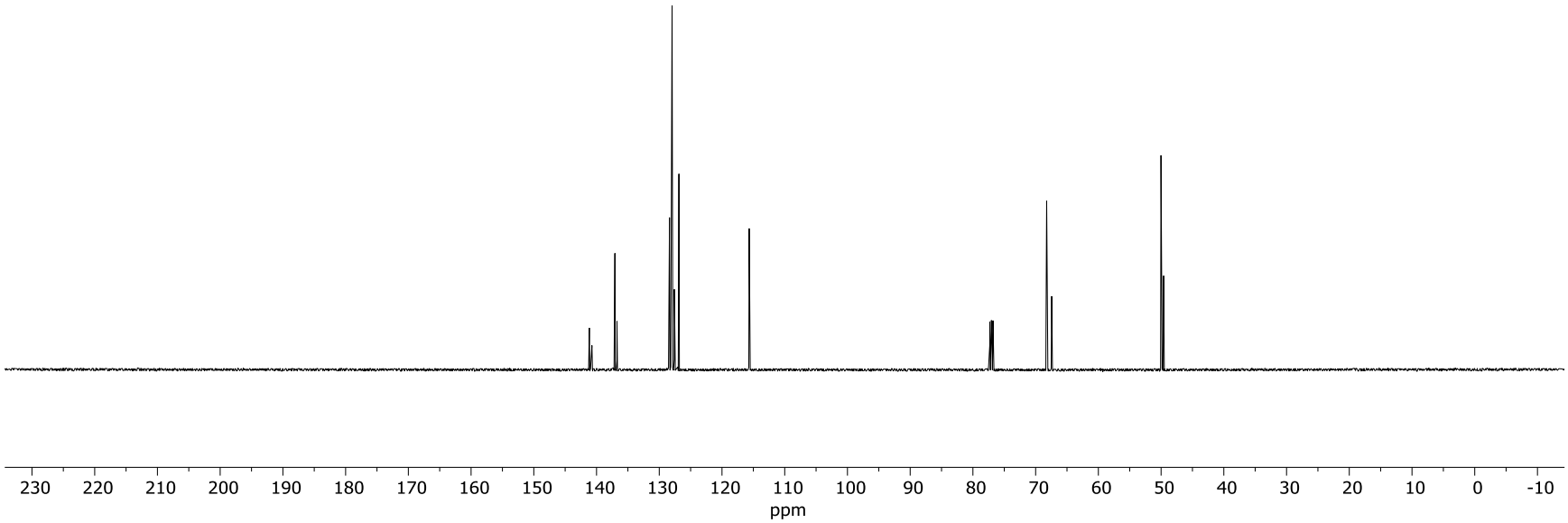
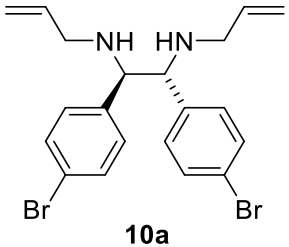


^{1}H 500 MHz, $CDCl_3$



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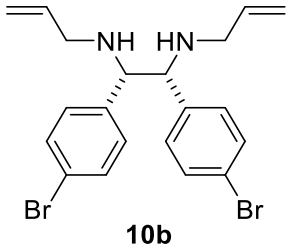

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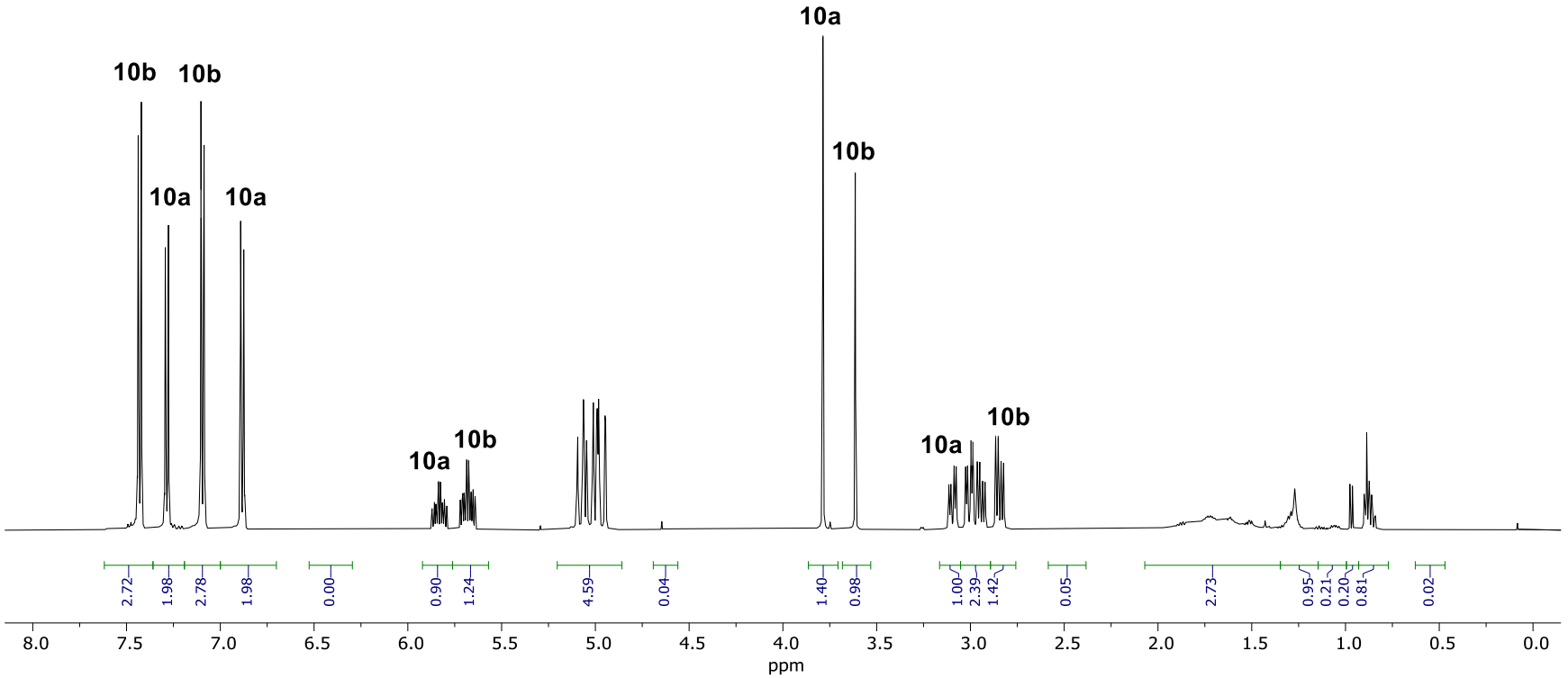

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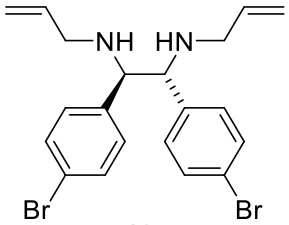

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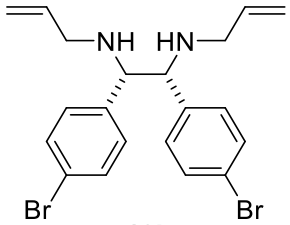

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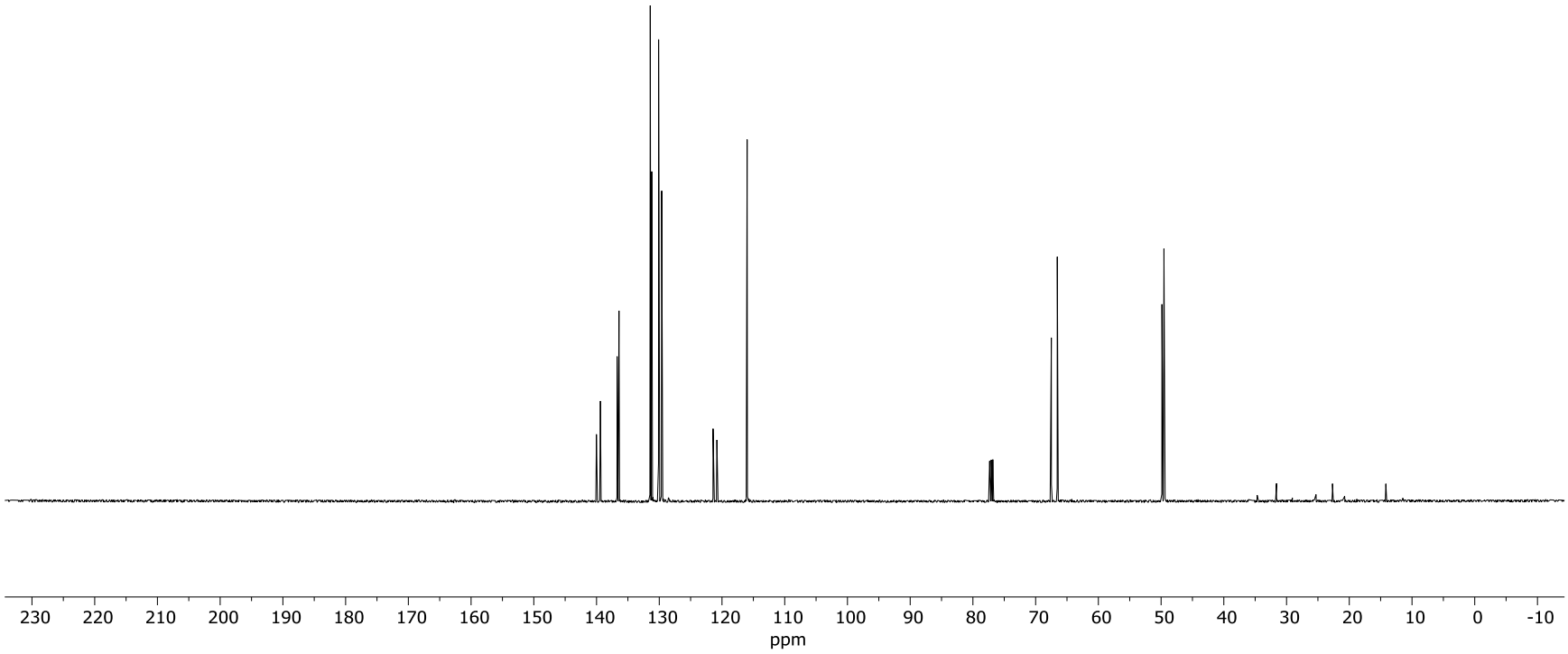
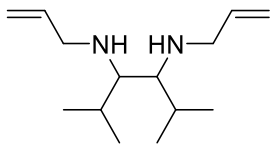


^{1}H 500 MHz, $CDCl_3$



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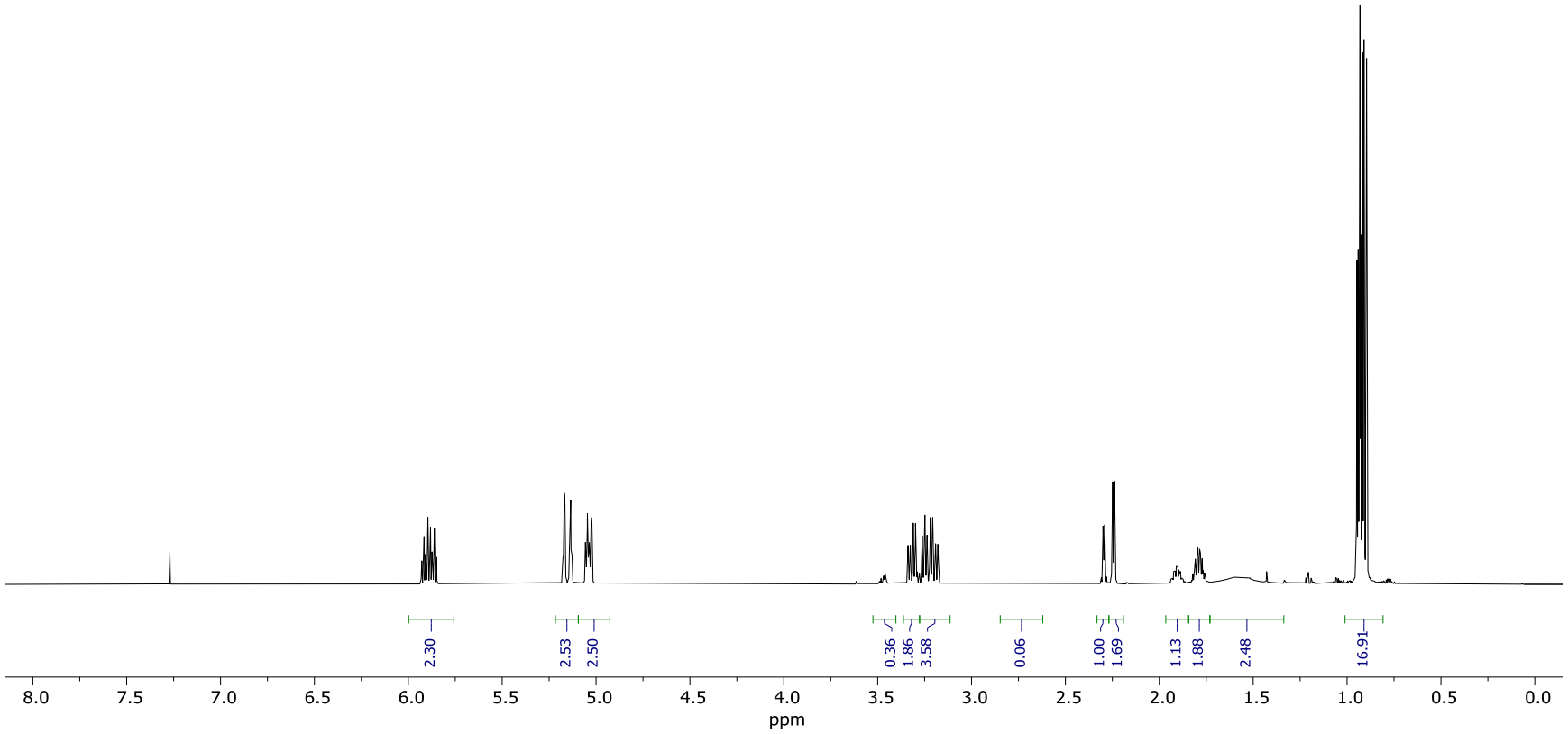

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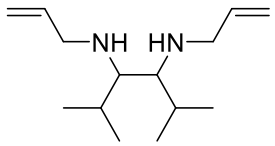

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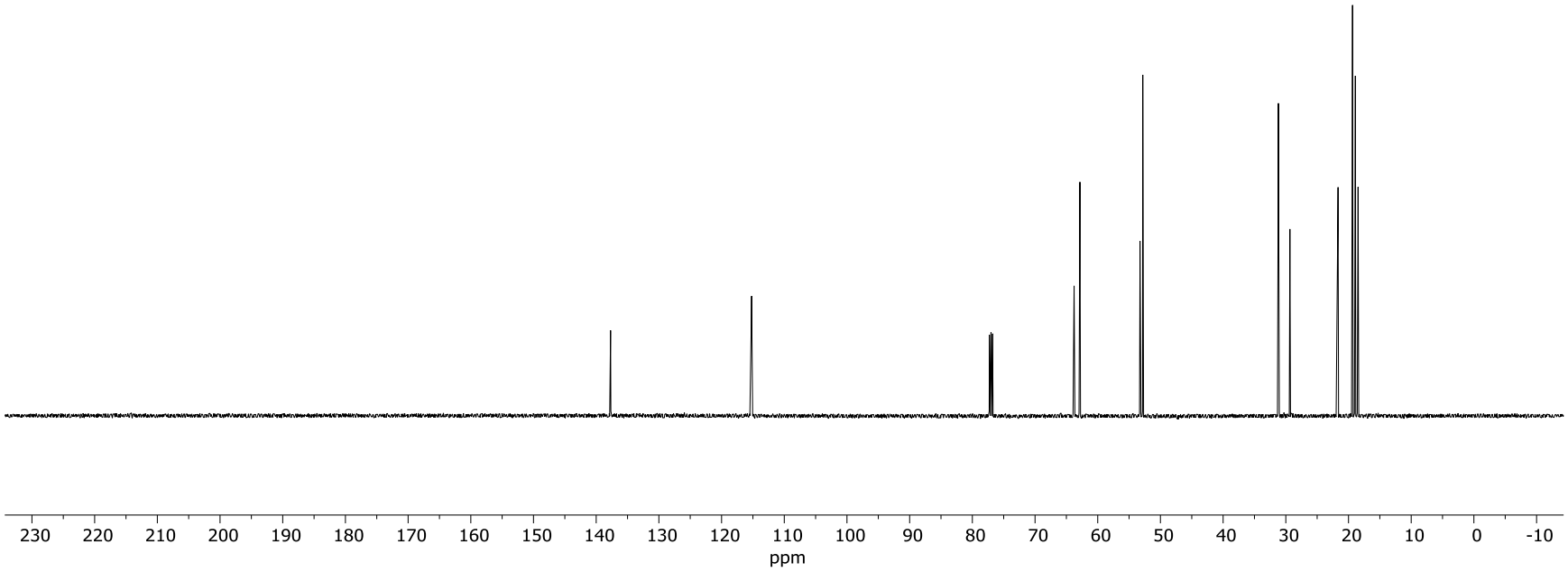

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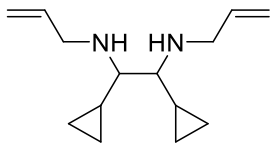

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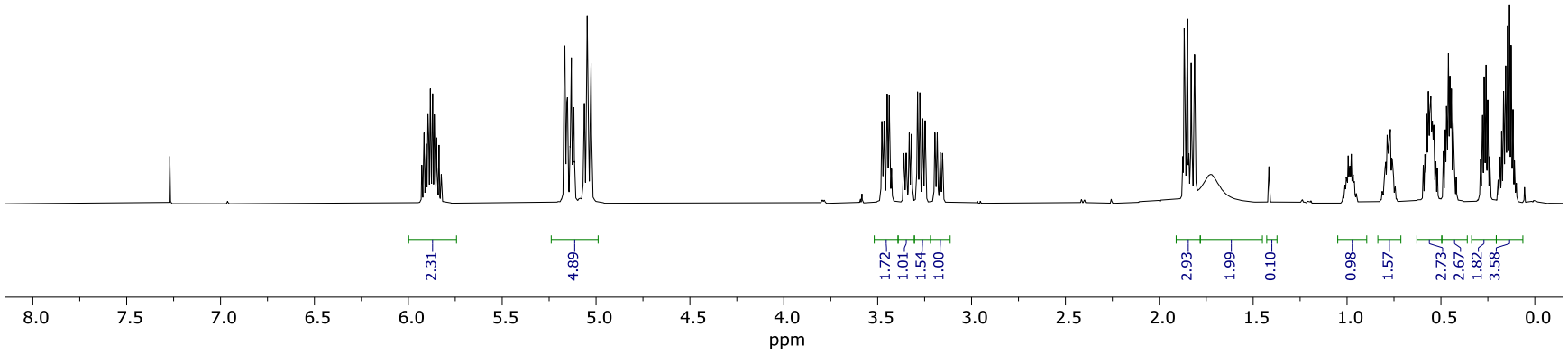

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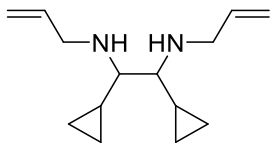

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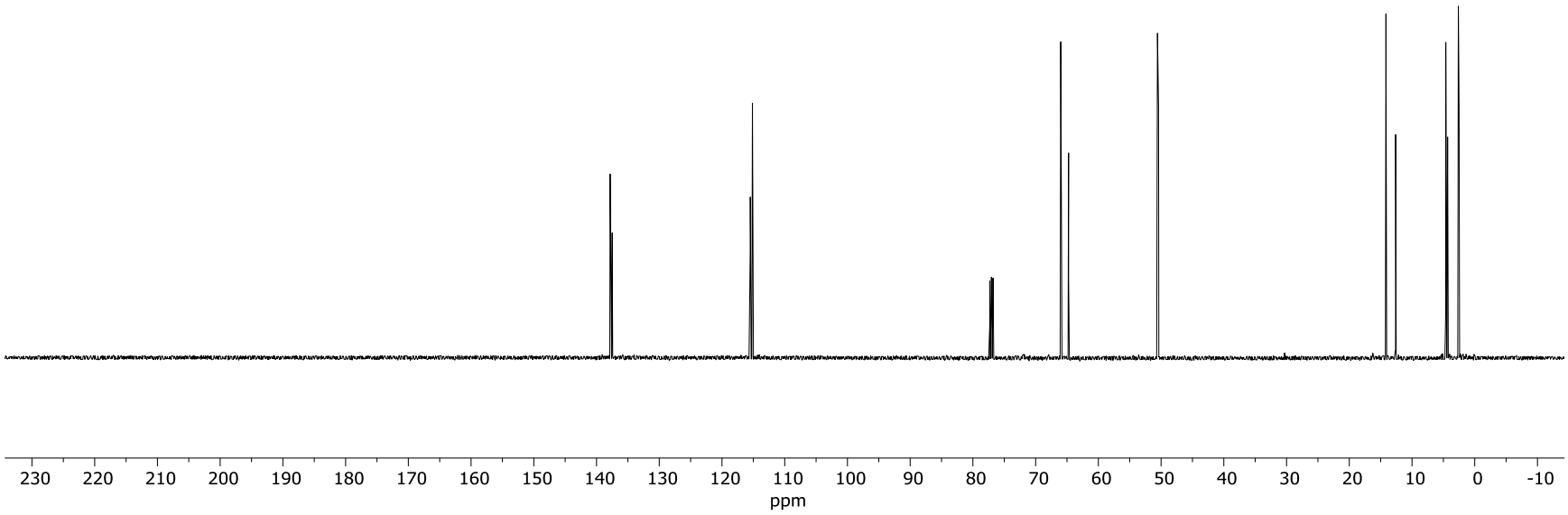

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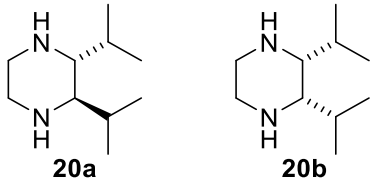

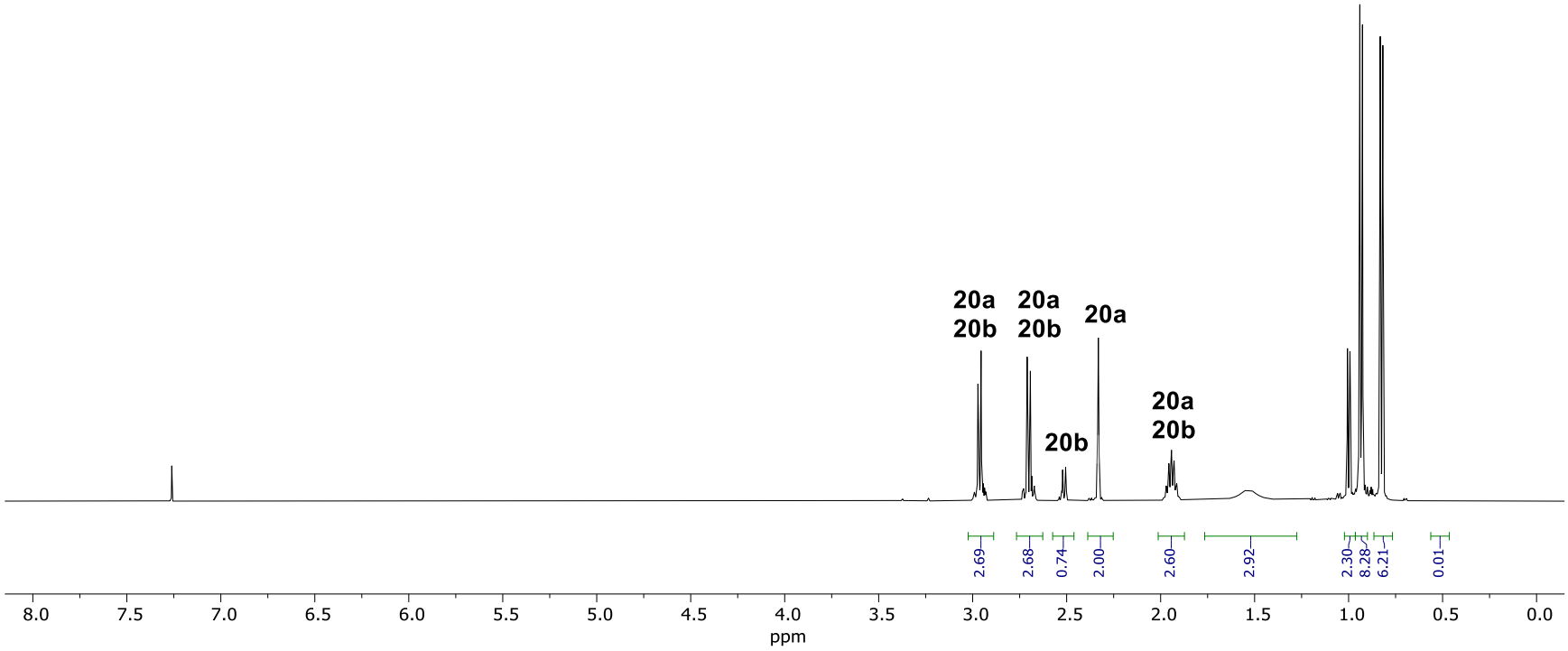

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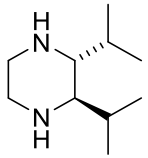

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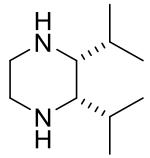

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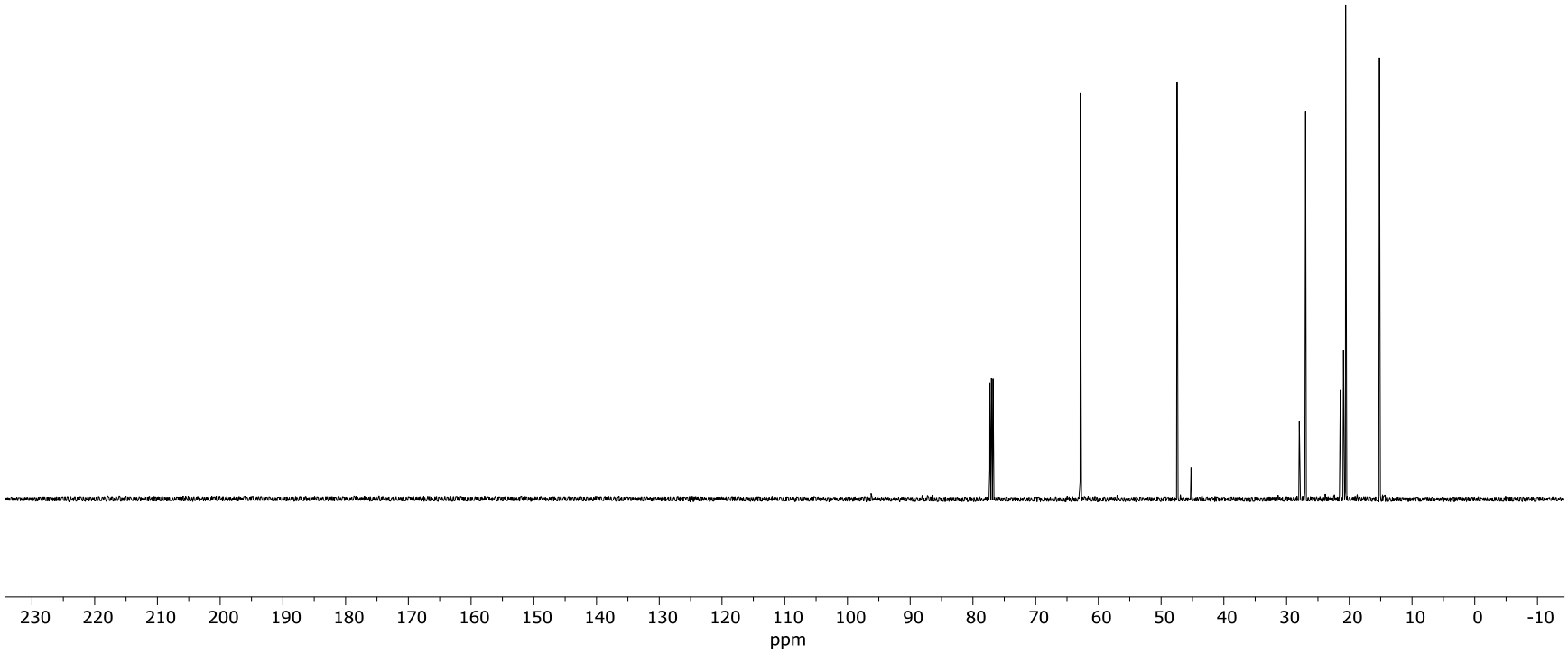
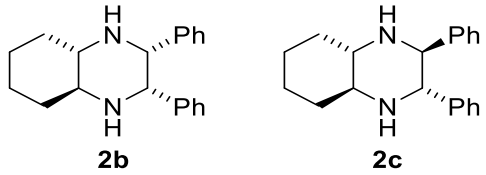
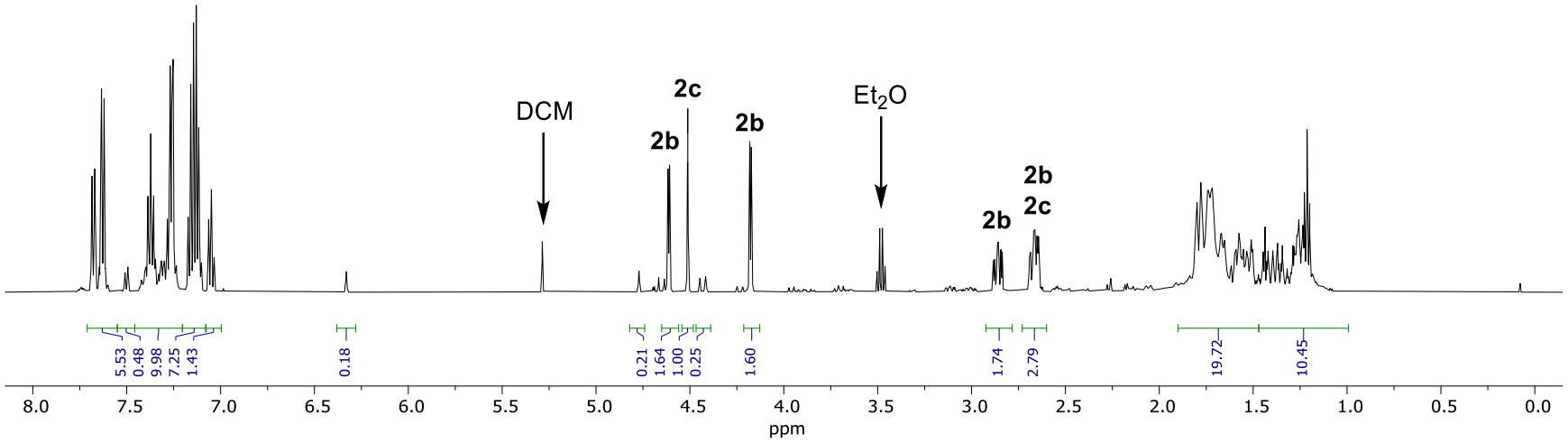


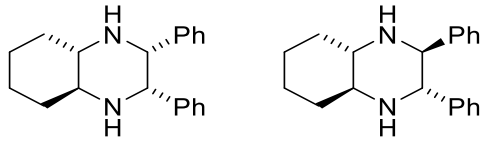
^{1}H 500 MHz, $CDCl_3$



2b **2c**

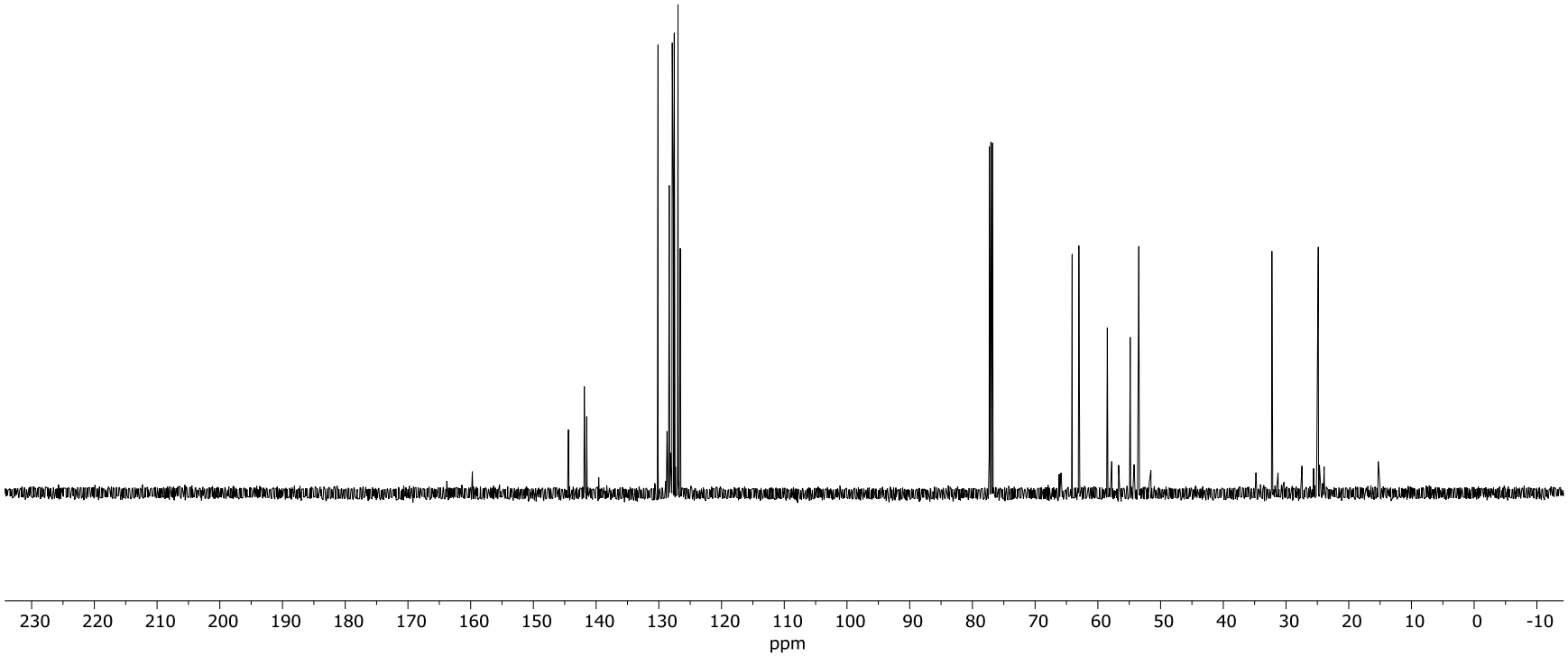


^{13}C 126 MHz, $CDCl_3$

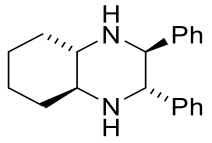


2b

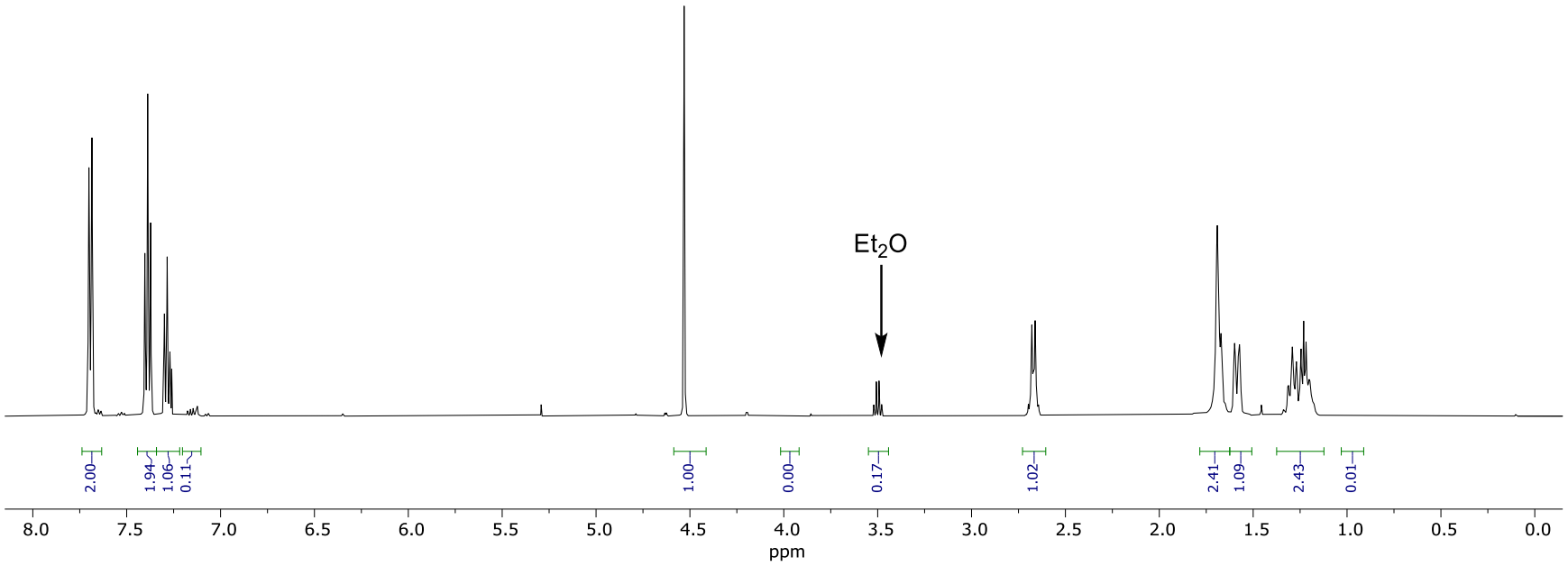
2c



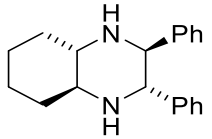
^{1}H 500 MHz, $CDCl_3$



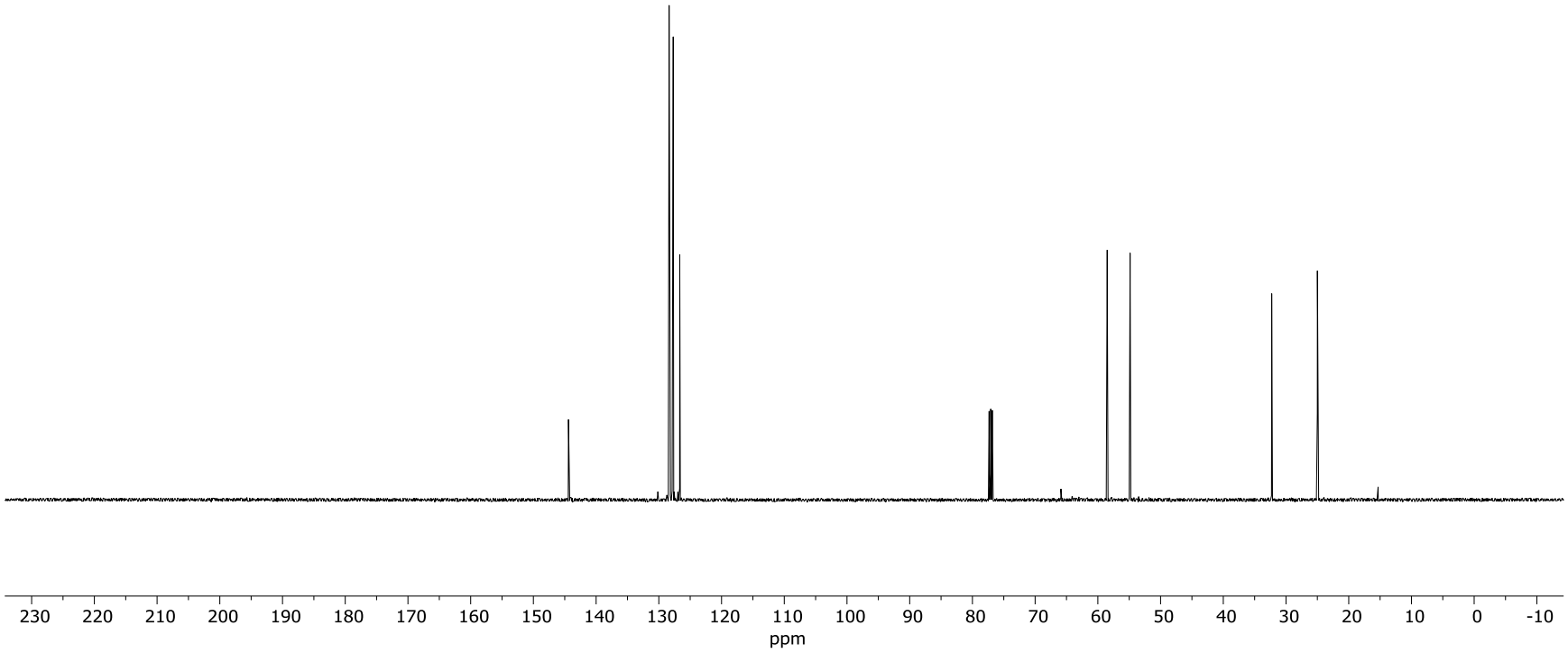
2c



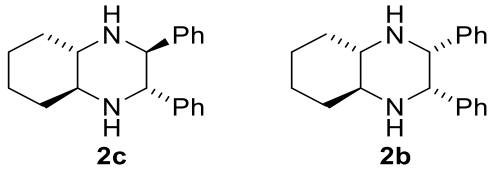
^{13}C 126 MHz, $CDCl_3$



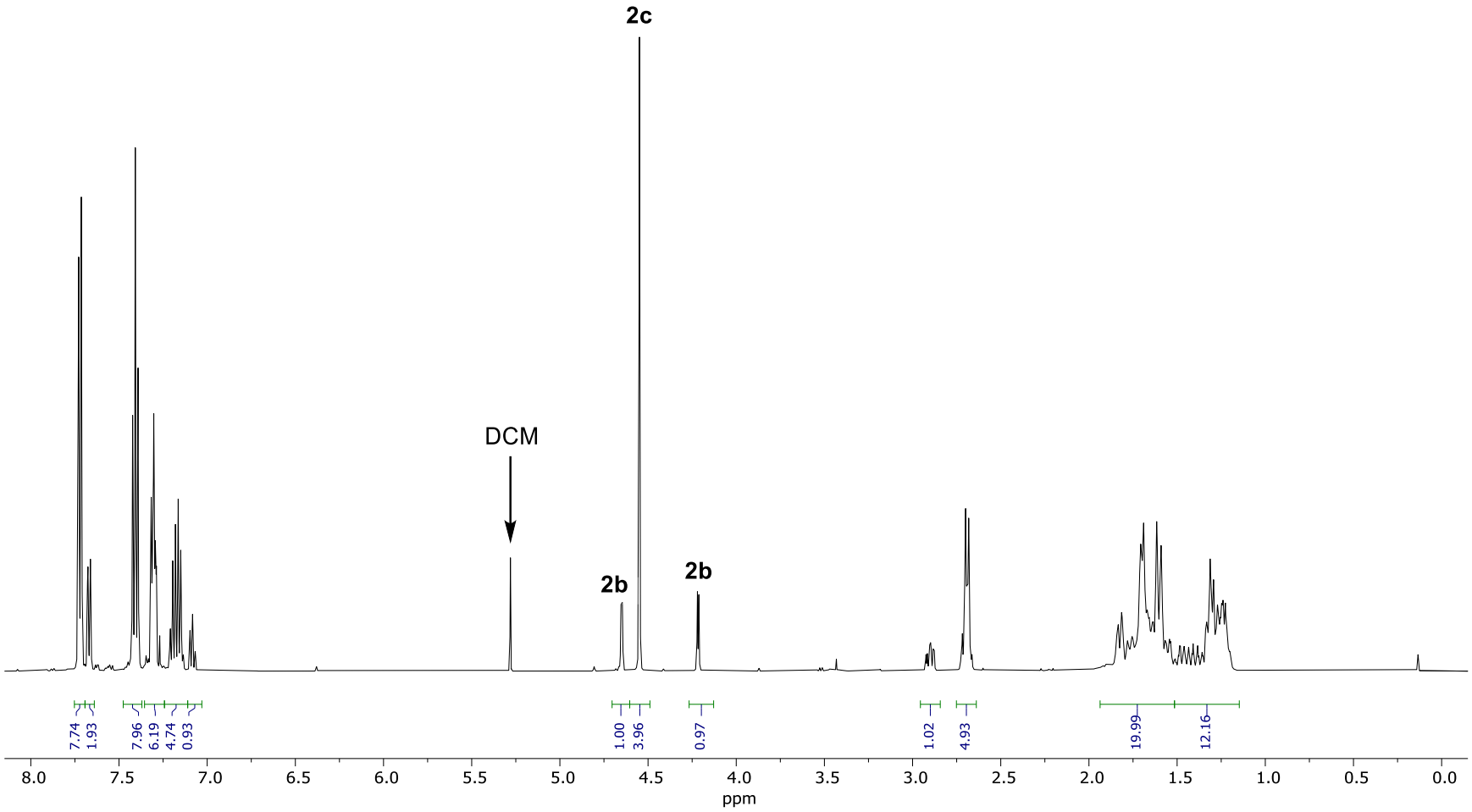
2c



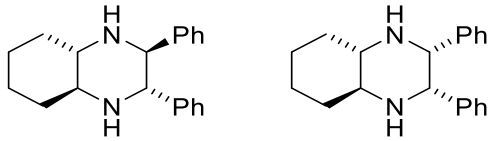
^{1}H 500 MHz, $CDCl_3$



2c **2b**

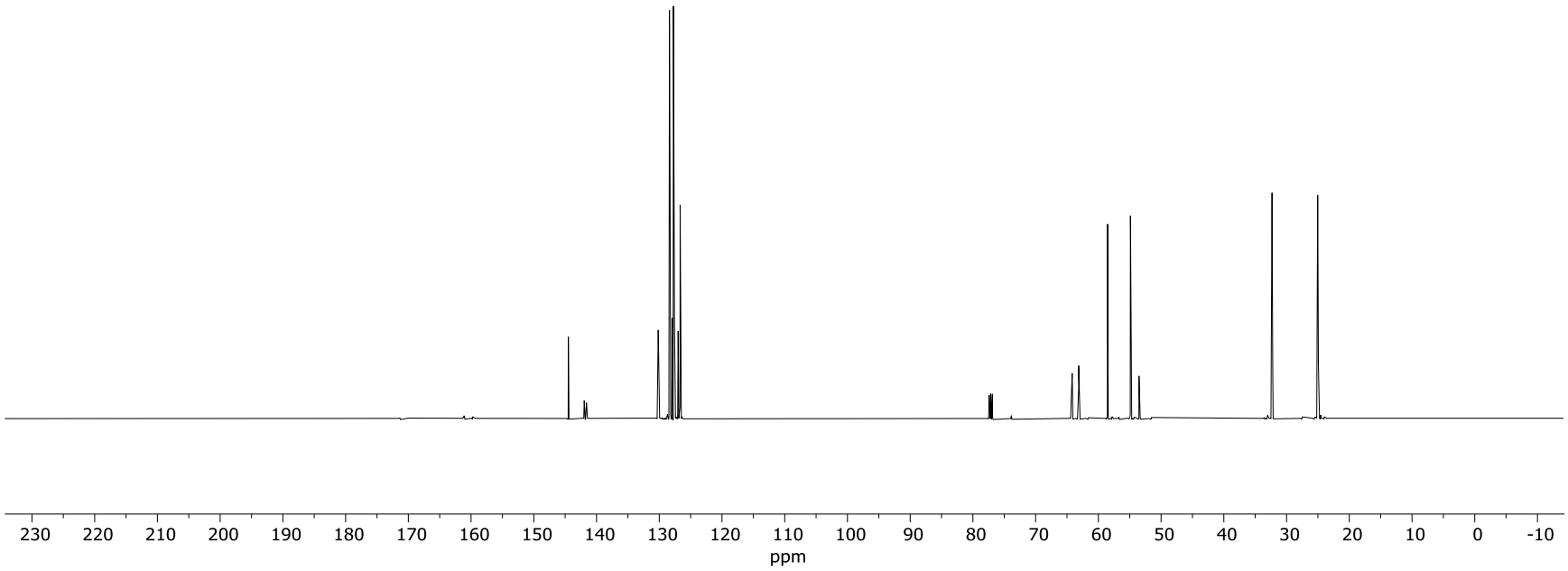


^{13}C 126 MHz, $CDCl_3$

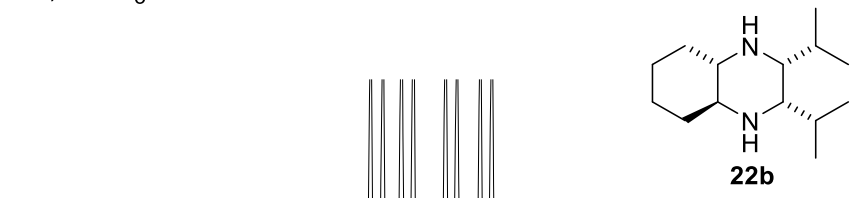


2c

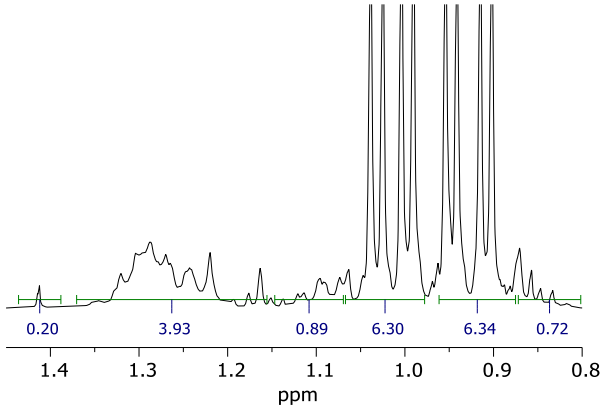
2b

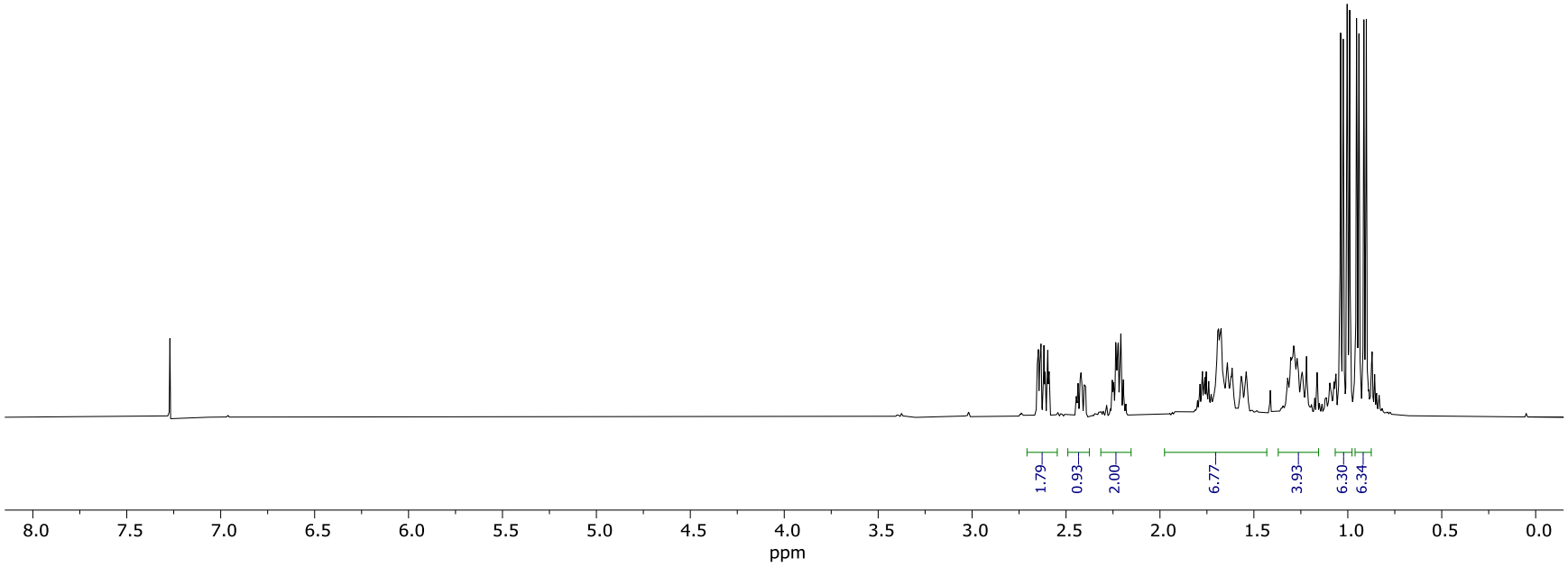


^{1}H 500 MHz, $CDCl_3$

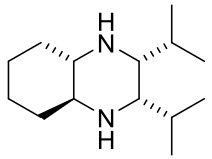


22b

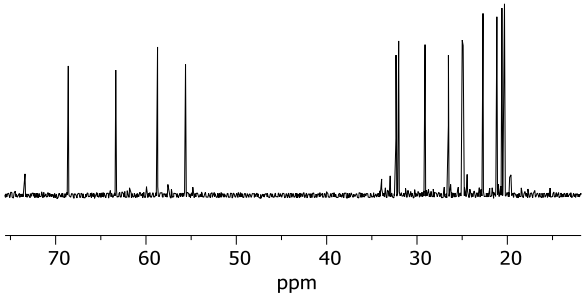


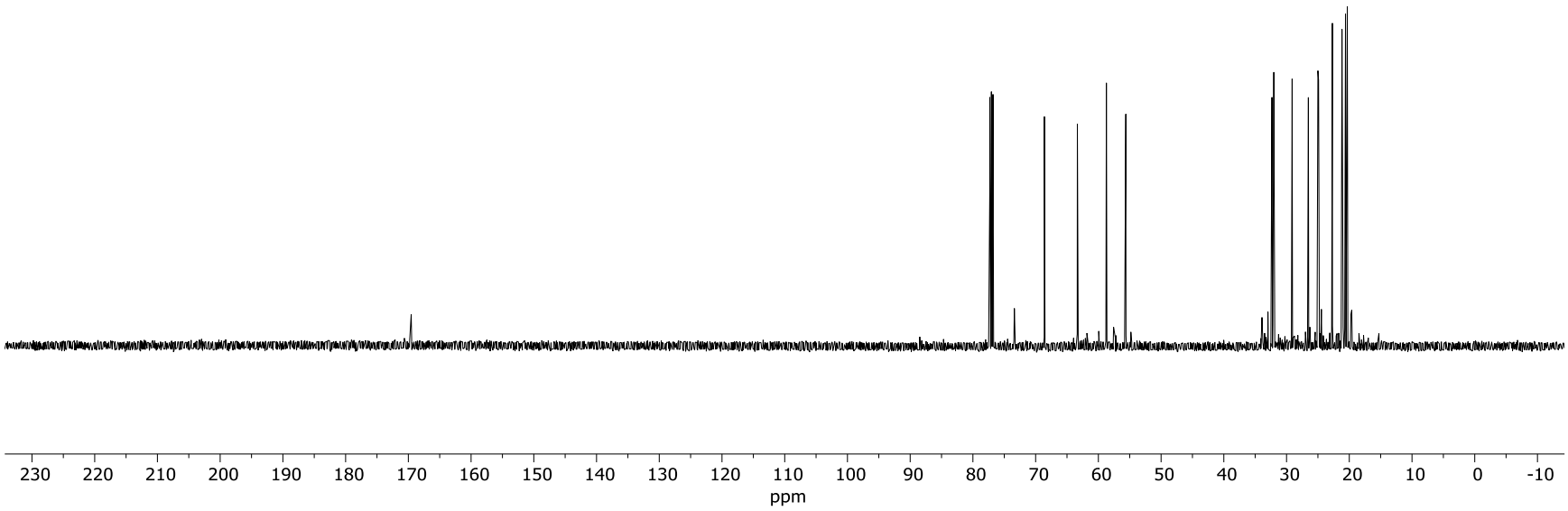


^{13}C 126 MHz, $CDCl_3$

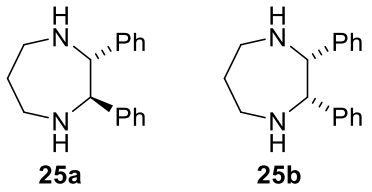


22b



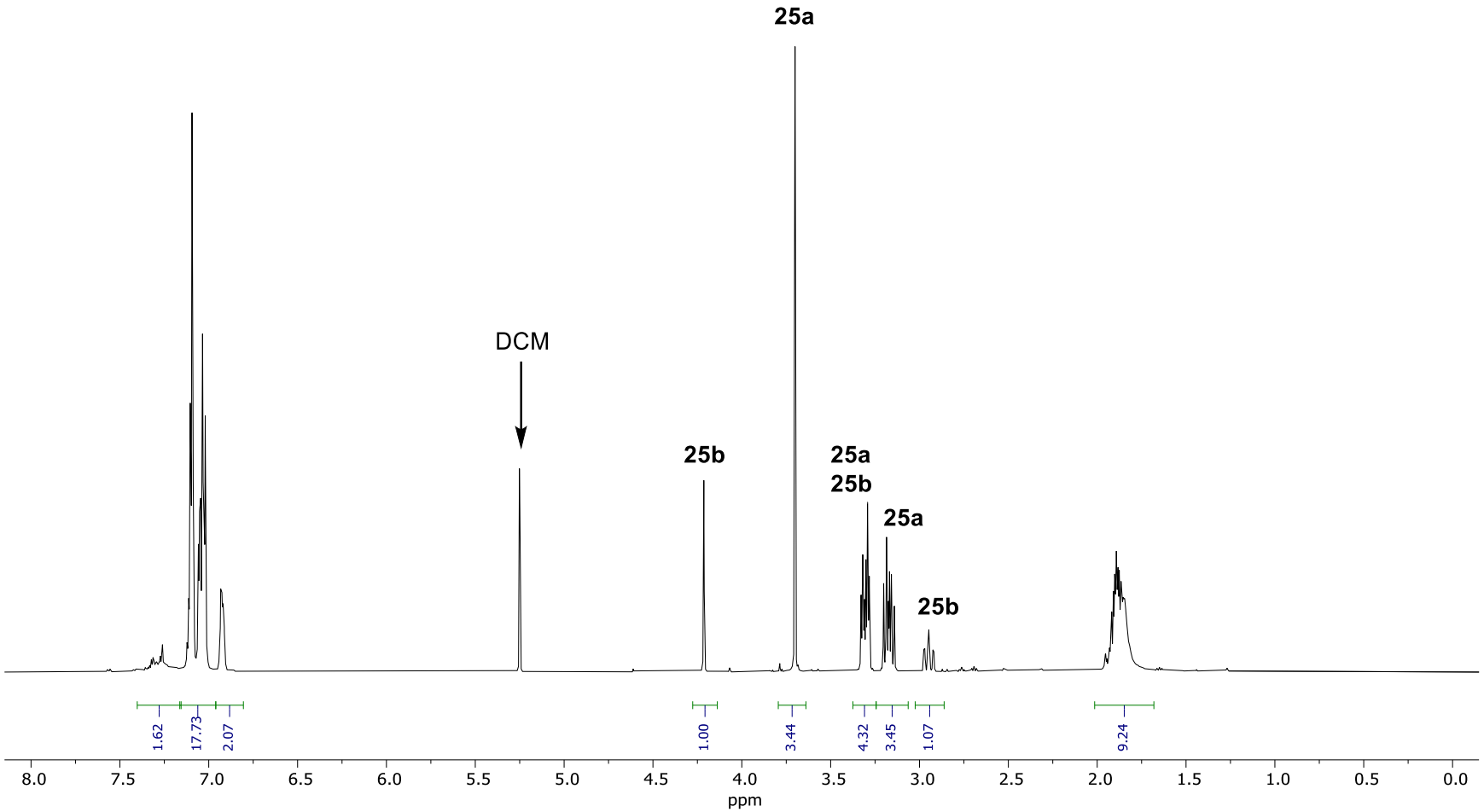


^{1}H 500 MHz, $CDCl_3$

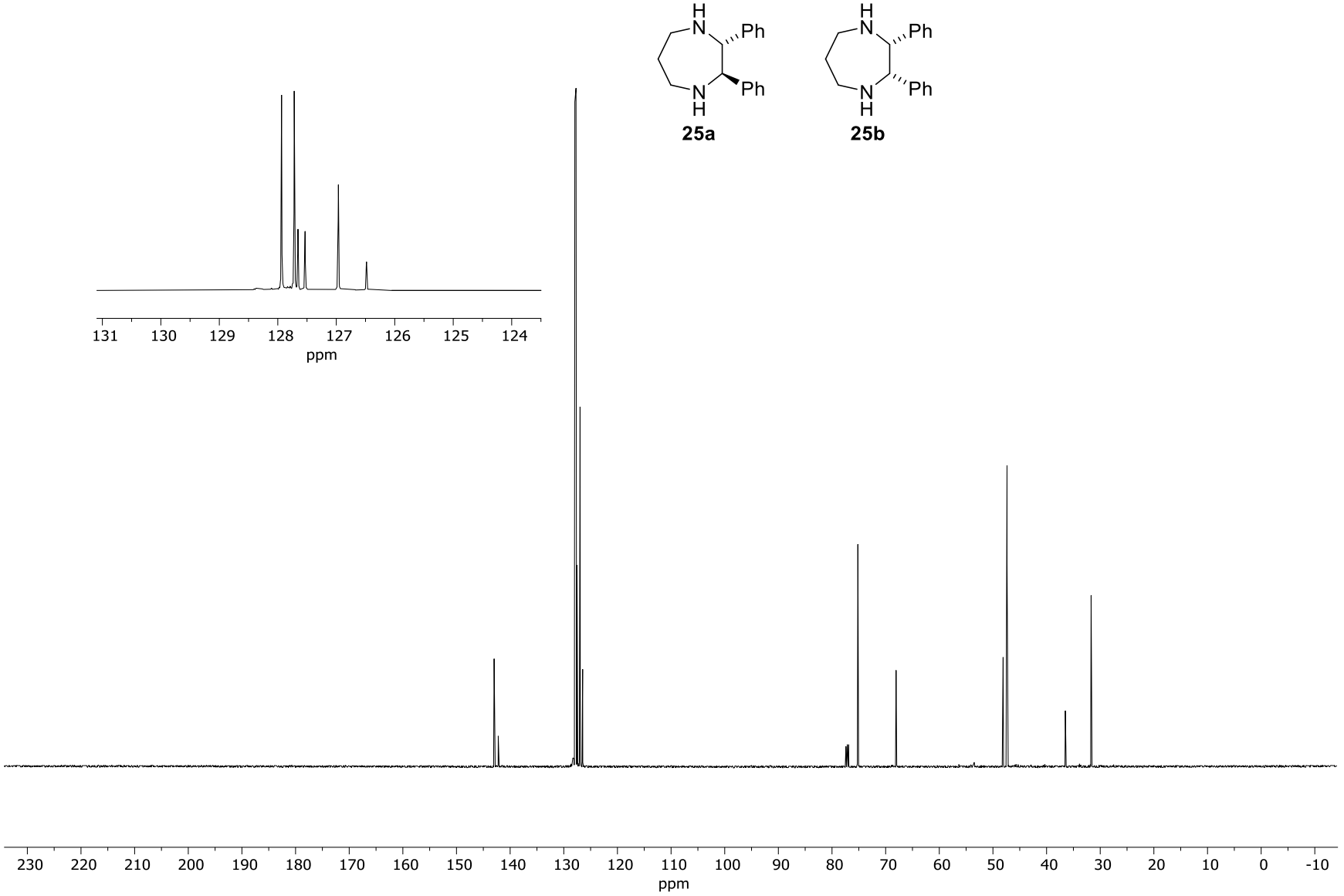


25a

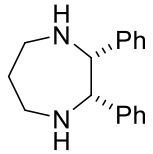
25b



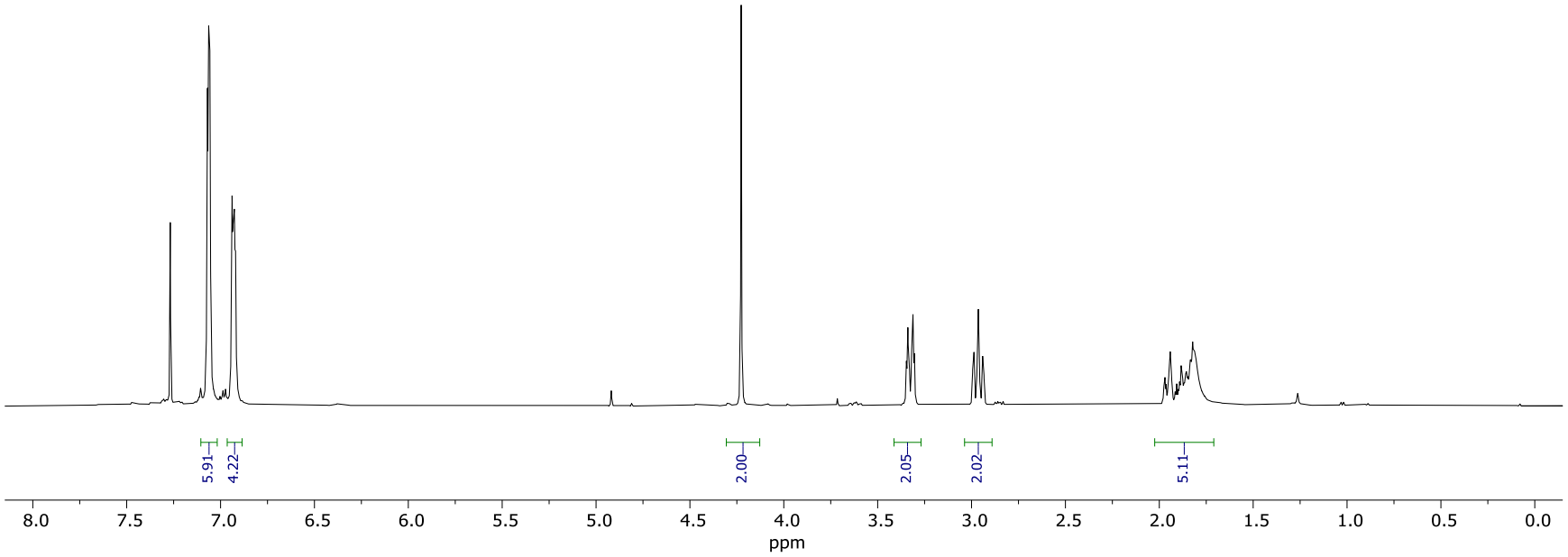
^{13}C 126 MHz, $CDCl_3$



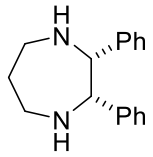
^{1}H 500 MHz, $CDCl_3$



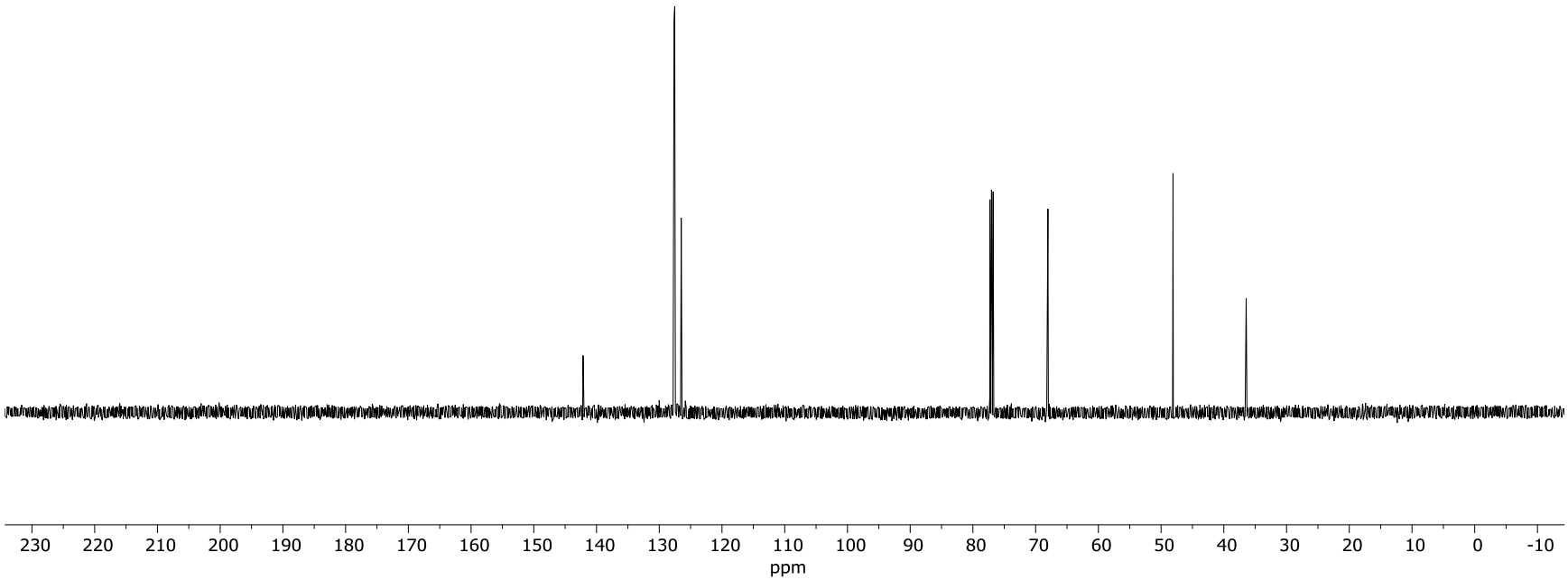
25b

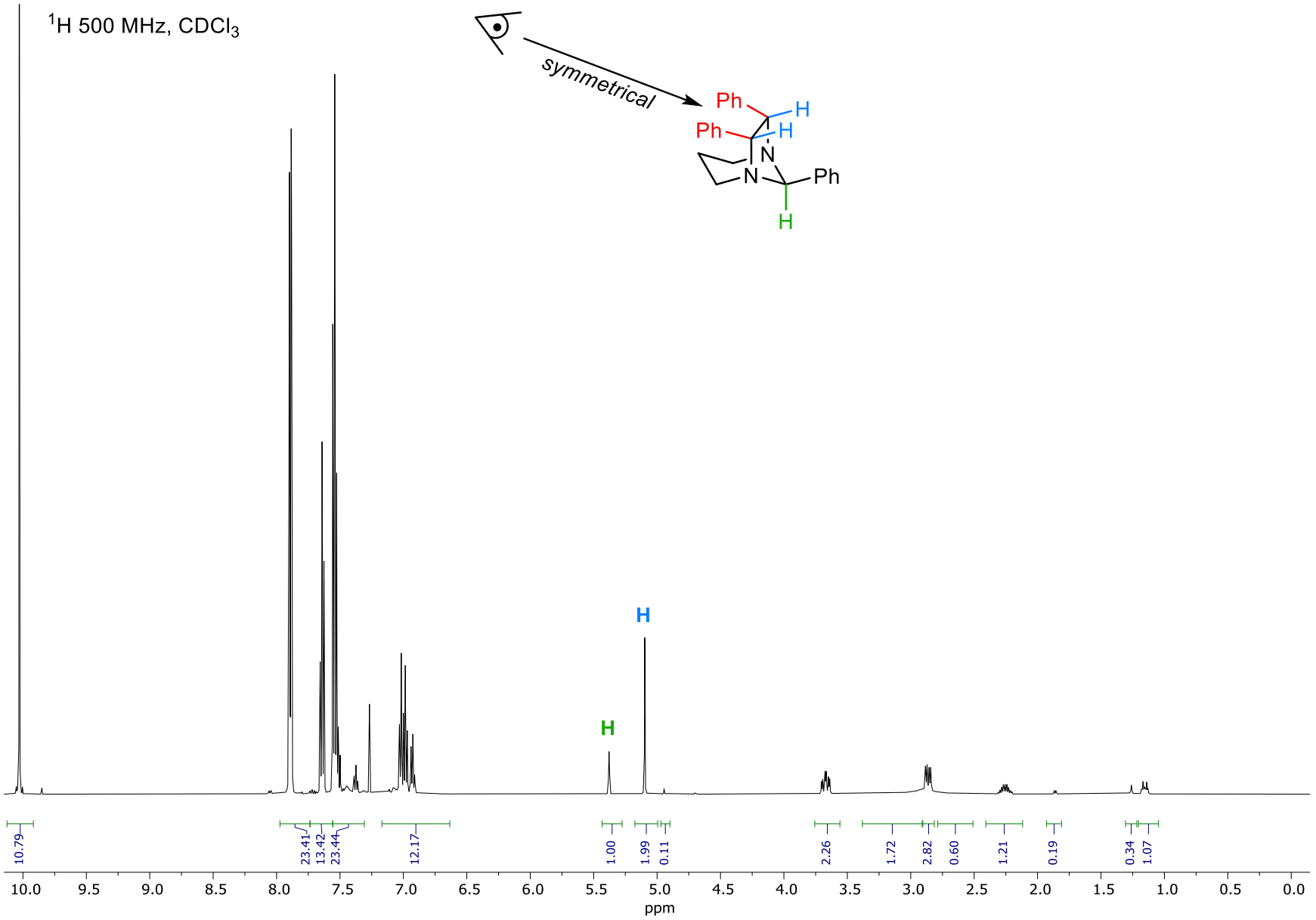


^{13}C 126 MHz, $CDCl_3$

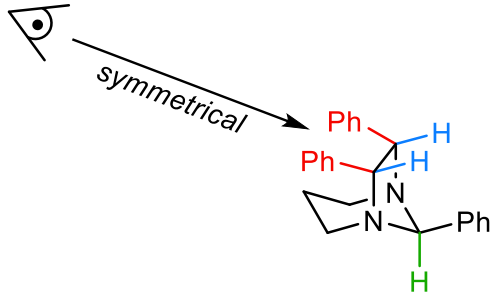


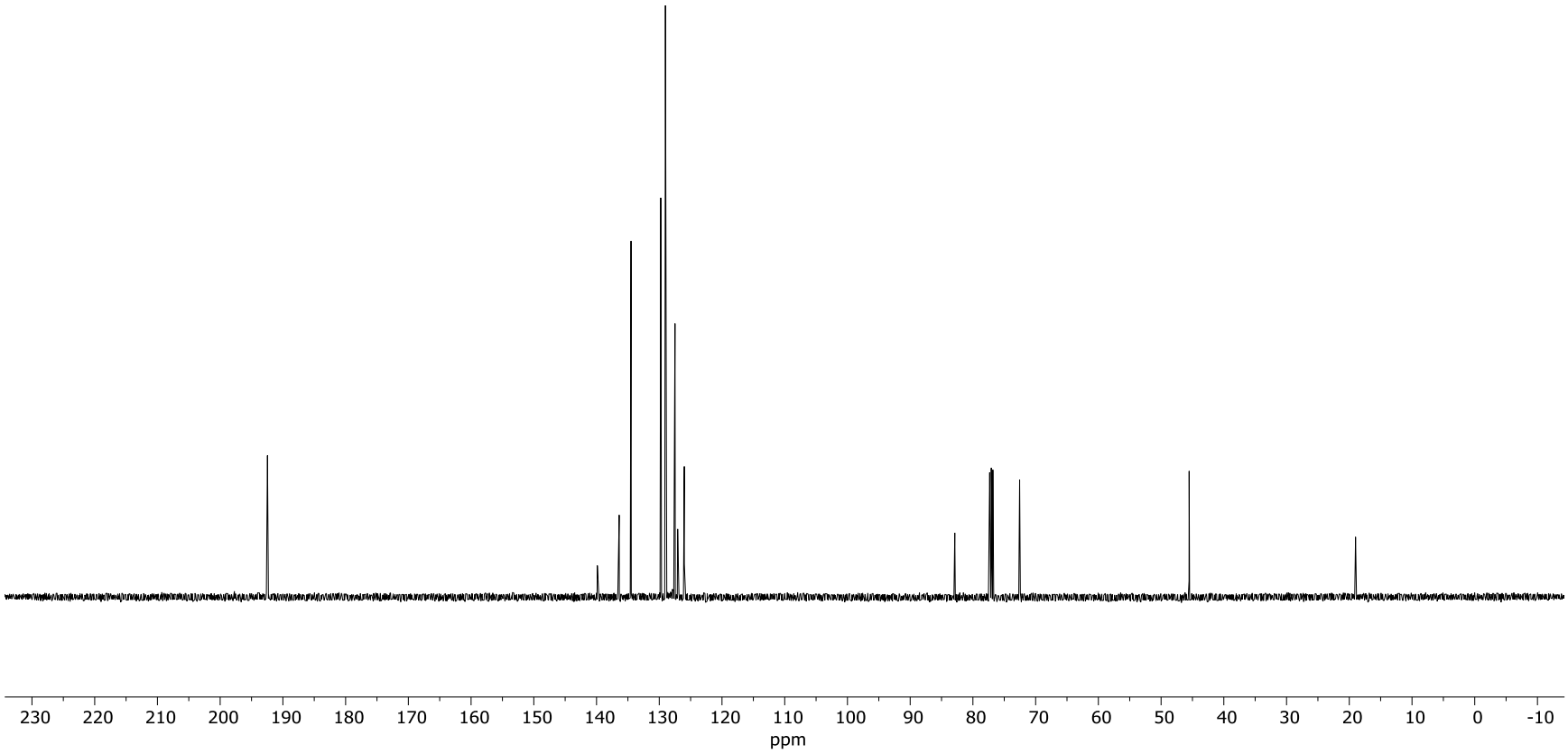
25b




1H 500 MHz, CDCl3
symmetrical
Ph
H
Ph
H
N
N
Ph
H
H
H
10.79
23.41
13.42
23.44
12.17
1.00
1.99
0.11
2.26
1.72
2.82
0.60
1.21
0.19
0.34
1.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

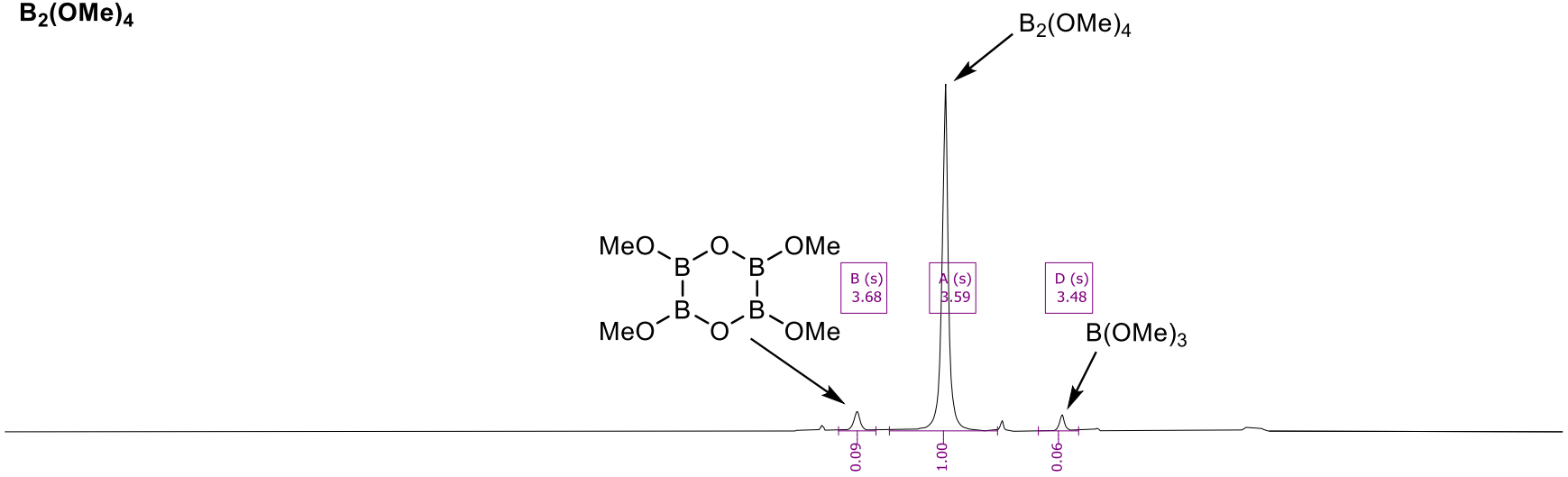
^{13}C 126 MHz, $CDCl_3$





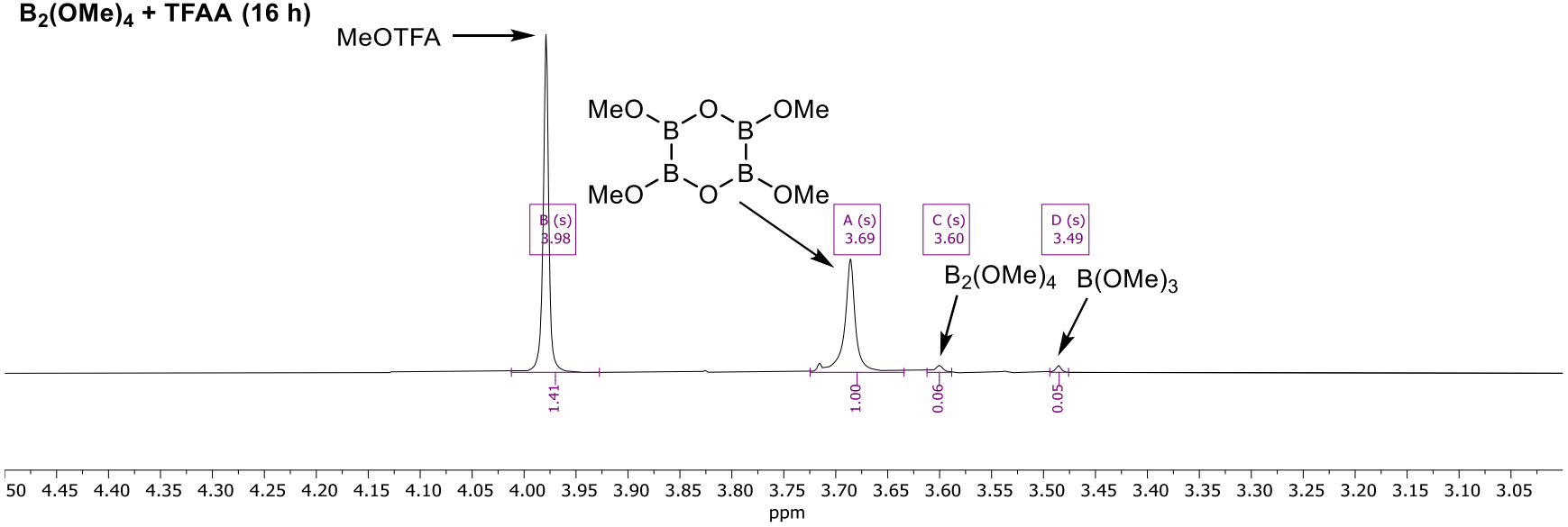
^{1}H 500 MHz, CD_3CN

$B_2(OMe)_4$



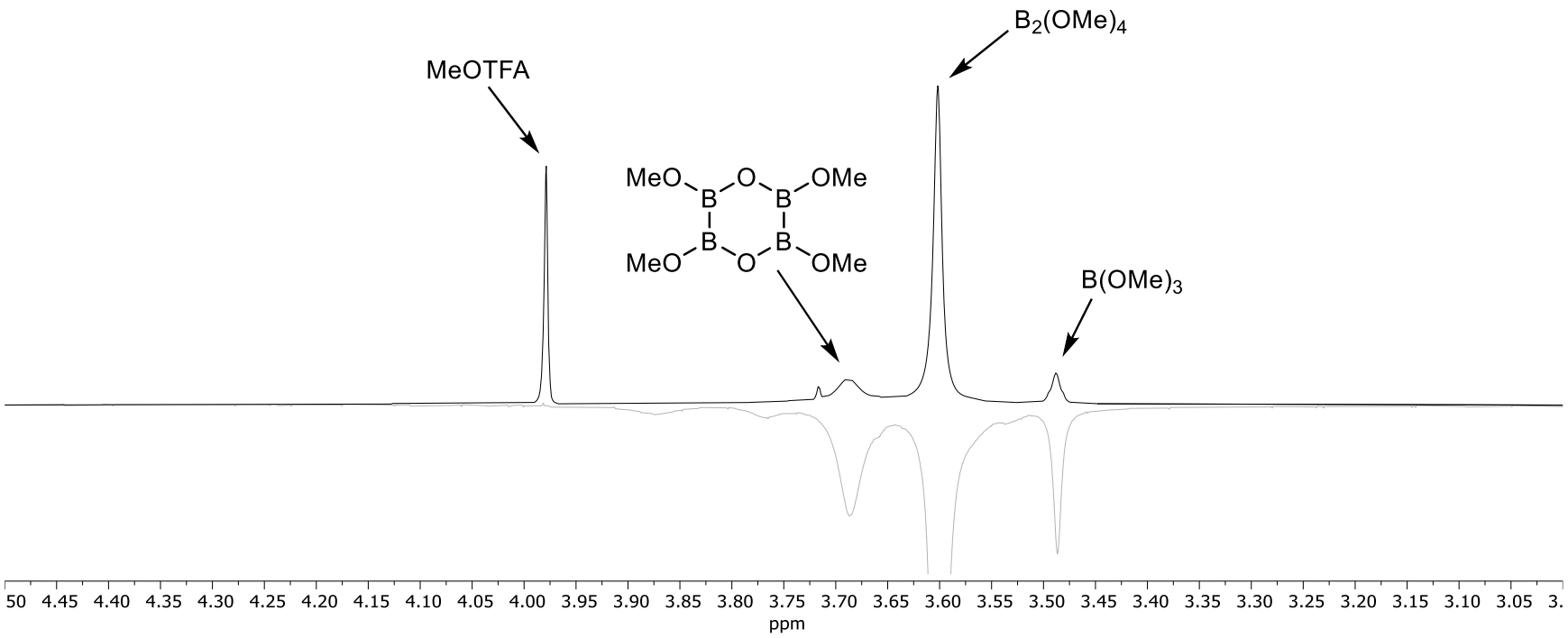
^{1}H 500 MHz, CD_3CN

$B_2(OMe)_4$ + TFAA (16 h)



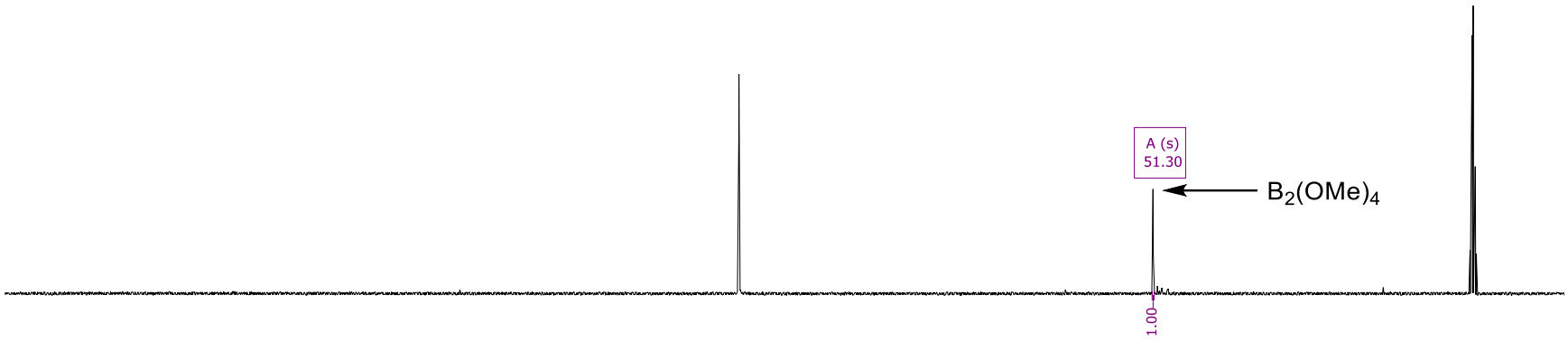
^{1}H 500 MHz, CD_3CN
$B_2(OMe)_4$ + TFAA (1 h)

(1D NOESY correlation below ^{1}H spectrum. Peak irradiated = 3.6 ppm)



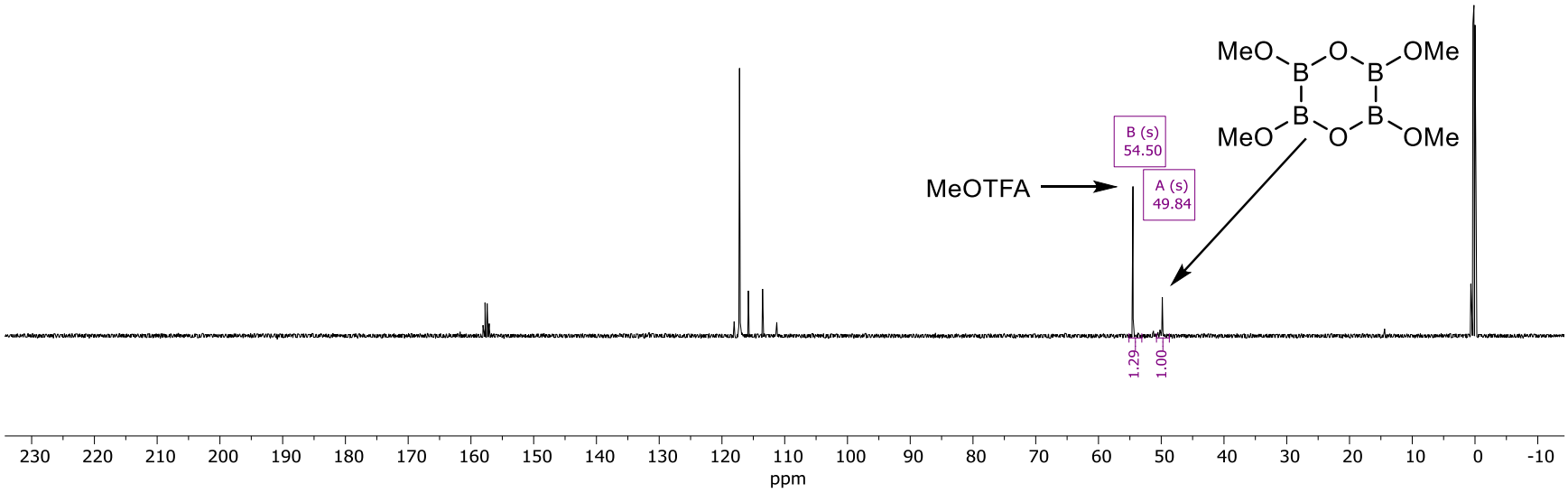
^{13}C 500 MHz, CD_3CN

$B_2(OMe)_4$



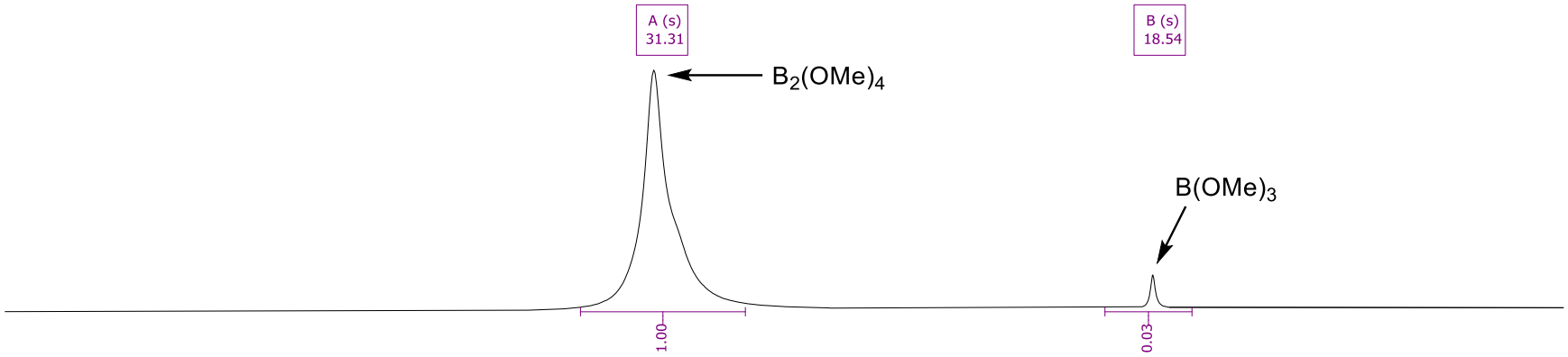
^{13}C 500 MHz, CD_3CN

$B_2(OMe)_4$ + TFAA (16 h)



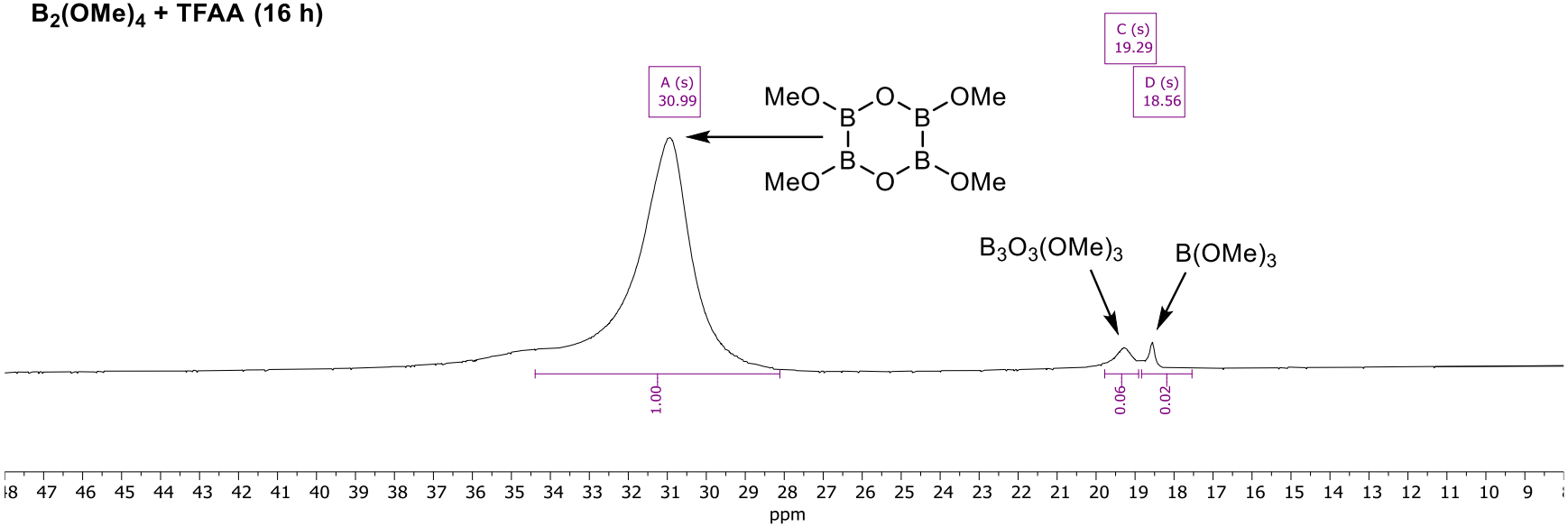
^{11}B 160 MHz, CD_3CN

$B_2(OMe)_4$



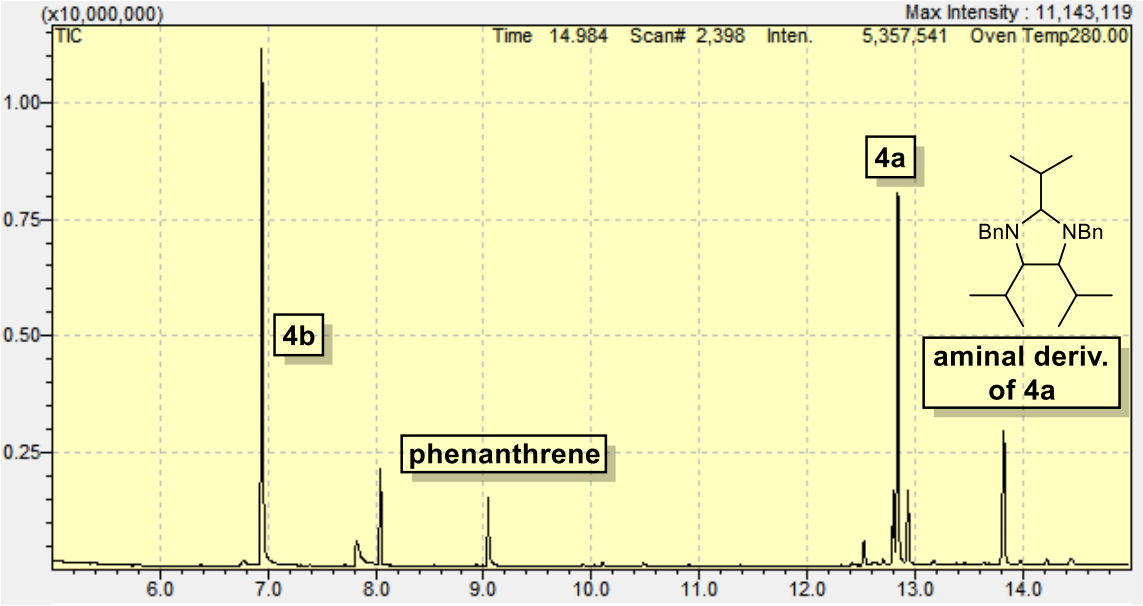
^{11}B 160 MHz, CD_3CN

$B_2(OMe)_4$ + TFAA (16 h)



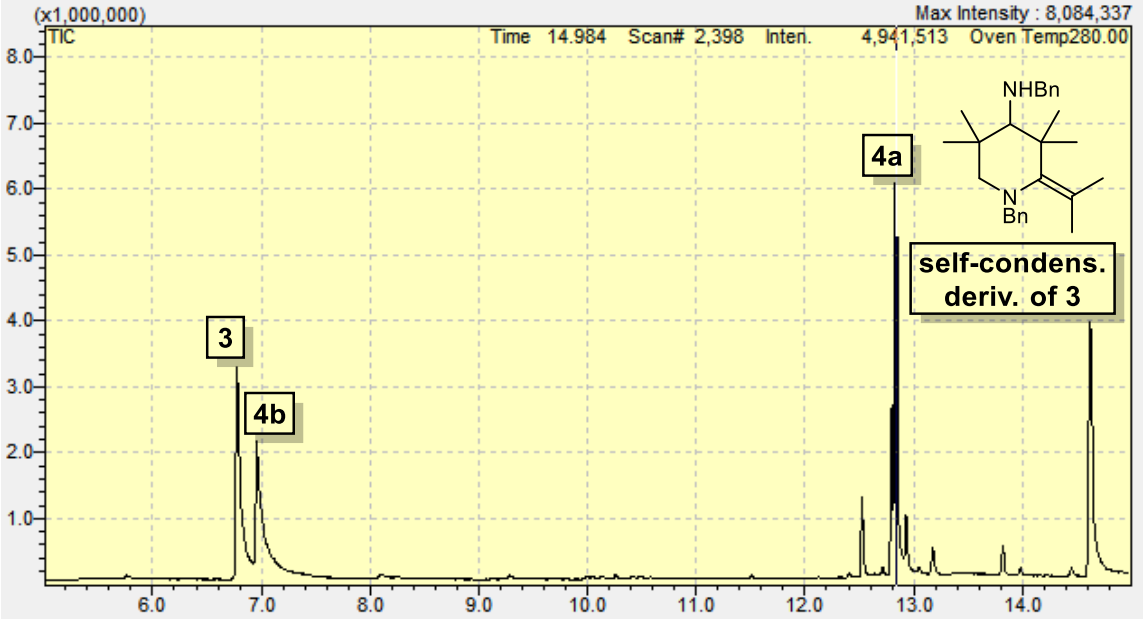
APPENDIX B: GC-MS Results for Table 3.1.

Entry 1



Entry 2

Entry 3



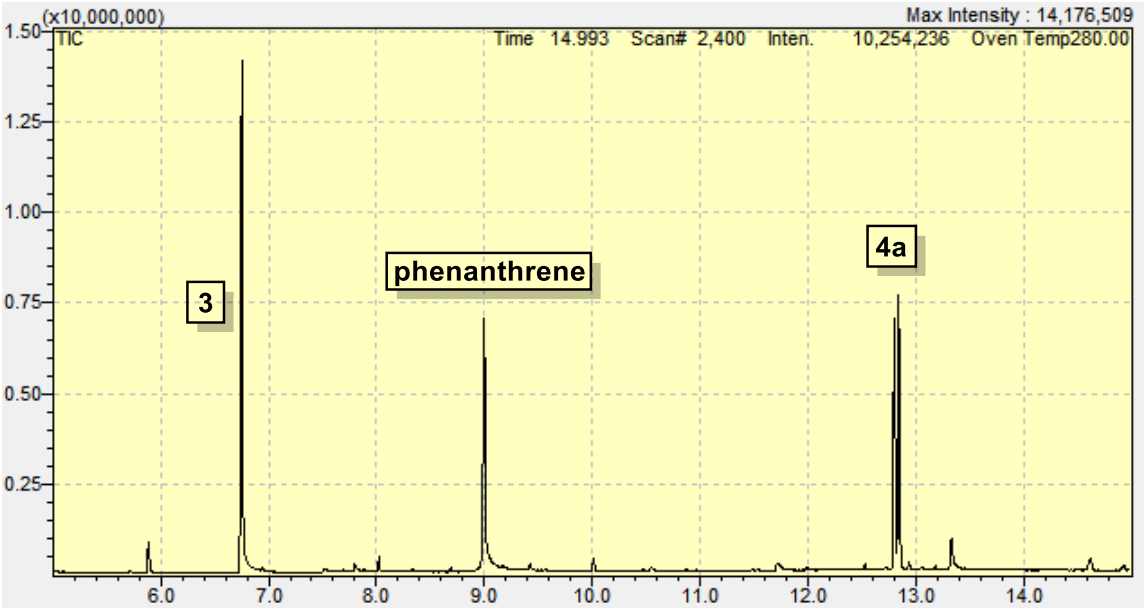
Entry 4

Entry 5

Entry 6

Entry 7

Entry 8



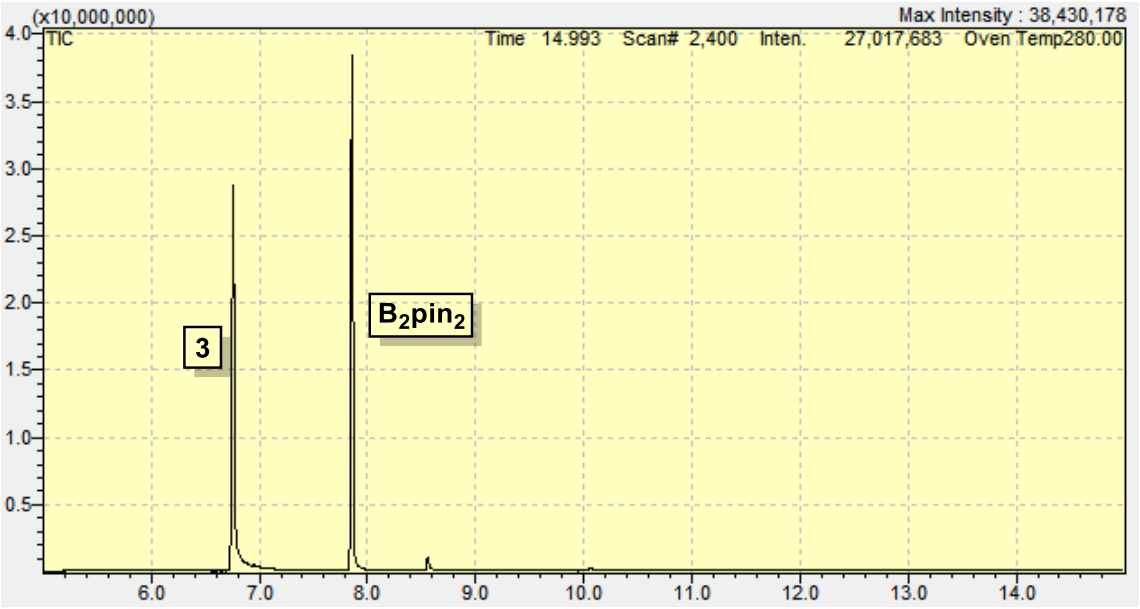
Entry 9

Entry 10a

Entry 11a

Entry 12

Entry 13


(x10,000,000)
Max Intensity : 38,430,178
TIC
Time 14.993 Scan# 2,400 Inten. 27,017,683 Oven Temp280.00
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
3
B2pin2
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0

APPENDIX C: Computational Coordinates.

The below coordinates use the M06-2X functional and the 6-31g(d,p) basis set with the SMD model for acetonitrile.

$B_2(OMe)_4$
B2OMe4_freqdp
M062X/6-31G(d,p)
E(RM062X) = -510.2014527

Zero-point correction= 0.182586 (Hartree/Particle)
Thermal correction to Energy= 0.196153
Thermal correction to Enthalpy= 0.197097
Thermal correction to Gibbs Free Energy= 0.142453
Sum of electronic and ZPE= -510.018866
Sum of electronic and thermal Energies= -510.005300
Sum of electronic and thermal Enthalpies= -510.004355
Sum of electronic and thermal Free Energies= -510.058999

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	123.088	43.757	115.008

B,0.012485,0.862721,-0.0572
B,-0.012485,-0.862721,-0.0572
O,1.088779,1.636814,0.273028
O,-1.119295,1.517117,-0.462081
O,-1.088779,-1.636814,0.273028
O,1.119295,-1.517117,-0.462081
C,2.310365,1.058009,0.706255
H,2.141907,0.218879,1.387176
H,2.879172,1.830449,1.228801
H,2.894296,0.703265,-0.147806
C,-1.119295,2.937412,-0.537493
H,-2.106394,3.251607,-0.882406
H,-0.36218,3.296668,-1.241051
H,-0.921718,3.385146,0.441144
C,1.119295,-2.937412,-0.537493
H,0.921718,-3.385146,0.441144
H,2.106394,-3.251607,-0.882406
H,0.36218,-3.296668,-1.241051
C,-2.310365,-1.058009,0.706255
H,-2.141907,-0.218879,1.387176
H,-2.879172,-1.830449,1.228801
H,-2.894296,-0.703265,-0.147806

$B_4O_2(OMe)_4$ (29)
b4o2ome4
M062X/6-31G(d,p)
E(RM062X) = -710.4984307

Zero-point correction= 0.201419 (Hartree/Particle)
Thermal correction to Energy= 0.218381
Thermal correction to Enthalpy= 0.219325
Thermal correction to Gibbs Free Energy= 0.156463
Sum of electronic and ZPE= -710.297011
Sum of electronic and thermal Energies= -710.280050
Sum of electronic and thermal Enthalpies= -710.279106
Sum of electronic and thermal Free Energies= -710.341967

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	137.036	55.908	132.303

B,0.86110955,1.2007384435,0.0172099256
O,1.5697484816,2.3553578005,0.0614605474
O,1.5535613226,0.0000000001,0.
B,-0.8611095502,1.2007384434,-0.0172099255
O,-1.5697484818,2.3553578003,-0.0614605474
O,-1.5535613226,-0.0000000001,0.
B,0.8611095502,-1.2007384434,-0.0172099255
B,-0.86110955,-1.2007384435,0.0172099256
O,1.5697484818,-2.3553578003,-0.0614605474
O,-1.5697484816,-2.3553578005,0.0614605474
C,2.9941840483,-2.3085441246,-0.0899548634
H,3.3893951925,-1.8221388754,0.8063816708
H,3.3565571453,-3.3370001355,-0.1299312872
C,-2.9941840481,-2.3085441249,0.0899548635
H,-3.356557145,-3.3370001359,0.1299312872
H,-3.3893951924,-1.8221388757,-0.8063816708
C,-2.9941840483,2.3085441246,-0.0899548634
H,-3.3565571453,3.3370001355,-0.1299312872
H,-3.3893951925,1.8221388754,0.8063816708
C,2.9941840481,2.3085441249,0.0899548635
H,3.356557145,3.3370001359,0.1299312872
H,3.3893951924,1.8221388757,-0.8063816708
H,-3.3523021594,1.7662119991,-0.9695899009
H,3.3523021592,1.7662119994,0.969589901
H,3.3523021594,-1.7662119991,-0.9695899009
H,-3.3523021592,-1.7662119994,0.969589901

$B(OMe)_3$
bome3
M062X/6-31G(d,p)
E(RM062X) = -370.2379722

Zero-point correction= 0.134218 (Hartree/Particle)
Thermal correction to Energy= 0.143868
Thermal correction to Enthalpy= 0.144813
Thermal correction to Gibbs Free Energy= 0.098272
Sum of electronic and ZPE= -370.103754
Sum of electronic and thermal Energies= -370.094104
Sum of electronic and thermal Enthalpies= -370.093160
Sum of electronic and thermal Free Energies= -370.139701

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	90.279	29.808	97.954

B,-0.0009657041,-0.0003167871,0.0001938615
O,1.2391729113,0.572432602,0.000041736
C,1.3398715183,1.9885153086,-0.0002822636
H,0.8684316288,2.4197358164,-0.8887740455
H,2.4008474798,2.2459180336,-0.0006674269
H,0.8690090899,2.4200952196,0.8883461419
O,-0.1241246458,-1.360799626,0.0009651853
O,-1.1172691659,0.78701062,-0.0003185521
C,-2.3933530533,0.164817481,-0.0001906231
H,-2.5267351929,-0.4672310653,-0.8834878093
H,-3.1474222573,0.9542390152,-0.0106285392
H,-2.5342470462,-0.4505633566,0.8937251505
C,1.0538141484,-2.1534339024,0.0003368955
H,0.7486181959,-3.2015680982,0.0060246816
H,1.6655412656,-1.9554361053,0.8858425091
H,1.6590528275,-1.9633221555,-0.8913729018

$B_3O_3(B(OMe)_2)_3$ (30)
brxbome23_from-b2ome4_not-symmetrized
M062X/6-31G(d,p)
E(RM062X) = -1065.7363152

Zero-point correction= 0.302458 (Hartree/Particle)
Thermal correction to Energy= 0.328879
Thermal correction to Enthalpy= 0.329824
Thermal correction to Gibbs Free Energy= 0.240173
Sum of electronic and ZPE= -1065.433857
Sum of electronic and thermal Energies= -1065.407436

Sum of electronic and thermal Enthalpies= -1065.406492
Sum of electronic and thermal Free Energies= -1065.496143

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.375	86.577	188.687

B,-1.1925331674,0.7206754312,0.1917696817
O,0.0279660393,1.3668910492,0.2160849699
O,-1.1998607869,-0.6630019468,0.2092700215
B,1.2226840763,0.669870897,0.2549655204
B,-0.0300342837,-1.3965869024,0.2515308714
O,1.171614242,-0.7104894544,0.2771272679
B,-0.0225492606,-3.1180984867,0.243965336
O,-1.082170523,-3.9262541042,0.5377662084
O,1.1530236106,-3.7208615241,-0.0995759765
C,-2.3405976967,-3.3838114327,0.9149122218
C,1.2221482604,-5.140669395,-0.1461433115
H,-2.2441918812,-2.7114669436,1.7724701199
H,-2.9896421321,-4.2172979008,1.1912664822
H,-2.7979281237,-2.8334270757,0.0882474943
H,1.0078669227,-5.5787197155,0.8333936105
H,2.2353946813,-5.4139431505,-0.4469890326
H,0.5101046493,-5.5478918284,-0.8703073573
B,-2.6877711023,1.5711516757,0.118677289
O,-2.8670787159,2.9036066466,0.3523279768
O,-3.7895086137,0.8363035039,-0.2125251526
C,-1.7790772037,3.7423376654,0.716903072
C,-5.0550270126,1.4786672804,-0.3045766183
H,-1.2694380495,3.3685096041,1.6096819562
H,-2.1841948139,4.7337017847,0.9302379528
H,-1.0503843388,3.8212083603,-0.0944320264
H,-5.3382872205,1.932014409,0.6501520123
H,-5.7929937933,0.7209586202,-0.5749299362
H,-5.0466040892,2.2609445264,-1.0696572189
B,2.705372039,1.5463424369,0.2597500463
O,3.9557701378,1.0165539163,0.3926221075
O,2.6093851164,2.8998865662,0.1099376879
C,4.1552200216,-0.3801228704,0.5640633908
C,3.7945965326,3.6857667317,0.0963306338
H,3.6469555978,-0.7468813963,1.4603117541
H,5.2287302308,-0.5487517912,0.6716134105
H,3.7905878943,-0.9428963564,-0.299557324
H,4.3578723923,3.5682308661,1.0269734309
H,3.4987640886,4.7307861823,-0.0145476302
H,4.4443624553,3.4061135716,-0.7385661621

$B_4O_2(NMe_2)_4$ (31)
b4o2nme24_antitwist
M062X/6-31G(d,p)
E(RM062X) = -788.1807893

Zero-point correction= 0.364858 (Hartree/Particle)
Thermal correction to Energy= 0.387071
Thermal correction to Enthalpy= 0.388015
Thermal correction to Gibbs Free Energy= 0.315114
Sum of electronic and ZPE= -787.815932
Sum of electronic and thermal Energies= -787.793719
Sum of electronic and thermal Enthalpies= -787.792775
Sum of electronic and thermal Free Energies= -787.865676

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	242.890	80.292	153.433

B,1.2219001866,-0.7860360962,-0.3499017548
B,-1.1481552504,-0.8557338118,0.1311510297
B,-1.1551825698,0.8535939895,-0.1206784142
B,1.2200768077,0.7997041366,0.3361122765
N,-2.1859619197,-1.6387516045,0.6819724865
C,-3.4046798385,-1.0868842806,1.2399786375
C,-2.0911139415,-3.0786211039,0.8441294533
H,-4.2939670092,-1.4276800393,0.6921056187
H,-3.3730622094,0.0037093352,1.2162226275
H,-3.5200169201,-1.4030046868,2.2851829647
H,-2.9351949325,-3.5799295001,0.3528401099
H,-2.1147311982,-3.3571891569,1.9060992931
H,-1.1618530643,-3.4426671569,0.4062336129
N,-2.2039238585,1.6296172008,-0.6605972175
C,-2.1204172891,3.070079334,-0.8237170936
C,-3.4246674554,1.0695696857,-1.2058757592
H,-1.1891216124,3.4403737412,-0.3954907155
H,-2.9626927591,3.565746758,-0.3236828011
H,-2.1569269763,3.348426945,-1.8853806211
H,-3.3855025116,-0.0207864879,-1.1824660803
H,-3.5530083788,1.3848488109,-2.2498181556
H,-4.3104610318,1.4044318905,-0.6487613577
N,2.2633674987,-1.3941397332,-1.0841093864
C,2.1760958768,-2.7433861919,-1.613671538
C,3.4791502333,-0.7103992591,-1.4785747525
H,1.2482310257,-3.2127037884,-1.2871560514
H,3.0221923839,-3.3508913602,-1.2669461561

H,2.2022846765,-2.7373413222,-2.7114853948
H,3.4416103016,0.3367689453,-1.1736420184
H,3.5962706116,-0.7448624297,-2.5697987017
H,4.3702294604,-1.1766362436,-1.0361529127
N,2.2648098262,1.4147603186,1.0598096131
C,2.1739814616,2.763486958,1.5901036789
C,3.4891374183,0.7392140067,1.4417779794
H,2.2120691661,2.7578179626,2.6875661627
H,1.2394284091,3.2263287576,1.2735697762
H,3.0120733362,3.3767481525,1.2341861064
H,3.6172380333,0.7746263344,2.5317329333
H,4.3724916619,1.2113122274,0.9901724323
H,3.455454057,-0.3082263787,1.1373169909
O,0.0306177165,1.5219819387,0.1990788113
O,0.0386845675,-1.5161781773,-0.2010575721

$B_3O_3(B(NMe_2)_2)_3$ (32)
b3o3bnme23_rst_nosymm
M062X/6-31G(d,p)
E(RM062X) = -1182.2327813

Zero-point correction= 0.546184 (Hartree/Particle)
Thermal correction to Energy= 0.581076
Thermal correction to Enthalpy= 0.582020
Thermal correction to Gibbs Free Energy= 0.475343
Sum of electronic and ZPE= -1181.686597
Sum of electronic and thermal Energies= -1181.651706
Sum of electronic and thermal Enthalpies= -1181.650761
Sum of electronic and thermal Free Energies= -1181.757439

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	364.630	123.211	224.521

B,-1.3970147611,-0.1109065542,0.0001437801
B,0.8018129708,-1.1519428476,-0.0008355068
B,0.6038353261,1.2728034796,-0.0017419248
B,-3.1152978937,-0.2515894198,0.007889003
N,-3.8743963948,0.6109145559,0.8596524903
N,-3.7328213649,-1.2266612539,-0.8362045708
C,-3.2840048483,1.3241449077,1.9761310702
C,-5.271220825,0.9635231657,0.6781798944
C,-5.056149729,-1.7930165759,-0.6448582675
C,-3.0435254517,-1.8439372086,-1.9531887949
H,-3.806184775,1.0853704148,2.9132911245
H,-3.3472524684,2.4127835037,1.8353803367

H,-2.2348115035,1.0536238838,2.1021636736
H,-5.3828796911,2.0546209631,0.7398476445
H,-5.9254347733,0.526577291,1.4463696966
H,-5.6273900715,0.6488593947,-0.3032907424
H,-5.4500811978,-1.5362900219,0.3390045945
H,-4.9961938354,-2.8881529423,-0.7056514779
H,-5.7758199641,-1.4644109848,-1.4084359419
H,-2.0480153401,-1.4173239373,-2.0820612531
H,-3.5982040586,-1.6904637198,-2.889510755
H,-2.9398245042,-2.9290331349,-1.8092835931
B,1.7775738212,-2.5734822111,-0.0078646029
N,1.3981590711,-3.6732724102,0.8241233285
N,2.9350173289,-2.615667164,-0.8464094076
C,0.4811301159,-3.5309691014,1.9387678518
C,1.7832976853,-5.0586460177,0.6221801887
C,4.0794524371,-3.4904108264,-0.6630279991
C,3.134548056,-1.6998214343,-1.9533186031
H,0.9432761401,-3.8797547757,2.8729782288
H,-0.4318645897,-4.1240177161,1.7849351002
H,0.1946504048,-2.4878388357,2.0782736299
H,0.8898150349,-5.6958327529,0.6708141022
H,2.4838705691,-5.4233267255,1.3872148531
H,2.2363114126,-5.1971380822,-0.3600252845
H,4.047936406,-3.9716606273,0.3149993213
H,5.0027973757,-2.8976430617,-0.7143120454
H,4.150283735,-4.2691753633,-1.4360045078
H,2.2740690259,-1.0408766048,-2.0754425566
H,3.2741667132,-2.2481376343,-2.8955920494
H,4.0287435412,-1.0782013341,-1.8020643831
B,1.3425447118,2.830855776,-0.0016071796
N,0.8115763363,3.8484774053,-0.8545487579
N,2.4666810984,3.0610810257,0.8521927486
C,-0.0606568915,3.5540325595,-1.9753962638
C,0.9855444412,5.278725873,-0.6734109765
C,3.4719727431,4.0923726264,0.6672211849
C,2.7846023697,2.1996704917,1.9748961073
H,0.3589766805,3.9457570416,-2.9126367357
H,-1.0505653366,4.0139841033,-1.8437289433
H,-0.1946120343,2.478120727,-2.0944686375
H,0.0089307582,5.7765601756,-0.7444103282
H,1.6358954516,5.7299874194,-1.4365503928
H,1.3991603459,5.4983620197,0.3113821863
H,3.3821309776,4.5505593286,-0.3182123099
H,4.4720904849,3.6433053958,0.7370293825
H,3.4177432152,4.8833870292,1.4290603864
H,2.0262686319,1.4255811178,2.0999153066

H,2.8328628821,2.7758659208,2.9095697039
H,3.7605530412,1.7111426732,1.841647511
O,-0.5833477423,-1.2345797918,0.0005265749
O,-0.7762473402,1.1300867447,-0.0054097063
O,1.3681480458,0.1145660571,0.0023424936

REFERENCES

REFERENCES

(1) Xia, Y.-T.; Sun, X.-T.; Zhang, L.; Luo, K.; Wu, L. Metal-Free Hydrogen Atom Transfer from Water: Expeditious Hydrogenation of N-Heterocycles Mediated by Diboronic Acid. *Chem. Eur. J.* **2016**, *22*, 17151–17155.

(2) Xuan, Q.; Zhao, C.; Song, Q. Umpolung of protons from H_2O: a metal-free chemoselective reduction of carbonyl compounds via B_2pin_2/H_2O systems. *Org. Biomol. Chem.* **2017**, *15*, 5140–5144.

(3) Flinker, M.; Yin, H.; Juhl, R. W.; Eikeland, E. Z.; Overgaard, J.; Nielsen, D. U.; Skrydstrup, T. Efficient Water Reduction with sp^3-sp^3 Diboron(4) Compounds: Application to Hydrogenations, H–D Exchange Reactions, and Carbonyl Reductions. *Angew. Chem. Int. Ed.* **2017**, *56*, 15910–15915.

(4) Carmalt, C. J.; Clegg, W.; Cowley, A. H.; Lawlor, F. J.; Marder, T. B.; Norman, N. C.; Rice, C. R.; Sandoval, O. J.; Scott, A. J. Isolation and structural characterization of novel compounds containing B_4O_2 rings. *Polyhedron* **1997**, *16*, 2325–2328.

(5) Wartik, T.; Apple, E. F. A New Modification of Boron Monoxide. *J. Am. Chem. Soc.* **1955**, *77*, 6400–6401. (b) McCloskey, A. L.; Brotherton, R. J.; Boone, J. L. The Preparation of Boron Monoxide and its Conversion to Diboron Tetrachloride. *J. Am. Chem. Soc.* **1961**, *83*, 4750–4754.

(6) Mercer, G. J.; Sigman, M. S. Diastereoselective Synthesis of Piperazines by Manganese-Mediated Reductive Cyclization. *Org. Lett.* **2003**, *5*, 1591–1594.

(7) Lappert, M. F. 568. Cyclic organic boron compounds. Part I. Preparation, characterisation, and stability of esters of metaboric acid. *J. Chem. Soc.* **1958**, *0*, 2790–2793.

(8) Bomio, C.; Kabeshov, M. A.; Lit, A. R.; Lau, S.-H.; Ehlert, J.; Battilocchio, C.; Ley, S. V. Unveiling the role of boroxines in metal-free carbon–carbon homologations using diazo compounds and boronic acids. *Chem. Sci.* **2017**, *8*, 6071–6075.

(9) Maringgele, W.; Noltemeyer, M.; Meller, A. Bis(diorganylamino)dihalodiboroxanes as Building Blocks for Boron Heterocycles. *Organometallics* **1997,** *16*, 2276–2284.

(10) Clegg, W.; Marder, T. B.; Nlate, S.; Scott, A. J. 2,3,5,6-Tetrakis[3,5-bis(trifluoro-methyl)phenoxy]-2,5-bis(dimethyl-amino)2,3,5,6-tetrabora-1,4-dioxane diethyl ether 0.667-solvate. *Acta. Cryst.* **2007**, *C63*, o603–o605.

(11) Kinjo, R.; Ota, K. A Neutral and Aromatic Boron-Rich Inorganic Benzene. *Angew. Chem. Int. Ed.* **2020**, *59*, 6572–6575.

(12) Su, B.; Ota, K.; Xu, K.; Hirao, H.; Kinjo, R. Zwitterionic Inorganic Benzene Valence Isomer with σ-Bonding between Two π-Orbitals. *J. Am. Chem. Soc.* **2018**, *140*, 11921−11925.

(13) Moezzi, A.; Olmstead, M. M.; Pestana, D. C.; Power, P. P. Synthesis and Structural Characterization of $[PhE(BNMe_2)_2]_2$ (E = P or As): Six-Membered P_2B_4 and As_2B_4 Rings with Unusual Structures. *Z. Anorg. Allg. Chem.* **1995**, *621*, 1933–1938.

(14) Malhotra, S. C. The Chemistry of Tetrakis(dimethylamino)diboron. *Inorg. Chem.* **1964**, *3*, 862–865.

(15) Wann, D. A.; Robertson, H. E.; Bramham, G.; Bull, A. E. A.; Norman, N. C.; Russell, C. A.; Rankin, D. W. H. Unusual chalcogen-boron ring compounds: the gas-phase structures of 1,4-$B_4S_2(NMe_2)_4$ and related molecules. *Dalton Trans.* **2009**, 1446–1449.

(16) Nöth, H.; Fußstetter, H.; Pommerening, H.; Taeger, T. Neue Ringsysteme mit Dibor-Einheiten als Ringglieder: Dithiadisilaboracyclopentane, Dithiatriborolane und Dithiatetraborinane. *Chem. Ber.* **1980**, *113*, 342–357.

(17) *Gmelin Handbuch der Anorganischen Chemie, Gmelin Handbook:* B: B-Verb.4, *9.1*, 268–279.

(18) Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

(19) Zhao, Y.; Schultz, N. E.;Truhlar, D. G. Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions *J. Chem. Theory. Comput.* **2006**, *2*, 364–382.

(20) Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101–194118.

(21) Zhao, Y.; Truhlar, D. G. Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. *J. Phys. Chem. A* **2006**, *110*, 13126–13130.

(22) Boone, M.; Chibale, K.; Combrinck, J.; D'hooghe, M.; Mangelinckx, S.; Smith, P. J.; Van Puyvelde, J.; Van de Walle, T. Synthesis and biological evaluation of novel quinoline-piperidine scaffolds as antiplasmodium agents. *Eur. J. Med. Chem.* **2020**, *198*, 112330–112343.

(23) Hatano, B.; Ogawa, A.; Hirao, T.; Cp_2VCl_2-Catalyzed Meso-Selective Pinacol Coupling Reaction of Aldimines in the Presence of Chlorosilane and Zinc Metal. *J. Org. Chem.* **1998**, *63*, 9421–9424.

(24) Kakaei, S.; and Xu, J. Synthesis of (2-alkylthiothiazolin-5-yl)methyl dodecanoates via tandem radical reaction. *Org. Biomol. Chem.* **2013**, *11*, 5481–5490.

(25) E. Benedetti, M. Lomazzi, F. Tibiletti, J.-P. Goddard, L. Fensterbank, M. Malacria, G. Palmisano, A. Penoni. Synthesis of Nitrogen-Containing Heterocycles via Ring-Closing Ene-Ene and Ene-Yne Metathesis Reactions: An Easy Access to 1- and 2-Benzazepine Scaffolds and Five- and Six-Membered Lactams. *Synthesis*, **2012**, *44*, 3523–3533.

(26) Cook, G. R.; Barta, N. S.; Stille, J. R. Lewis acid-promoted 3-aza-Cope rearrangement of *N*-alkyl-*N*-allyl enamines. *J. Org. Chem.* **1992**, 57, 461–467.

(27) Xu, J.-K.; Li, S.-J.; Wang, H.-Y.; Xu, W.-C.; Tian, S.-K. Three-component carboarylation of unactivated imines with arynes and carbon nucleophiles. *Chem. Commun*. **2017**, *53*, 1708–1711.

(28) Nayak, M. K.; Suhr, S.; Chrysochos, N.; Rawat, H.; Schulzke, C.; Chandrasekhar, V.; Sarkar, B.; Jana, A. Tethered CAAC–CAAC dimers: oxidation to persistent radical cations and bridging-unit dependent reactivity/stability of the dications. *Chem. Commun.* **2021**, *57*, 1210–1213.

(29) Staab, H. A.; Vögtle, F. Untersuchungen über Schiffsche Basen, II: Darstellung von 1.2-Diamino-cyclopropanen und von Schiffschen Basen dieser Diamine. *Chem. Ber.* **1965**, *98*, 2691–2700.

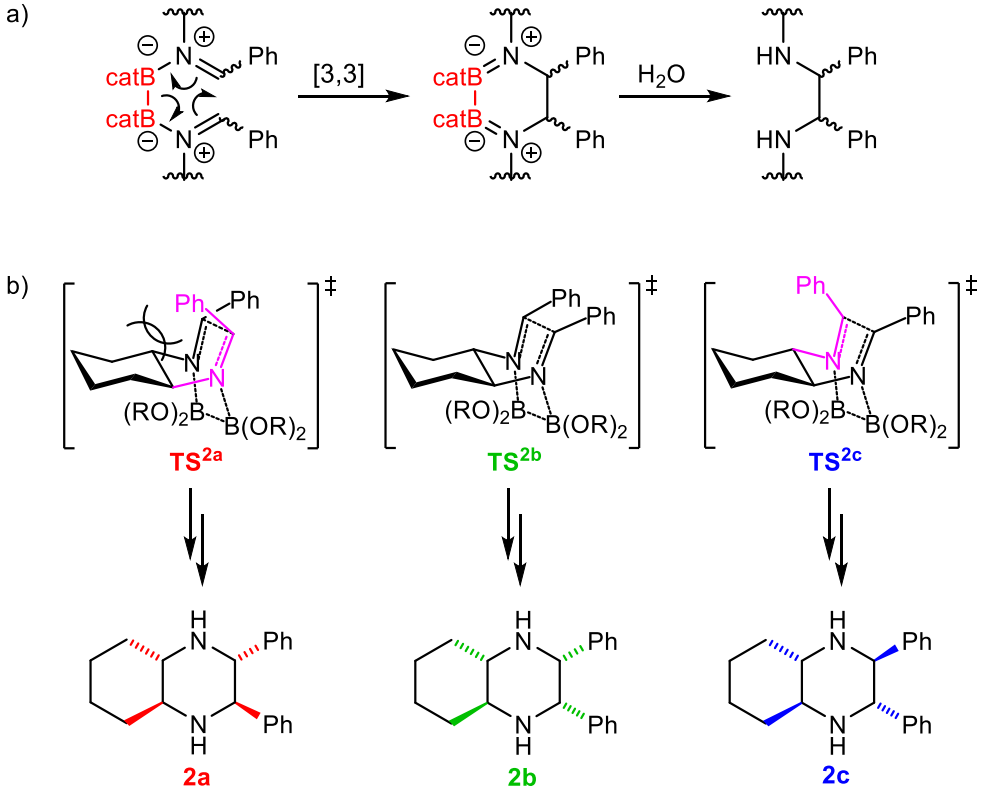
(30) Pirali, T.; Callipari, G.; Ercolano, E.; Genazzani, A. A.; Giovenzana, G. B.; Tron, G. C. A Concise Entry into Nonsymmetrical Alkyl Polyamines. *Org. Lett.* **2008**, *10*, 4199–4202.

Chapter 4. Probing the Origins of Diastereoselectivity Using Computational Models and New Experimental Conditions

Introduction.

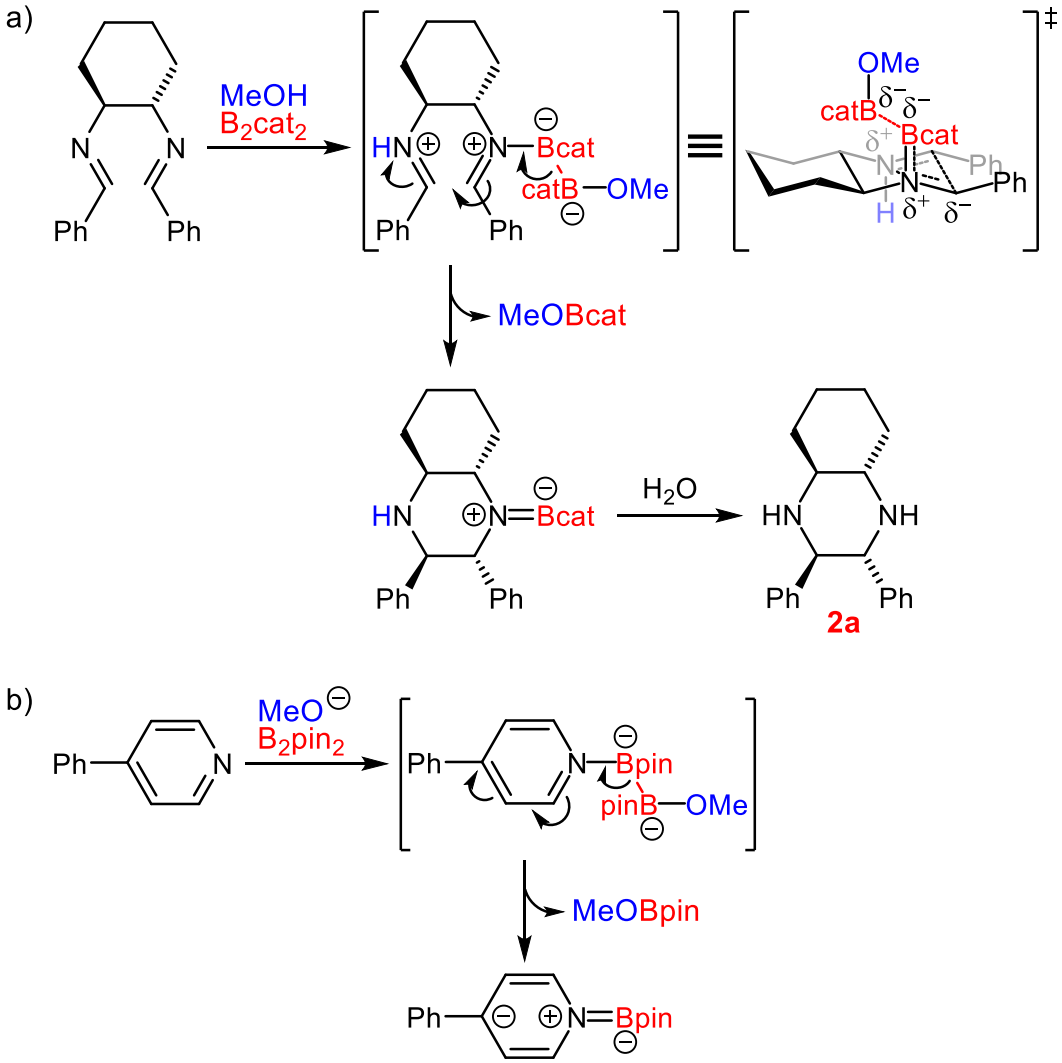
Intrigued by the mechanistic questions raised by our previous report (Chapter 2) of diboron-mediated reductive couplings of diimine **1** where variation of solvent (and the ligands on the diboron) enables diastereoselective access to all three diastereomers of a diamine **2a**-**2c**, we next investigated the proposed mechanisms for this reaction via computational modeling to investigate what influence choice of solvent may have on the mechanism.

Scheme 4.1. Concerted [3,3]-sigmatropic rearrangement mechanism[1-3] (a) and proposed transition states (b) as discussed in Chapter 2.



Two mechanisms were proposed in our initial report (Chapter 2): (1) A concerted [3,3]-sigmatropic rearrangement of a dicoordinate diimine-diboron complex (Scheme 4.1a), affording two potential kinetic products (**2b** and **2c**) via a closed boat-like transition state (Scheme 4.1b), and (2) heterolytic B-B cleavage of a monocoordinate diimine-diboron complex, affording the thermodynamic product (**2a**) via an ionic, open chair-like transition state (Scheme 4.2b) as previously reported in the literature for pyridines[4] (Scheme 4.2b).

Scheme 4.2. (a) Proposed ionic mechanism and transition state and (b) literature precedent.[4]



Investigation of the Sigmatropic Mechanism.

We began by considering the concerted [3,3]-sigmatropic rearrangement mechanism. *E*/*Z* imine isomerization (which is facile in the presence of electrophilic boron reagents[5]) is required to access the *trans*-diaxial diamine (**2c**), but we were unable to locate a transition state for this isomerization process. Two scenarios are possible for conditions leading to the *cis*-diamine (**2b**): (1) *E*/*Z* isomerization is slower than the reductive coupling

step, or (2) reductive coupling of the *E,E*-diimine is faster than reductive coupling of the *Z,E*-diimine.

Given prior reports of isomerization of 1,1-B_2cat_2 (**BC[1,1]**) to 1,2-B_2cat_2 (**BC[1,2]**) occurring in the presence of DBN or 4-picoline,[6] it is plausible that this transformation (Scheme 4.3, below) could also proceed at a rate competitive with the reductive coupling step. This would likely proceed through a highly polar ligand reorganization step requiring the presence of a nucleophile to stabilize the buildup of positive charge during dissociation of one of the catecholate ligands. As the steric profiles of these regioisomeric forms are different, we decided to consider reductive coupling transition states derived from both. Unfortunately, we also have yet to locate a transition state for the conversion of 1,1-B_2cat_2 into 1,2-B_2cat_2.

Scheme 4.3. Isomerization of 1,1-B_2cat_2 into 1,2-B_2cat_2.[6]

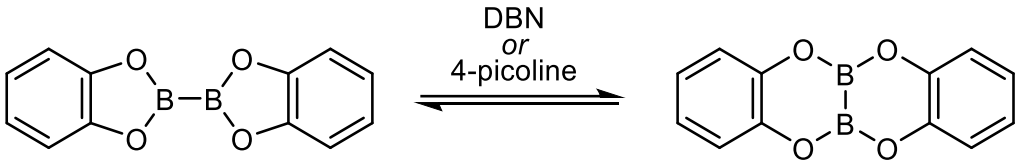
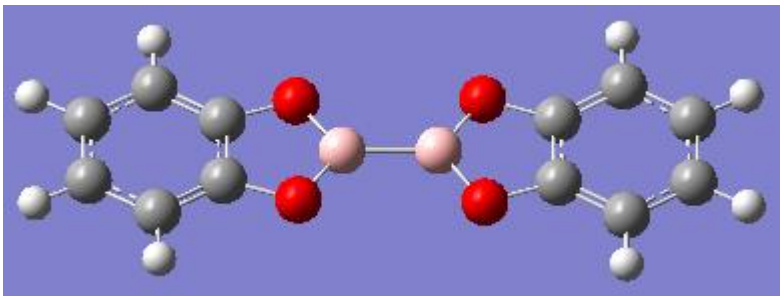
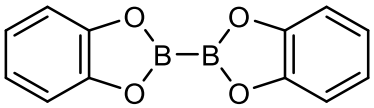


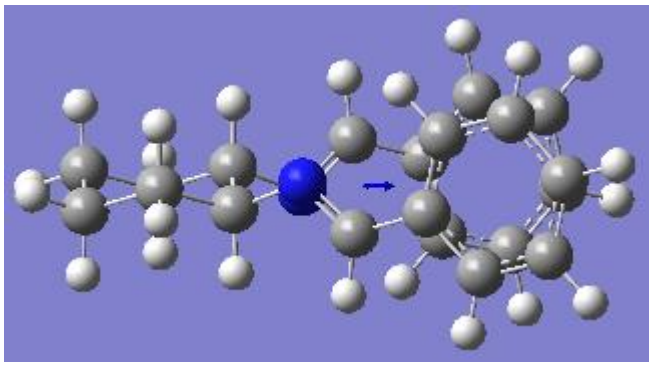
Figure 4.1. Dipole moments of representative examples of substrates, intermediate complexes, transition states, and products.[a]

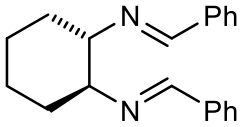




1,1-B_2cat_2

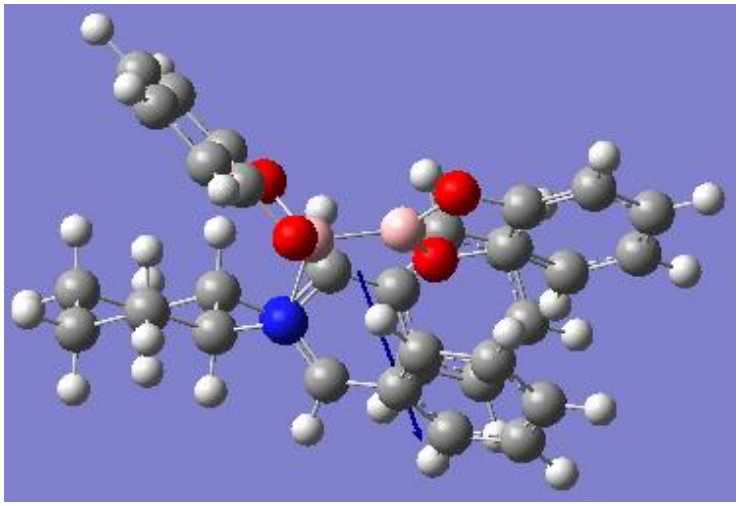
1,1-$B_2cat_2^{DMF}$ (1,1-B_2cat_2 in DMF)
Dipole moment = 0



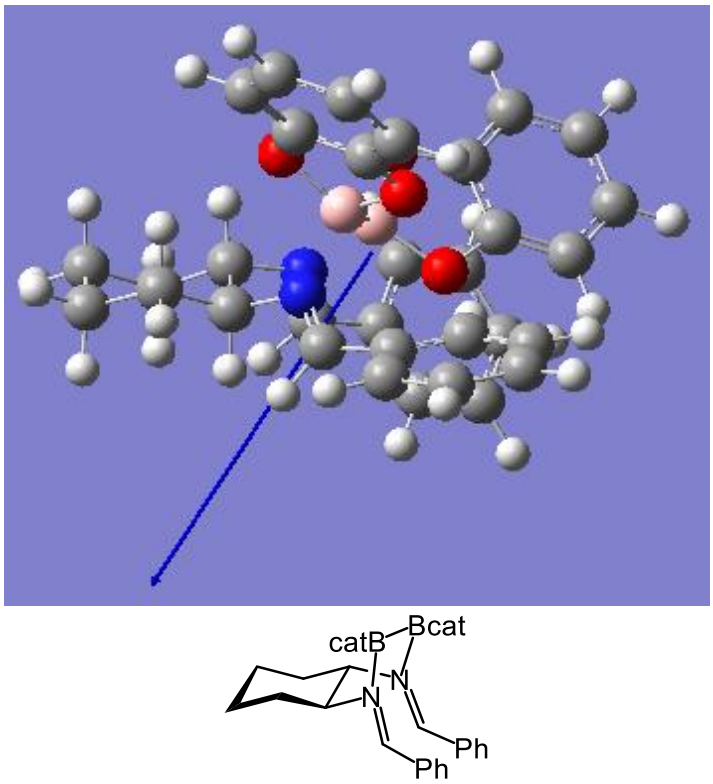


***E,E*-(1)^{DMF}** (*E,E*-diimine **1** in DMF)
Dipole moment = 1.03

Figure 4.1 (cont'd)

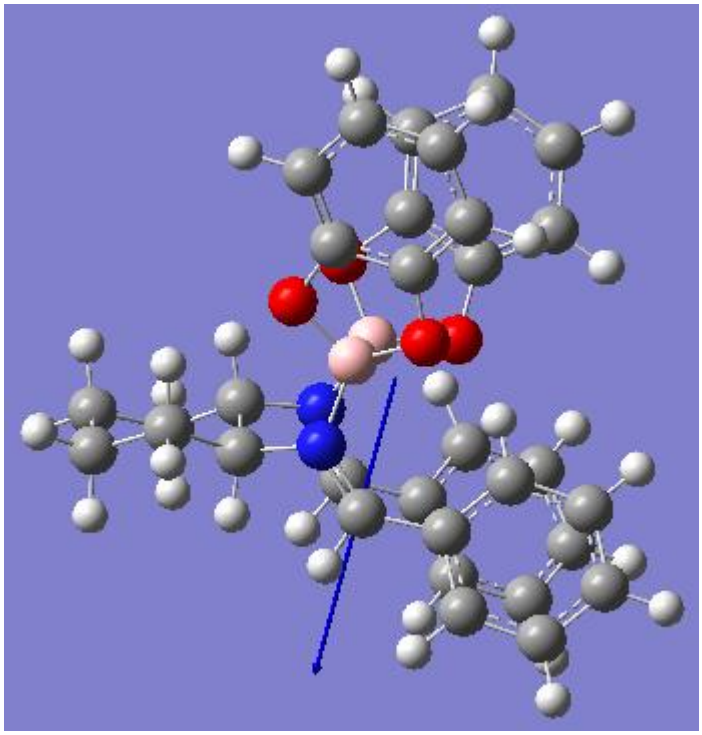


IA-*E*,*E*[1,1]^{DMF} (Intermediate monocoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in DMF
Dipole moment = 7.11



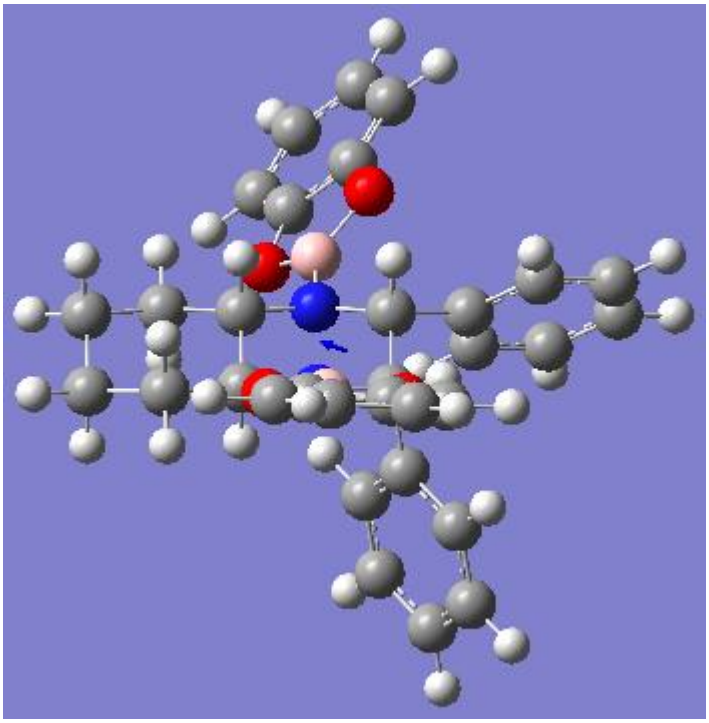
IB-*E*,*E*[1,1]^{DMF} (Intermediate dicoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
Dipole moment = 14.14

Figure 4.1 (cont'd)



TS-*E,E*[1,1]^{DMF} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E,E*-diimine **1** complex in DMF)
Dipole moment = 10.57

Figure 4.1 (cont'd)



P-*E,E*[1,1]^{DMF} (*N,N*-diborylated product **2c** from reductive coupling transition state **TS-*E,E*[1,1]^{DMF}** in DMF)
Dipole moment = 0.96

[a] Dipole moments and direction are indicated by blue arrows.

The strong influence solvent polarity has over reactivity and diastereoselectivity in this system offers insight into the relative energies of key intermediates and transition states, if their dipole moments are considered. Following the reaction pathway, they are: (1) Relatively non-polar: the substrate diimine and B_2cat_2; (2) very polar: the intermediate diimine-diboron Lewis acid-base complex, due to charge separation; (3) moderately polar: the transition state for reductive coupling, which should be less polar than the intermediate diimine-diboron Lewis acid-base complex, due to a partial shift of electron density from

the breaking B-B bond to the forming C-C bond. Our computational models were consistent with these predictions: intermediate dicoordinate diimine-diboron complexes **IB** had the highest dipole moments, and diimine **1** and B_2cat_2 substrates had the lowest dipole moments (Figure 4.1 and Table 4.2).

Given these considerations, if formation of diimine-diboron complexes **IA** or **IB** is exothermic, non-polar solvents should accelerate the reaction.

Table 4.1. Calculated energies (ΔG).[a]

Solvent	Product	Diimine (1) Geometry	$IA^{1,1}$	$IA^{1,2}$	$IB^{1,1}$	$IB^{1,2}$	$TS^{1,1}$	$TS^{1,2}$	$P^{1,1}$	$P^{1,2}$
MeOH	2b	*E*,*E*	-0.4	0.3	3.9	-4.1	18.1	16.6	-50.8	-28.7
DMF	2b	*E*,*E*	2.4	2.0	8.3	0.5	21.4	18.1	-49.6	-26.6
C_6H_6	2b	*E*,*E*	4.7	3.1	14.2	6.0	24.3	19.8	-50.9	-26.6
MeOH	2c	*Z*,*E*	-1.6	-0.5	2.9	-3.7	18.0	17.1	-58.2	-36.1
DMF	2c	*Z*,*E*	-0.5	1.5	6.9	0.4	20.5	18.8	-57.5	-34.8
C_6H_6	2c	*Z*,*E*	2.2	3.4	13.2	5.1	21.6	19.5	-59.4	-35.8
MeOH	2a	*E*,*Z*	6.7	6.8	5.6	-0.5	27.7	21.7	-51.6	-32.1
DMF	2a	*E*,*Z*	10.3	9.5	10.3	3.4	29.6	23.5	-50.0	-30.6
C_6H_6	2a	*E*,*Z*	9.3	11.5	14.4	8.6	30.7	25.6	-50.7	-31.4
MeOH	2b	*Z*,*Z*	5.5	7.6	5.3	-1.2	27.4	25.0	-50.8	-29.9
DMF	2b	*Z*,*Z*	8.0	9.7	9.5	2.0	30.1	26.5	-49.6	-29.0
C_6H_6	2b	*Z*,*Z*	8.2	12.2	11.4	6.7	30.6	27.2	-50.9	-29.8

[a] ΔG given in kcal/mol. 1,1-B_2cat_2 and *E*,*E*-diimine **1** were used as the ground state.

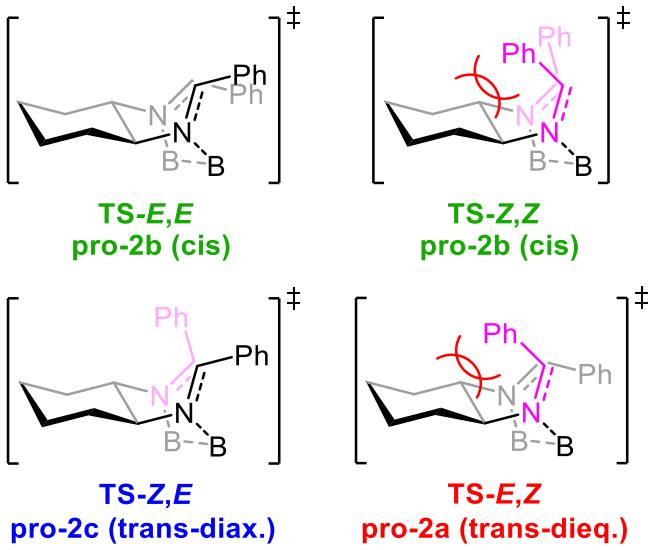
Table 4.2. Dipole moments.[a]

Solvent	Product	Diimine (1) Geometry	$IA^{1,1}$	$IA^{1,2}$	$IB^{1,1}$	$IB^{1,2}$	$TS^{1,1}$	$TS^{1,2}$	$P^{1,1}$	$P^{1,2}$
MeOH	2b	*E*,*E*	7.13	8.58	14.38	15.11	10.41	7.05	0.94	0.82
DMF	2b	*E*,*E*	7.11	8.41	14.14	14.65	10.57	7.07	0.96	0.90
C_6H_6	2b	*E*,*E*	5.83	6.85	10.91	11.39	7.87	5.42	0.71	0.93
MeOH	2c	*Z*,*E*	8.51	9.91	15.76	16.72	9.64	7.67	0.61	3.45
DMF	2c	*Z*,*E*	8.55	9.48	15.67	16.22	10.47	7.88	0.70	3.22
C_6H_6	2c	*Z*,*E*	7.53	8.26	12.55	13.17	8.46	6.63	0.69	2.56
MeOH	2a	*E*,*Z*	6.65	8.11	16.04	16.30	11.17	9.70	0.66	3.14
DMF	2a	*E*,*Z*	6.64	7.97	15.49	15.86	11.59	9.67	0.82	2.93
C_6H_6	2a	*E*,*Z*	5.22	6.62	12.47	13.11	9.22	8.05	0.67	2.36
MeOH	2b	*Z*,*Z*	7.99	9.61	17.69	18.43	9.68	8.02	0.94	3.34
DMF	2b	*Z*,*Z*	8.05	9.38	17.26	17.93	10.08	8.10	0.96	3.08
C_6H_6	2b	*Z*,*Z*	7.06	8.16	15.12	15.29	8.73	7.02	0.71	2.48

[a] ΔG given in kcal/mol. 1,1-B_2cat_2 and *E*,*E*-diimine **1** were used as the ground state.

However, experimental results indicate the reverse: *polar* solvents accelerate the reaction, implying that formation of diimine-diboron complexes is *endothermic* (or approximately thermoneutral). Consistent with these observations, our models indicated that all stereoisomers of dicoordinate diimine-1,1-B_2cat_2 (**IB^{1,1}**) and dicoordinate diimine-1,2-B_2cat_2 (**IB^{1,2}**) complexes were endothermic in both DMF and benzene (Table 4.1).

Figure 4.2 Concerted [3,3]-sigmatropic rearrangement transition states.[a]



[a] Each of these four possible E/Z diimine configurations in diimine-diboron reductive coupling transition states have two combinations with diboron isomers (1,1- and 1,2-), signified as TS-*E*/*Z*,*E*/*Z*[1,1]/[1,2].

Consistent with observed diastereoselectivity (as illustrated by Figure 4.2 and Table 4.3) we found that the relative energies of transition states **TS-*E*,*Z*** leading to *trans*-diequatorial product (**2a**) were dramatically higher than those leading to either *trans*-diaxial product (**2c**) via **TS-*Z*,*E***, or *cis*-product (**2b**) via **TS-*E*,*E***, suggesting that this mechanism is unlikely to explain the formation of **2a**. We also found that **TS-*Z*,*Z*** were even higher than those leading to the *trans*-diequatorial product (**2a**). Given these results, we decided to limit our discussion of transition states to **TS-*E*,*E*** and **TS-*Z*,*E***.

These results reveal the likely mechanistic scenarios for each set of conditions:

With polar aprotic solvents (using DMF to model conditions selective for *cis*-product **2b**), either: (1) *E*/*Z* isomerization is **slower** than reductive coupling, as **TS-*E*,*E*[1,1]** is higher energy than **TS-*Z*,*E*[1,1]**, or (2) diboron isomerization is faster than reductive coupling, as **TS-*E*,*E*[1,2]** is lower energy than **TS-*Z*,*E*[1,2]**, **TS-*E*,*E*[1,1]**, and **TS-*Z*,*E*[1,1].**

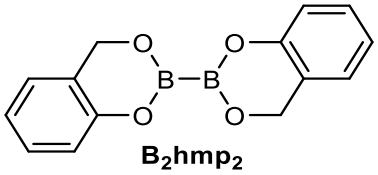
Table 4.3. Calculated transition state energies ($\Delta G^{\ddagger}$).[a]

Product	Transition State	1,1-B_2cat_2 (MeOH)	1,2-B_2cat_2 (MeOH)	1,1-B_2cat_2 (DMF)	1,2-B_2cat_2 (DMF)	1,1-B_2cat_2 (Benzene)	1,2-B_2cat_2 (Benzene)
2b	TS-*E*,*E*	19.6	**18.0**	21.4	**18.2**	24.3	19.8
2c	TS-*Z*,*E*	**19.4**	18.6	**20.5**	18.8	**21.6**	**19.5**
2a	TS-*E*,*Z*	29.1	23.2	29.6	23.5	30.7	25.6
2b	TS-*Z*,*Z*	28.8	26.5	30.1	26.5	30.6	27.2

[a] $\Delta G^{\ddagger}$ given in kcal/mol. 1,1-B_2cat_2 and *E*,*E*-diimine **1** were used as the ground state, unless the monocoordinate intermediates **IA** or dicoordinate intermediates **IB** were lower in energy. The lowest energy transition state for each solvent is highlighted in bold.

With non-polar aprotic solvents (using benzene to model conditions selective for *trans*-diaxial product **2a**), *E*/*Z* isomerization is **faster** than reductive coupling, and the relative rate of diboron isomerization is unclear, as **TS-*Z*,*E*[1,1]** and **TS-*Z*,*E*[1,2]** are *both* lower energy than **TS-*E*,*E*[1,1]** or **TS-*E*,*E*[1,2]**. However, since the energy gap between **TS-*Z*,*E*[1,2]** and **TS-*E*,*E*[1,2]** is *less* than the gap between **TS-*Z*,*E*[1,1]** and **TS-*E*,*E*[1,1]**, future work should consider means to reduce the rate of diboron isomerization. Future work should also include locating transition states for reductive coupling with B_2hmp_2 (Figure 4.3), which eliminates the aforementioned 1,2-diboron isomers from consideration. It is also expected that $A^{1,3}$ strain derived from steric clashes between the diimine and this bulkier diboron will further lower the energy of **TS-*Z*,*E*** relative to **TS-*E*,*E*,** consistent with the experimentally observed improvement in selectivity for **2c** with B_2hmp_2.

Figure 4.3. Structure of B_2hmp_2.

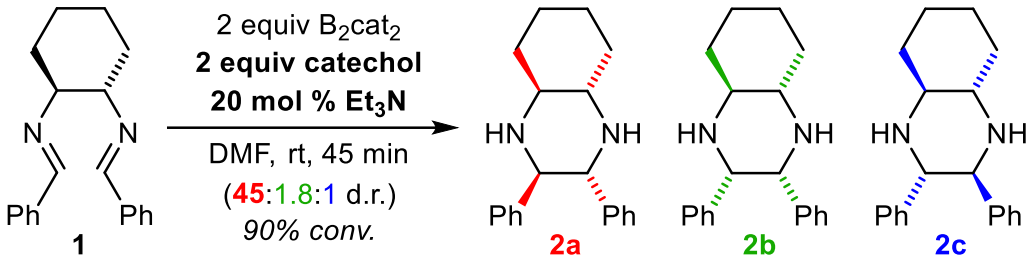


Investigation of the Ionic Mechanism.

Here we describe our preliminary investigations into the viability of the second proposed mechanism: Heterolytic B-B cleavage of a monocoordinate diimine-diboron complex, affording the thermodynamic product via an open chair-like transition state (Scheme 4.2a). The formation of the *trans*-diequatorial product (**2a**), consistent with our expectations, appears to be ruled out by our computational studies on the [3,3]-sigmatropic pathway that proceeds through concerted transition states. We found that transition states leading to **2a** were significantly higher in energy in MeOH, DMF, and benzene (Table 4.3), suggesting another mechanism is operative.

We postulated that catechol is present in solution (liberated by exchange with methanol) and a base is present (possibly **2a-c** themselves, generated by deborylation of the *N*,*N*-diboryl diamine product by methanol or catechol), and that both components may be necessary for the reaction to proceed, as deprotonation of catechol would provide access to anionic B_2cat_2 complexes such as the one shown in Scheme 4.2a.

Scheme 4.4. Reductive coupling of **1** with added base and catechol.[a]



[a] Conversion and diastereomeric ratio estimated by GC-MS analysis.

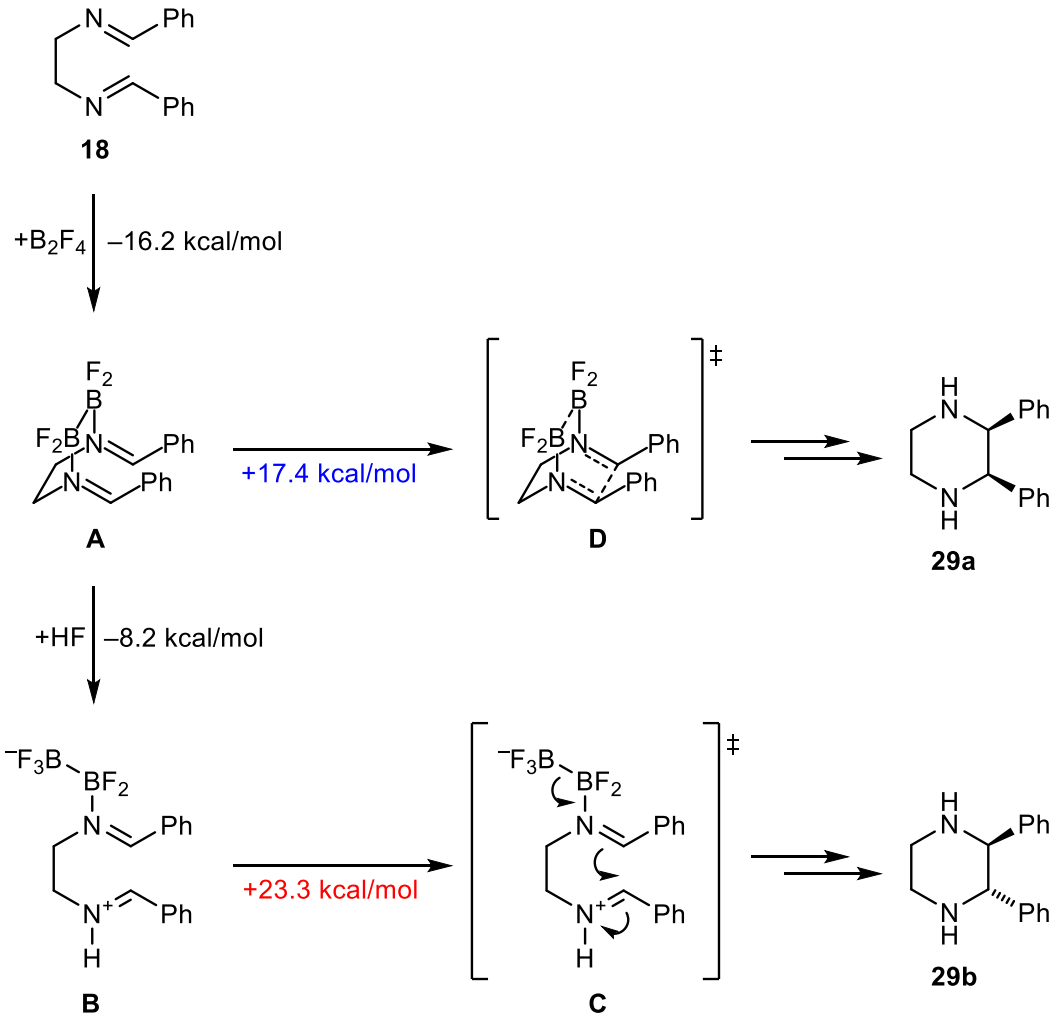
To test this hypothesis, the reductive coupling was again performed with two conditions changed: a) solvent was replaced with polar aprotic DMF, and b) both catechol and Et_3N were added prior to diimine **1** (Scheme 4.4). Intruigingly, unlike the system in DMF *without* catechol and Et_3N, which affords the *cis*-product (**2b**), this system was highly selective for the *trans*-diequatorial product **2a** (45:1.8:1, **2a**:**2b**:**2c** d.r.). Catechol was essential for the dramatic reversal in diastereoselectivity (without Et_3N, 9.6:3.4:1 **2a**:**2b**:**2c** d.r.), suggesting a change in the mechanism. Addition of Et_3N alone did not reverse selectivity (1:4.9:2.9 **2a**:**2b**:**2c** d.r.). It is currently unclear whether Et_3N plays the role of a catalyst or an initiator (due to generation of the basic diamine product throughout the reaction).

We developed a substantially simplified computational system (Scheme 4.5) to establish the theoretical framework (bond distances, angles, etc.) for finding transition states for the proposed ionic mechanism for the transformation shown in Scheme 4.4. We found that formation of diimine-B_2F_4 complex (**A**) from diimine **18** and B_2F_4 was exothermic (–16.2 kcal/mol), as was the reaction of **18** with HF to form ionized diimine-B_2F_5H complex (**B**) (–8.2 kcal/mol). Reductive cyclization of **18** to **29b** via open transition state (**C**) was found with a reasonable barrier (23.3 kcal/mol), while elimination of HF to

return to the initial diimine-B_2F_4 complex (**A**) and reductive cyclization to **29a** via concerted [3,3]-sigmatropic rearrangement transition state (**D**) had an overall barrier of 25.6 kcal/mol (higher by 2.3 kcal/mol), suggesting that in this system, the other pathway is preferred. However, given the influence solvent and the structure of the diboron has over product selectivity (Chapter 2), it is critical to note that this system is only a demonstration of the theoretical feasibility of the ionic mechanism (not evidence that it is operative), and is intended primarily to establish a framework for models of the experimental system.

Due to the difficulty of locating global minima in this experimental system (a consequence of the greatly increased conformational flexibility and atom count with the diimine, B_2cat_2, and added catechol), studies on the experimental system have thus far been unsuccessful.

Scheme 4.5. Modeling the ionic mechanism**.**



Conclusions.

We have used computational modeling to rationalize the divergent diastereochemical outcomes of diboron-mediated reductive coupling reactions of diimines (see Figure 4.4 for reaction coordinates for reactions in DMF and benzene for products **2b** and **2c**). It is unlikely that *trans*-diequatorial compound **2a** is formed via a concerted [3,3]-sigmatropic rearrangement of a diimine-diboron complex due to significant $A^{1,3}$ strain in these transition states. It is proposed that an alternative, ionic mechanism accounts for its selective synthesis in protic solvents.

Figure 4.4. Generalized reaction coordinates for reactions in DMF and benzene for products **2b** and **2c** (relative energies given in kcal/mol).

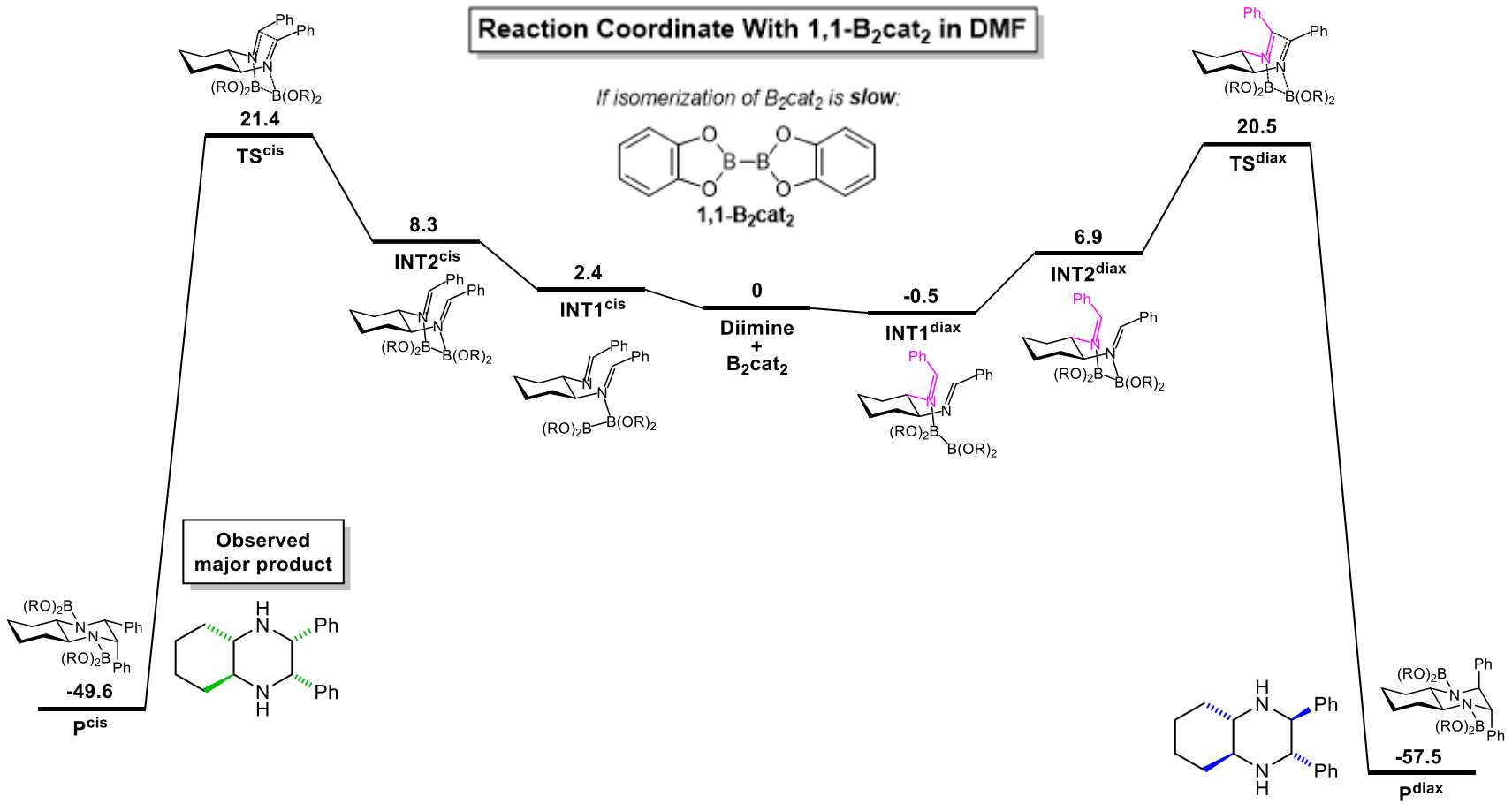


Figure 4.4 (cont'd)

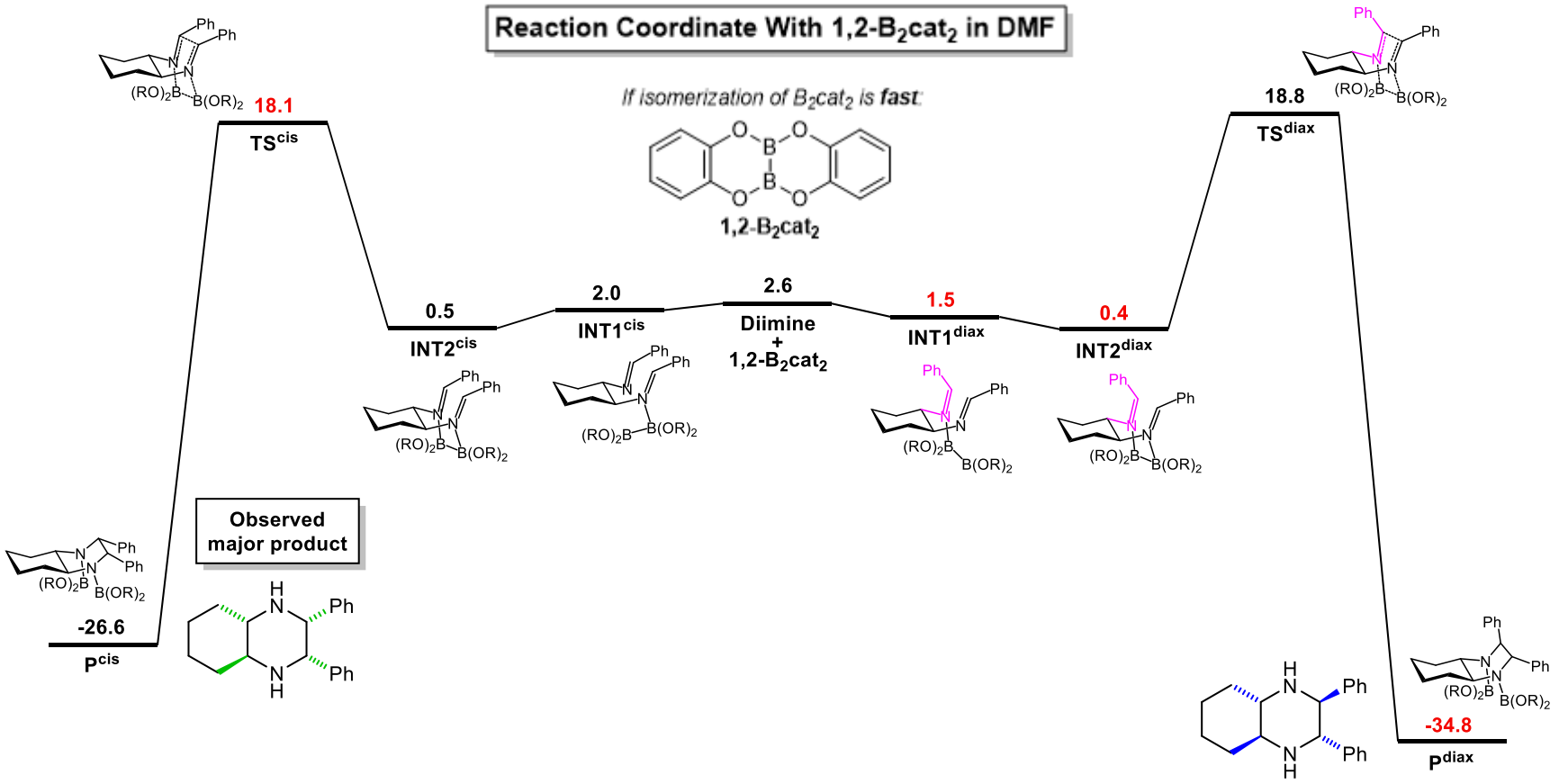


Figure 4.4 (cont'd)

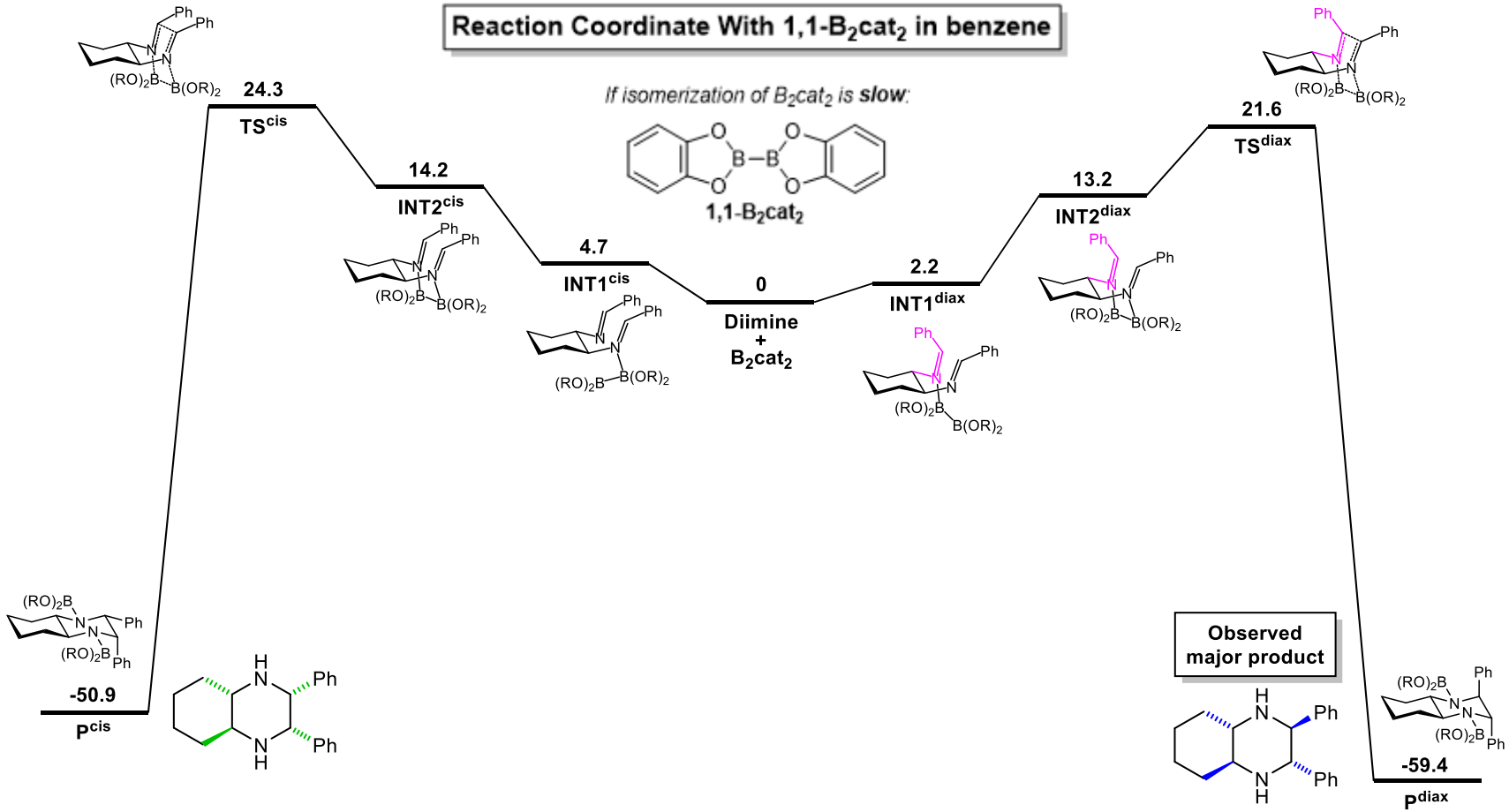
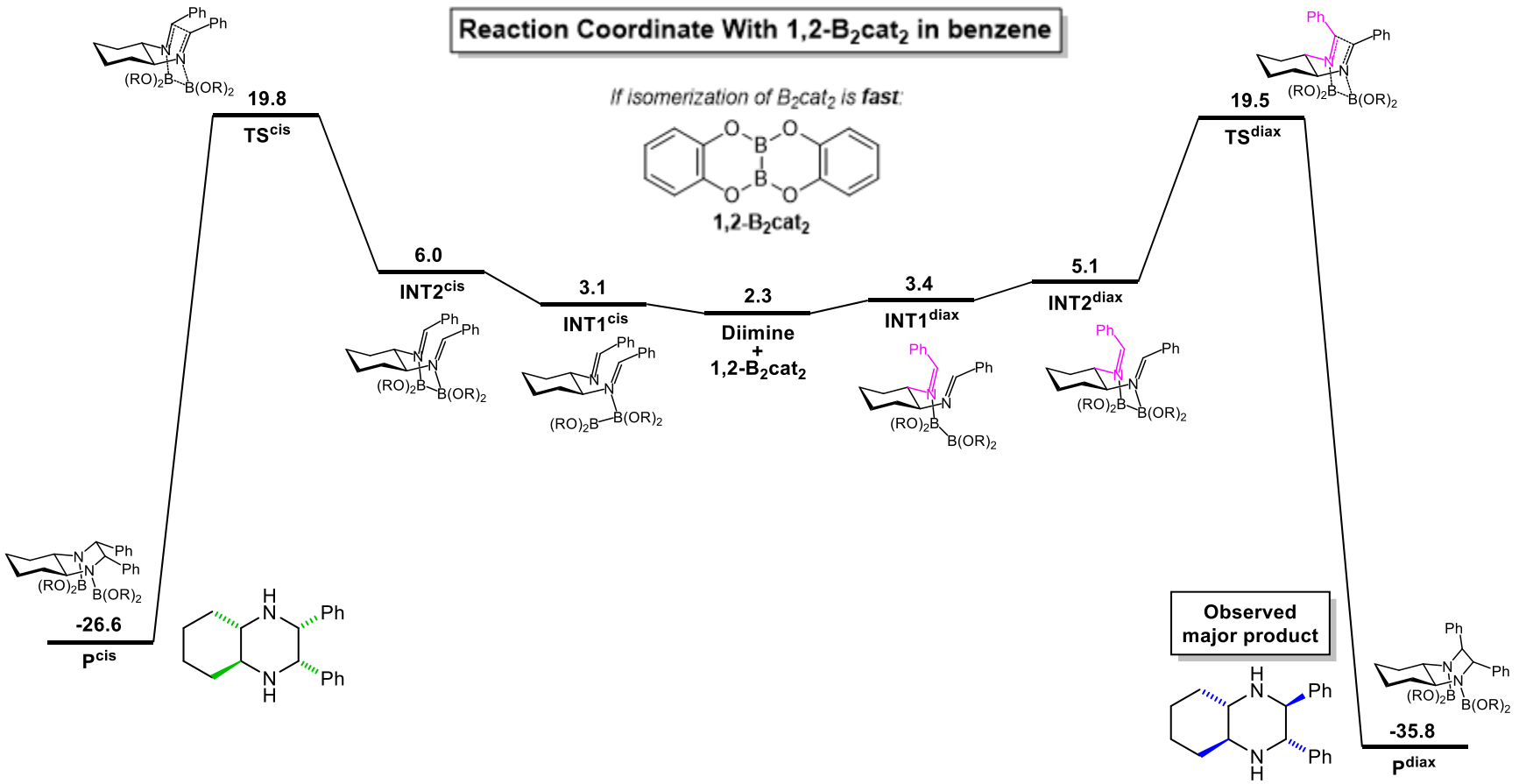


Figure 4.4 (cont'd)



Experimental Section.

Computational Methods. DFT quantum chemical calculations for diimine **1**, complexes, and transition states, were carried out using the Gaussian 16 software suite (Revision A.03)[7] using the M06-2X functional[8-10] and the 6-31G(d,p) basis set for all atoms. Structures were minimized until program default convergence limits were reached. Gaussian 16 was also utilized for solution-phase optimizations and calculation of harmonic vibrational frequencies (at 298.15 ˚K). The frequency calculations were performed to ensure that one imaginary frequency exists for all transition states and no imaginary frequencies exist for all local minima. Solvation effects were included by performing optimizations and frequency calculations with the SMD model for DMF and benzene. Diimine **3** (Scheme 4.5) complexes, and transition states used the 6-31+G(d,p) basis set with the SMD model for acetonitrile. Coordinates are provided in Appendix C for this chapter.

Reductive coupling of 1 with added base and catechol. B_2cat_2[11] (59.5 mg, 0.25 mmol) and catechol (27.5 mg, 0.25 mmol) were added to a 4 mL vial, followed by a stir bar and 0.25 mL DMF. Then, while stirring, Et_3N (3.5 µL, 0.025 mmol) was added, followed by diimine **1** (36.3 mg, 0.125 mmol), and the vial flushed with N_2 before sealing with a PTFE cap. After stirring the reaction mixture for 45 minutes, a sample was withdrawn (5-10 µL) and diluted with 1.0 mL MeOH. GC-MS analysis of this solution found 90% conversion of **1**, and that the reaction was highly selective for **2a** (45:1.8:1 **2a**:2b:2c d.r.).

Reductive coupling of 1 with added catechol. B_2cat_2[11] (59.5 mg, 0.25 mmol) and catechol (27.5 mg, 0.25 mmol) were added to a 4 mL vial, followed by a stir bar and 0.25

mL DMF. Then, while stirring, diimine **1** (36.3 mg, 0.125 mmol) was added, and the vial flushed with N_2 before sealing with a PTFE cap. After stirring the reaction mixture for 1.25 hours, a sample was withdrawn (5-10 µL) and diluted with 1.0 mL MeOH. GC-MS analysis of this solution found 98% conversion of **1**, and that the reaction was highly selective for **2b** (9.6:3.4:1 **2b**:2c:2a d.r.).

Reductive coupling of 1 with added base. B_2cat_2[11] (59.5 mg, 0.25 mmol) was added to a 4 mL vial, followed by a stir bar and 0.25 mL DMF. Then, while stirring, Et_3N (35 µL, 0.25 mmol) was added, followed by diimine **1** (36.3 mg, 0.125 mmol), and the vial flushed with N_2 before sealing with a PTFE cap. After stirring the reaction mixture for 1 hour, a sample was withdrawn (5-10 µL) and diluted with 1.0 mL MeOH. GC-MS analysis of this solution found 93% conversion of **1**, and that the reaction was selective for **2c** (1:4.9:2.9 2b:**2c**:2a d.r.).

APPENDICES

APPENDIX A: Bond Distances

Table 4.4. Bond distance change from intermediate complex to transition state (Å).[a]

Solvent	Product	Transition State	B-B^{1,1}	B-B^{1,2}	C-C^{1,1}	C-C^{1,2}	DM^{1,1}	DM^{1,2}
MeOH	2b	TS-*E*,*E*	0.27	0.35	-1.82	-1.85	-3.97	-8.06
DMF	2b	TS-*E*,*E*	0.27	0.35	-1.78	-1.77	-3.57	-7.58
C_6H_6	2b	TS-*E*,*E*	0.28	0.33	-1.67	-1.73	-3.03	-5.97
MeOH	2c	TS-*Z*,*E*	0.31	0.34	-1.53	-1.66	-6.12	-9.05
DMF	2c	TS-*Z*,*E*	0.29	0.33	-1.43	-1.58	-5.20	-8.34
C_6H_6	2c	TS-*Z*,*E*	0.24	0.33	-1.32	-1.70	-4.09	-6.54
MeOH	2a	TS-*E*,*Z*	0.26	0.26	-1.50	-1.96	-4.88	-6.60
DMF	2a	TS-*E*,*Z*	0.24	0.26	-1.29	-1.90	-3.90	-6.19
C_6H_6	2a	TS-*E*,*Z*	0.26	0.24	-1.37	-1.80	-3.24	-5.06
MeOH	2b	TS-*Z*,*Z*	0.33	0.34	-1.42	-1.38	-8.00	-10.42
DMF	2b	TS-*Z*,*Z*	0.32	0.34	-1.31	-1.33	-7.18	-9.83
C_6H_6	2b	TS-*Z*,*Z*	0.27	0.32	-0.78	-1.21	-6.39	-8.27

[a] DM = dipole moment.

Table 4.5. B-B bond distances (Å).

Solvent	Product	Diimine (1) Geometry	IA^{1,1}	IA^{1,2}	IB^{1,1}	IB^{1,2}	TS^{1,1}	TS^{1,2}	P^{1,1}	P^{1,2}
MeOH	2b	*E*,*E*	1.72	1.69	1.73	1.73	2.00	2.09	5.57	2.67
DMF	2b	*E*,*E*	1.72	1.69	1.73	1.75	2.00	2.09	5.56	2.67
C_6H_6	2b	*E*,*E*	1.72	1.69	1.73	1.75	2.01	2.08	5.57	2.67
MeOH	2c	*Z*,*E*	1.71	1.69	1.73	1.74	2.04	2.07	5.49	2.69
DMF	2c	*Z*,*E*	1.71	1.69	1.74	1.73	2.02	2.07	5.78	2.69
C_6H_6	2c	*Z*,*E*	1.71	1.69	1.74	1.72	1.98	2.05	5.48	2.69
MeOH	2a	*E*,*Z*	1.72	1.69	1.73	1.73	1.99	1.99	4.70	2.70
DMF	2a	*E*,*Z*	1.72	1.69	1.74	1.73	1.98	1.99	4.98	2.69
C_6H_6	2a	*E*,*Z*	1.72	1.69	1.73	1.73	1.99	1.98	5.07	2.69
MeOH	2b	*Z*,*Z*	1.71	1.69	1.74	1.72	2.07	2.06	5.57	2.70
DMF	2b	*Z*,*Z*	1.71	1.69	1.74	1.72	2.06	2.06	5.56	2.70
C_6H_6	2b	*Z*,*Z*	1.71	1.69	1.74	1.73	2.01	2.05	5.57	2.70

Table 4.6. C-C bond distances (Å).

Solvent	Product	Diimine (1) Geometry	IA^{1,1}	IA^{1,2}	IB^{1,1}	IB^{1,2}	TS^{1,1}	TS^{1,2}	P^{1,1}	P^{1,2}
MeOH	2b	*E*,*E*	3.82	4.00	4.67	4.51	2.85	2.66	1.55	1.61
DMF	2b	*E*,*E*	3.82	4.02	4.60	4.49	2.82	2.71	1.55	1.61
C_6H_6	2b	*E*,*E*	3.80	3.52	4.51	4.55	2.84	2.82	1.55	1.61
MeOH	2c	*Z*,*E*	4.47	4.04	4.59	4.43	3.06	2.77	1.54	1.59
DMF	2c	*Z*,*E*	4.59	3.77	4.57	4.41	3.13	2.83	1.54	1.59
C_6H_6	2c	*Z*,*E*	4.50	3.76	4.51	4.61	3.18	2.91	1.54	1.59
MeOH	2a	*E*,*Z*	3.96	4.08	4.31	4.47	2.82	2.51	1.54	1.59
DMF	2a	*E*,*Z*	3.97	4.08	4.16	4.45	2.87	2.55	1.56	1.59
C_6H_6	2a	*E*,*Z*	3.94	4.00	4.18	4.46	2.81	2.67	1.56	1.59
MeOH	2b	*Z*,*Z*	4.59	4.17	4.49	4.15	3.08	2.76	1.55	1.61
DMF	2b	*Z*,*Z*	4.59	4.12	4.46	4.15	3.16	2.82	1.55	1.61
C_6H_6	2b	*Z*,*Z*	4.63	4.08	4.02	4.11	3.24	2.90	1.55	1.61

APPENDIX B: Computational Coordinates

The below coordinates use the M06-2X functional and the 6-31g(d,p) basis set with the SMD model for methanol, dimethylformamide, benzene.

BC[1,1]^{MeOH} (1,1-B_2cat_2 in MeOH)
b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -812.5933855

Zero-point correction= 0.189451 (Hartree/Particle)
Thermal correction to Energy= 0.202147
Thermal correction to Enthalpy= 0.203091
Thermal correction to Gibbs Free Energy= 0.149421
Sum of electronic and ZPE= -812.403934
Sum of electronic and thermal Energies= -812.391238
Sum of electronic and thermal Enthalpies= -812.390294
Sum of electronic and thermal Free Energies= -812.443964

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.849	50.954	112.958

H,0.000165166,2.5158521927,-4.0888466982
C,0.0000950817,1.4317116791,-4.1022801999
C,-0.0000950817,-1.4317116791,-4.1022801999
C,0.0000463472,0.6953608417,-2.9338545125
C,0.0000464736,0.698766121,-5.2938892975
C,-0.0000464736,-0.698766121,-5.2938892975
C,-0.0000463472,-0.6953608417,-2.9338545125
H,0.0000812112,1.2305814511,-6.2395542787
H,-0.0000812112,-1.2305814511,-6.2395542787
H,-0.000165166,-2.5158521927,-4.0888466982
O,-0.0000722737,-1.1421241566,-1.630757619
O,0.0000722737,1.1421241566,-1.630757619
B,0.,0.,-0.8436190705
H,-0.000165166,2.5158521927,4.0888466982
C,-0.0000950817,1.4317116791,4.1022801999
C,0.0000950817,-1.4317116791,4.1022801999
C,-0.0000463472,0.6953608417,2.9338545125
C,-0.0000464736,0.698766121,5.2938892975
C,0.0000464736,-0.698766121,5.2938892975
C,0.0000463472,-0.6953608417,2.9338545125
H,-0.0000812112,1.2305814511,6.2395542787
H,0.0000812112,-1.2305814511,6.2395542787
H,0.000165166,-2.5158521927,4.0888466982

O,0.0000722737,-1.1421241566,1.630757619
O,-0.0000722737,1.1421241566,1.630757619
B,0.,0.,0.8436190705

BC[1,2]^{MeOH} (1,2-B_2cat_2 in MeOH)
b2cat2_1-2_meoh
M062X/6-31G(d,p)
E(RM062X) = -812.5909938

Zero-point correction= 0.189355 (Hartree/Particle)
Thermal correction to Energy= 0.201835
Thermal correction to Enthalpy= 0.202779
Thermal correction to Gibbs Free Energy= 0.150369
Sum of electronic and ZPE= -812.401639
Sum of electronic and thermal Energies= -812.389159
Sum of electronic and thermal Enthalpies= -812.388215
Sum of electronic and thermal Free Energies= -812.440625

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.653	51.665	110.307

O,-1.1930663301,1.4900300643,-0.0001878816
O,-1.1930696977,-1.4900202385,-0.0000029388
B,0.0000036021,0.8249662003,0.0000279868
B,-0.0000031129,-0.8249589352,-0.0000629173
O,1.1930693217,1.4900314893,-0.0001327603
O,1.193064597,-1.4900271811,0.0000554991
C,2.3352635366,-0.7060468186,0.0000681794
C,2.3352681609,0.706044287,-0.0000787296
C,3.5483286462,-1.3862634851,0.0001520855
C,3.5483337003,1.3862585251,-0.000130826
C,4.7552663177,-0.6962171074,0.000087386
H,3.5162168953,-2.4712121012,0.0002437633
C,4.7552692488,0.6962085133,-0.0000333981
H,3.5162236672,2.4712072112,-0.000230358
H,5.688872516,-1.248467988,0.0001456487
H,5.6888775707,1.2484556769,-0.0000680086
C,-2.3352696994,-0.7060388248,0.0000793902
C,-3.548333531,-1.386253392,0.0002050664
C,-2.3352660137,0.7060545922,-0.0000614761
C,-4.7552708547,-0.6962024544,0.00018842
H,-3.5162264111,-2.4712020329,0.0002882404
C,-3.5483299657,1.3862698673,-0.0000695099
C,-4.7552685331,0.6962211889,0.0000664943
H,-5.6888781675,-1.2484514027,0.0002778098

H,-3.5162221089,2.4712185247,-0.0001687361
H,-5.6888743547,1.2484728214,0.0000655707

BC[1,1]^{DMF} (1,1-B_2cat_2 in DMF)
cfc_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -812.596877

Zero-point correction= 0.189874 (Hartree/Particle)
Thermal correction to Energy= 0.202530
Thermal correction to Enthalpy= 0.203474
Thermal correction to Gibbs Free Energy= 0.150023
Sum of electronic and ZPE= -812.407003
Sum of electronic and thermal Energies= -812.394347
Sum of electronic and thermal Enthalpies= -812.393403
Sum of electronic and thermal Free Energies= -812.446854

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	127.089	50.808	112.497

H,-0.0618359336,2.5148634153,4.0875615353
C,-0.0352427789,1.4310720269,4.0995684179
C,0.0352427789,-1.4310720269,4.0995684179
C,-0.0170904348,0.69573955,2.929757997
C,-0.017375414,0.6986750944,5.2910107976
C,0.017375414,-0.6986750944,5.2910107976
C,0.0170904348,-0.69573955,2.929757997
H,-0.0305396861,1.2302413972,6.2366315423
H,0.0305396861,-1.2302413972,6.2366315423
H,0.0618359336,-2.5148634153,4.0875615353
O,0.0279257629,-1.141423706,1.6311987801
O,-0.0279257629,1.141423706,1.6311987801
B,0.,0.,0.8442614863
H,0.0618359336,2.5148634153,-4.0875615353
C,0.0352427789,1.4310720269,-4.0995684179
C,-0.0352427789,-1.4310720269,-4.0995684179
C,0.0170904348,0.69573955,-2.929757997
C,0.017375414,0.6986750944,-5.2910107976
C,-0.017375414,-0.6986750944,-5.2910107976
C,-0.0170904348,-0.69573955,-2.929757997
H,0.0305396861,1.2302413972,-6.2366315423
H,-0.0305396861,-1.2302413972,-6.2366315423
H,-0.0618359336,-2.5148634153,-4.0875615353
O,-0.0279257629,-1.141423706,-1.6311987801

O,0.0279257629,1.141423706,-1.6311987801
B,0.,0.,-0.8442614863

BC[1,2]^{DMF} (1,2-B_2cat_2 in DMF)
b2cat2_1-2_dmf
M062X/6-31G(d,p)
E(RM062X) = -812.5932204

Zero-point correction= 0.189554 (Hartree/Particle)
Thermal correction to Energy= 0.202065
Thermal correction to Enthalpy= 0.203010
Thermal correction to Gibbs Free Energy= 0.150443
Sum of electronic and ZPE= -812.403666
Sum of electronic and thermal Energies= -812.391155
Sum of electronic and thermal Enthalpies= -812.390211
Sum of electronic and thermal Free Energies= -812.442777

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.798	51.609	110.636

O,-1.1933532468,-1.4885184996,0.0003087531
O,-1.1933536778,1.4886129388,0.0000989657
B,0.0000197107,-0.8255900125,-0.0002383572
B,-0.0000020607,0.8256636318,-0.0000331686
O,1.193344285,-1.4885744219,-0.0000794324
O,1.1933653491,1.4886192642,-0.0001876347
C,2.3324763166,0.7065314113,-0.000241635
C,2.3324800371,-0.706491262,-0.0000994098
C,3.5468811956,1.385861238,-0.0002709578
C,3.5468586095,-1.3858596664,-0.000031594
C,4.7537534375,0.6962492212,-0.0001704272
H,3.5165211112,2.4706364698,-0.0003268166
C,4.7537473623,-0.6962679343,-0.0000897307
H,3.5164697445,-2.4706318884,0.000047283
H,5.6872508681,1.2485170449,-0.0001779318
H,5.6872381159,-1.2485461683,-0.0000408498
C,-2.3325034861,0.7065614792,-0.0001521461
C,-3.5468798823,1.385908741,-0.0003408229
C,-2.332484721,-0.7064765057,0.0000212019
C,-4.7537650256,0.6962954731,-0.0003681191
H,-3.5165168325,2.4706825947,-0.0004344742
C,-3.5468701135,-1.3858181037,0.0000036256
C,-4.7537566559,-0.6962131324,-0.0001946158
H,-5.6872556366,1.2485750971,-0.0005145222
H,-3.5165120176,-2.470593919,0.0001648347

H,-5.6872387867,-1.2485070911,-0.0002210181

BC[1,1]^{benzene} (1,1-B_2cat_2 in benzene)
cfc_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -812.5955254

Zero-point correction= 0.190125 (Hartree/Particle)
Thermal correction to Energy= 0.202766
Thermal correction to Enthalpy= 0.203710
Thermal correction to Gibbs Free Energy= 0.150377
Sum of electronic and ZPE= -812.405401
Sum of electronic and thermal Energies= -812.392760
Sum of electronic and thermal Enthalpies= -812.391816
Sum of electronic and thermal Free Energies= -812.445148

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	127.237	50.746	112.248

H,-0.1101493422,2.5117991696,4.084255457
C,-0.0627929433,1.4291518907,4.098448836
C,0.0627929433,-1.4291518907,4.098448836
C,-0.0305386962,0.6952521939,2.9284714958
C,-0.0307363149,0.6979058823,5.2892385344
C,0.0307363149,-0.6979058823,5.2892385344
C,0.0305386962,-0.6952521939,2.9284714958
H,-0.0540751362,1.2285799709,6.2349611256
H,0.0540751362,-1.2285799709,6.2349611256
H,0.1101493422,-2.5117991696,4.084255457
O,0.0500088093,-1.1400737832,1.630976836
O,-0.0500088093,1.1400737832,1.630976836
B,0.,0.,0.8444972095
H,0.1101493422,2.5117991696,-4.084255457
C,0.0627929433,1.4291518907,-4.098448836
C,-0.0627929433,-1.4291518907,-4.098448836
C,0.0305386962,0.6952521939,-2.9284714958
C,0.0307363149,0.6979058823,-5.2892385344
C,-0.0307363149,-0.6979058823,-5.2892385344
C,-0.0305386962,-0.6952521939,-2.9284714958
H,0.0540751362,1.2285799709,-6.2349611256
H,-0.0540751362,-1.2285799709,-6.2349611256
H,-0.1101493422,-2.5117991696,-4.084255457
O,-0.0500088093,-1.1400737832,-1.630976836
O,0.0500088093,1.1400737832,-1.630976836
B,0.,0.,-0.8444972095

BC[1,2]^{benzene} (1,2-B_2cat_2 in benzene)
b2cat2_1-2_benzene
M062X/6-31G(d,p)
E(RM062X) = -812.5923852

Zero-point correction= 0.189856 (Hartree/Particle)
Thermal correction to Energy= 0.202332
Thermal correction to Enthalpy= 0.203276
Thermal correction to Gibbs Free Energy= 0.150838
Sum of electronic and ZPE= -812.402529
Sum of electronic and thermal Energies= -812.390053
Sum of electronic and thermal Enthalpies= -812.389109
Sum of electronic and thermal Free Energies= -812.441547

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.965	51.541	110.366

O,-1.1937588339,-1.4873268215,0.0002946201
O,-1.1937524673,1.4874063009,0.0000875264
B,0.000021909,-0.8267927043,-0.0002131784
B,-0.0000054656,0.8268568985,-0.0000430018
O,1.1937443564,-1.4873882361,-0.0000620655
O,1.1937634658,1.487424734,-0.0001816513
C,2.3327027581,0.7062545936,-0.0002430059
C,2.3327107525,-0.7062167587,-0.0000850779
C,3.5466555106,1.3853166535,-0.0002794274
C,3.5466398408,-1.3853114682,-0.0000127243
C,4.7527577883,0.6959493856,-0.0001716008
H,3.5125832537,2.4695585801,-0.0003428068
C,4.7527549829,-0.695960681,-0.0000899727
H,3.5125402969,-2.4695509508,0.0000791254
H,5.6863743313,1.2476668277,-0.0001913554
H,5.6863677521,-1.2476836841,-0.0000342655
C,-2.3327322046,0.7062812267,-0.0001931245
C,-3.5466485968,1.3853647838,-0.0003397091
C,-2.3327162333,-0.7062083194,-0.000040496
C,-4.7527652844,0.6959943959,-0.0003587594
H,-3.5125779577,2.4696057117,-0.0004010677
C,-3.5466488642,-1.3852765054,-0.0000245271
C,-4.7527618141,-0.6959044204,-0.0001890348
H,-5.6863747406,1.2477233266,-0.0004737354
H,-3.5125914731,-2.4695190424,0.0001311336
H,-5.6863690632,-1.2476378264,-0.000190818

***E,E*-(1)^{MeOH}** (*E,E*-diimine **1** in MeOH)
cydiimph2_EE_meoh
M062X/6-31G(d,p)
E(RM062X) = -884.5343065

Zero-point correction= 0.378938 (Hartree/Particle)
Thermal correction to Energy= 0.397837
Thermal correction to Enthalpy= 0.398782
Thermal correction to Gibbs Free Energy= 0.328304
Sum of electronic and ZPE= -884.155368
Sum of electronic and thermal Energies= -884.136469
Sum of electronic and thermal Enthalpies= -884.135525
Sum of electronic and thermal Free Energies= -884.206002

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	249.647	74.440	148.332

C,4.9125242396,0.6961166937,-0.3156333221
C,3.6514440834,1.4642558439,0.0760221424
C,2.3776438973,0.7095419593,-0.3105335298
C,2.3776442589,-0.7095401833,0.3105326245
C,3.6514446254,-1.4642535841,-0.0760234089
C,4.9125245989,-0.6961139555,0.3156316863
H,3.6376133901,1.6246732016,1.1621118504
H,3.6327975245,2.4529215074,-0.3952085259
H,4.9566515658,0.5979822368,-1.4085829334
H,5.8007264264,1.2582039944,-0.0092869951
H,2.3370590996,-0.5852178898,1.40573541
H,3.6327985754,-2.4529192568,0.3952072656
H,3.6376136755,-1.6246709593,-1.162113112
H,4.9566522084,-0.5979794803,1.4085812844
H,5.8007269126,-1.2582009138,0.0092850989
H,2.3370584769,0.5852196494,-1.4057363031
N,1.2168873687,1.4296995052,0.1853285839
N,1.2168878661,-1.4296981536,-0.1853291724
C,0.2039098763,1.5034877846,-0.5792280618
H,0.2126184963,1.0885049744,-1.597777685
C,0.2039106527,-1.5034868933,0.5792277991
H,0.2126195598,-1.0885044686,1.5977775765
C,-1.0658788504,2.1314626845,-0.1629474282
C,-2.1355051289,2.1526332749,-1.0622692795
C,-1.2258666944,2.6898803273,1.1116053493
C,-3.350739981,2.7278866791,-0.6982881626
H,-2.0102958963,1.7137712678,-2.0490599387
C,-2.437693635,3.2644934,1.4732217914

H,-0.3928656681,2.6662918587,1.8072295268
C,-3.50244995,3.2849249641,0.5692154925
H,-4.1770197103,2.740565355,-1.4022301567
H,-2.5575835505,3.6973593976,2.4616848865
H,-4.4484009816,3.7344507768,0.8555686659
C,-1.065877707,-2.1314629595,0.1629478055
C,-2.1355035318,-2.1526344704,1.0622701725
C,-1.2258656698,-2.6898807751,-1.1116048807
C,-3.3507380662,-2.7278889144,0.6982896393
H,-2.0102942072,-1.7137723384,2.0490607644
C,-2.43769229,-3.2644948938,-1.4732207369
H,-0.3928650036,-2.6662915936,-1.8072294624
C,-3.5024481589,-3.2849273586,-0.569213932
H,-4.1770174511,-2.7405682882,1.4022320251
H,-2.5575823081,-3.6973610122,-2.4616837673
H,-4.4483989385,-3.7344539937,-0.8555666464

***E,Z*-(1)^{MeOH}** (*E,Z*-diimine **1** in MeOH)
cydiimph2_EZ_meoh
M062X/6-31G(d,p)
E(RM062X) = -884.5265055

Zero-point correction= 0.379505 (Hartree/Particle)
Thermal correction to Energy= 0.398134
Thermal correction to Enthalpy= 0.399078
Thermal correction to Gibbs Free Energy= 0.330344
Sum of electronic and ZPE= -884.147001
Sum of electronic and thermal Energies= -884.128372
Sum of electronic and thermal Enthalpies= -884.127428
Sum of electronic and thermal Free Energies= -884.196161

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	249.833	74.165	144.662

C,2.0936070703,-0.5274269693,0.4162908905
C,4.262980688,-1.5109731306,-0.4487648556
C,2.0631562244,-2.4526136747,-1.2204819219
C,3.5229432289,-2.7701145839,-0.89988508
C,1.3494489628,-1.8046133476,-0.0324401481
C,3.554145545,-0.8642835481,0.740543292
H,4.3045225846,-0.7966942095,-1.2818592428
H,2.0106423262,-1.7608567898,-2.0716879914
H,3.5653163961,-3.5207789838,-0.0994283599
H,1.3543457886,-2.4980785715,0.8258936522
H,3.5680223932,-1.5475759167,1.5997823715

H,2.074553038,0.1931706193,-0.4127870733
H,5.2975124392,-1.7483509349,-0.1800808817
H,1.5196330981,-3.3590662357,-1.5081697623
H,4.0099648109,-3.209958748,-1.7762474548
H,4.0667455528,0.0531609197,1.0493660817
N,-0.0081778308,-1.4539146396,-0.4135318116
N,1.4693173021,-0.0283039353,1.6313479543
C,0.8553745419,1.0854770168,1.6852808316
H,0.4885730815,1.3714747248,2.6775752275
C,-0.9363848119,-1.6968405195,0.4202349248
H,-0.7382110124,-2.200974495,1.3772452659
C,-2.3415294759,-1.315430145,0.1776917974
C,-5.014252955,-0.5981161147,-0.2067205635
C,-2.7334838221,-0.661990159,-0.9980765455
C,-3.2985001789,-1.6058458553,1.1543300358
C,-4.631066619,-1.2486817394,0.9637077187
C,-4.0630870129,-0.3062307422,-1.1870343417
H,-1.9887913054,-0.4438472261,-1.7575192582
H,-2.9922076021,-2.1124693592,2.0662070074
H,-5.3680930867,-1.4774877296,1.7271000004
H,-4.3629387673,0.1995856042,-2.0996995295
H,-6.0522992099,-0.3180078441,-0.3579615458
C,0.5748449789,2.1170180665,0.6474314302
C,0.0015831752,4.1893968201,-1.1483720082
C,0.1732430132,1.8266227678,-0.6627607151
C,0.6544114572,3.4557330372,1.0529631157
C,0.3860194904,4.4864803811,0.1584215272
C,-0.1135177512,2.8604134964,-1.5512171192
H,0.0605165047,0.7932028997,-0.9757556557
H,0.9342415638,3.6845002794,2.0784260307
H,0.4654024379,5.5193617529,0.4828714947
H,-0.4330069874,2.6244908121,-2.5618802202
H,-0.219346265,4.9911749502,-1.8463155643

***E,E*-(1)^{DMF}** (*E,E*-diimine **1** in DMF)
cydiimph2_EE_dmf
M062X/6-31G(d,p)
E(RM062X) = -884.5337399

Zero-point correction= 0.379075 (Hartree/Particle)
Thermal correction to Energy= 0.397991
Thermal correction to Enthalpy= 0.398935
Thermal correction to Gibbs Free Energy= 0.328306
Sum of electronic and ZPE= -884.154665
Sum of electronic and thermal Energies= -884.135749

Sum of electronic and thermal Enthalpies= -884.134805
Sum of electronic and thermal Free Energies= -884.205433

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	249.743	74.382	148.651

C,4.7758083554,-0.7039236572,0.2982286775
C,3.5130953552,-1.4644197849,-0.1060689076
C,2.2457544361,-0.7077373469,0.303008107
C,2.2457532623,0.7077414365,-0.3030082157
C,3.5130930344,1.4644258641,0.1060687017
C,4.7758072489,0.7039317212,-0.2982287951
H,3.4941738739,-1.6051555281,-1.1947607274
H,3.4923401261,-2.4605664669,0.3487650106
H,4.8223316118,-0.6327129703,1.3929881618
H,5.6633497247,-1.257782262,-0.0241224501
H,2.2208305426,0.5998210161,-1.401181193
H,3.4923362756,2.4605724835,-0.3487653114
H,3.4941713087,1.6051617172,1.1947604997
H,4.8223306725,0.6327211282,-1.3929882735
H,5.6633476825,1.2577917603,0.0241224298
H,2.2208316051,-0.5998169694,1.4011810928
N,1.0793330969,-1.4239110845,-0.1847473708
N,1.0793309061,1.4239133292,0.1847473417
C,0.2076720084,-1.7816133579,0.6670759781
H,0.3232237566,-1.5685815501,1.7399795277
C,0.2076690407,1.7816140952,-0.6670758597
H,0.3232209489,1.5685822017,-1.7399793944
C,-1.0216184252,-2.5087409661,0.2900774754
C,-1.9177791921,-2.8909236526,1.2919721517
C,-1.3064296337,-2.8215474628,-1.0451595345
C,-3.0849955263,-3.5789086151,0.9682410332
H,-1.695526321,-2.6466660483,2.3277597335
C,-2.4709282022,-3.5069210971,-1.3672160773
H,-0.6060743539,-2.5206186356,-1.8179945135
C,-3.3624042566,-3.8874939944,-0.3612939735
H,-3.7758028139,-3.8729668265,1.7521055104
H,-2.6883214189,-3.7468974879,-2.4034212
H,-4.2714796742,-4.423291235,-0.6165998773
C,-1.0216226585,2.5087394249,-0.290077287
C,-1.9177842163,2.8909203566,-1.2919718907
C,-1.3064343201,2.8215455747,1.0451597253
C,-3.0850018244,3.5789032373,-0.968240689
H,-1.6955311563,2.6466630879,-2.3277595127
C,-2.4709340643,3.5069171055,1.3672164082

H,-0.6060783207,2.520618116,1.8179945936
C,-3.3624108962,3.8874882224,0.3612942909
H,-3.7758097256,3.8729600519,-1.7521051363
H,-2.6883275747,3.7468932592,2.4034215128
H,-4.2714872984,4.4232838105,0.616600227

***E,Z*-(1)^{DMF}** (*E,Z*-diimine **1** in DMF)
cydiimph2_ZE_dmf
M062X/6-31G(d,p)
E(RM062X) = -884.5260424

Zero-point correction= 0.379399 (Hartree/Particle)
Thermal correction to Energy= 0.398083
Thermal correction to Enthalpy= 0.399027
Thermal correction to Gibbs Free Energy= 0.329614
Sum of electronic and ZPE= -884.146644
Sum of electronic and thermal Energies= -884.127960
Sum of electronic and thermal Enthalpies= -884.127016
Sum of electronic and thermal Free Energies= -884.196428

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	249.801	74.205	146.091

C,-0.5443266139,1.5753111893,1.0370017163
C,-0.6914767658,2.5272420542,3.3790439375
C,-1.0454354774,0.0657512136,2.9984489201
C,-1.430212594,1.2744859309,3.8507917715
C,-1.3043929524,0.318076085,1.5115629305
C,-0.9492938783,2.7809198243,1.8943993158
H,0.3860640126,2.3959363958,3.5444935779
H,0.021657552,-0.1583818514,3.1278614366
H,-2.5125427005,1.443277938,3.7743768331
H,-2.3789099661,0.5107230382,1.3490610407
H,-2.0161082602,2.9792070564,1.7274339898
H,0.5321965433,1.3969322818,1.1654289461
H,-1.0008663245,3.3990109944,3.9645654743
H,-1.6019349747,-0.8252317094,3.3085290088
H,-1.2117324599,1.0724770168,4.9043134174
H,-0.398450511,3.661294415,1.5462374127
N,-0.8547334937,-0.8272891306,0.7393609187
N,-0.9268214189,1.8579996677,-0.3373180722
C,-0.1027326728,1.8202906063,-1.3060514665
H,-0.503015407,2.127014266,-2.2789440541
C,-1.6255291228,-1.2680892397,-0.1697668868
H,-2.6169619281,-0.8283058525,-0.3517952536

C,-1.2471169945,-2.3868394439,-1.0558820531
C,-0.5767048253,-4.4779445998,-2.7827396345
C,-0.0246758716,-3.0558153145,-0.9107627376
C,-2.1284046744,-2.7765897359,-2.0683262593
C,-1.7946229748,-3.8184041705,-2.9303487327
C,0.3067088814,-4.0954684376,-1.7706139217
H,0.652412461,-2.755001788,-0.1170201725
H,-3.0768172106,-2.2568316548,-2.178648849
H,-2.4834475453,-4.1141258583,-3.7152926679
H,1.2545837867,-4.6118157694,-1.654664336
H,-0.3141743511,-5.2904384434,-3.4532152978
C,1.3446812018,1.4684215522,-1.3557041178
C,4.0717582932,0.8899626348,-1.6200409157
C,1.9044146328,0.3774730386,-0.6787369538
C,2.1598749252,2.2432076554,-2.1906161832
C,3.5181531155,1.9673102997,-2.3103465245
C,3.26096371,0.0921999083,-0.8147759051
H,1.2713052463,-0.2584227076,-0.0667286437
H,1.7212762451,3.0702455744,-2.7434086087
H,4.1416729825,2.5845766179,-2.9494956674
H,3.6843496601,-0.7603183539,-0.2924631306
H,5.1293687102,0.6659668163,-1.7192035819

***E,E*-(1)$^{\text{benzene}}$** (*E*,*E*-diimine **1** in benzene)
cydiimph2_EE_benzene
M062X/6-31G(d,p)
E(RM062X) = -884.5340406

Zero-point correction= 0.379381 (Hartree/Particle)
Thermal correction to Energy= 0.398259
Thermal correction to Enthalpy= 0.399203
Thermal correction to Gibbs Free Energy= 0.328976
Sum of electronic and ZPE= -884.154659
Sum of electronic and thermal Energies= -884.135782
Sum of electronic and thermal Enthalpies= -884.134838
Sum of electronic and thermal Free Energies= -884.205065

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	249.911	74.316	147.806

C,4.8218430184,-0.6944317495,0.3199343352
C,3.5600659875,-1.466265207,-0.064166903
C,2.2874966858,-0.7038073909,0.3163589062
C,2.2874955803,0.7038115769,-0.3163590086
C,3.5600637038,1.466271372,0.0641667662

C,4.8218419266,0.6944398789,-0.3199345104
H,3.5410573421,-1.6392431158,-1.1478514537
H,3.5384123657,-2.450508234,0.4153054796
H,4.8678782599,-0.5887280166,1.4120330382
H,5.7105129838,-1.2576833182,0.0177685927
H,2.2476421176,0.5683817978,-1.4116039015
H,3.5384085339,2.4505143655,-0.4153056148
H,3.5410548214,1.6392492511,1.1478513178
H,4.8678773006,0.5887362182,-1.4120332149
H,5.7105110226,1.2576928319,-0.017768794
H,2.2476430462,-0.5683776695,1.4116038016
N,1.1322726722,-1.4306412176,-0.17493245
N,1.1322704507,1.4306436157,0.1749323814
C,0.1838637736,-1.6621939259,0.635744264
H,0.226466141,-1.339338589,1.6872748235
C,0.1838611578,1.6621948319,-0.6357442981
H,0.2264639001,1.3393393661,-1.6872748035
C,-1.0462714162,-2.3720919649,0.2319761069
C,-2.0585737809,-2.5772545299,1.1716448705
C,-1.2145605793,-2.8410526649,-1.0761189427
C,-3.2278564587,-3.2426661352,0.8133130703
H,-1.9273125939,-2.2102228698,2.1864904054
C,-2.3803109836,-3.505087756,-1.4323318237
H,-0.4182948667,-2.6740380659,-1.794468075
C,-3.3893783563,-3.7071922464,-0.488676064
H,-4.0109929144,-3.3973205875,1.5486353456
H,-2.5075951045,-3.8681685257,-2.4474095522
H,-4.2998133746,-4.2267106824,-0.7709554744
C,-1.0462753475,2.3720904965,-0.2319759752
C,-2.0585782012,2.5772511715,-1.1716446296
C,-1.2145652676,2.8410508258,1.0761191055
C,-3.2278620956,3.2426605589,-0.8133126924
H,-1.9273164172,2.2102197934,-2.1864901887
C,-2.3803168946,3.5050837024,1.4323321284
H,-0.418299166,2.6740377185,1.7944681545
C,-3.3893847414,3.7071863162,0.488676479
H,-4.0109989191,3.3973135605,-1.54863488
H,-2.5076015953,3.8681641951,2.4474098821
H,-4.2998207168,4.2267030183,0.770955996

***E,Z*-(1)$^{\text{benzene}}$** (*E*,*Z*-diimine **1** in benzene)
cydiimph2_ZE_benzene
M062X/6-31G(d,p)
E(RM062X) = -884.5266089
Zero-point correction= 0.379932 (Hartree/Particle)
Thermal correction to Energy= 0.398551

Thermal correction to Enthalpy= 0.399495
Thermal correction to Gibbs Free Energy= 0.330768
Sum of electronic and ZPE= -884.146677
Sum of electronic and thermal Energies= -884.128058
Sum of electronic and thermal Enthalpies= -884.127114
Sum of electronic and thermal Free Energies= -884.195841

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	250.095	74.061	144.648

C,1.8104221567,-1.1158623515,0.3776759321
C,3.5278475406,-2.7314001161,-0.5502699796
C,1.116650754,-2.9263556859,-1.2427312222
C,2.4121841755,-3.6895764488,-0.9690484552
C,0.6878124248,-2.0901782884,-0.0344359439
C,3.1013562792,-1.8960373239,0.6566899801
H,3.7660608605,-2.0648375745,-1.3897597262
H,1.2516649008,-2.2491034601,-2.0959597681
H,2.2426208061,-4.4189531394,-0.1658332482
H,0.5068688153,-2.7520953119,0.8307069452
H,2.9278248085,-2.5451356027,1.5244747334
H,1.9883419223,-0.4228222071,-0.4566049622
H,4.4423947936,-3.2854789994,-0.3156771209
H,0.3039677315,-3.6117464945,-1.5053392588
H,2.7059819702,-4.2580692327,-1.8572239304
H,3.8860419049,-1.1867633953,0.9400232588
N,-0.5016857579,-1.3316368861,-0.3744851401
N,1.4155552038,-0.4560349669,1.6104676445
C,1.2348675736,0.7992703605,1.6921462074
H,1.0101658529,1.1776060776,2.6960920767
C,-1.4741355094,-1.3505020036,0.4414704594
H,-1.4343780174,-1.9334223963,1.3740944615
C,-2.7174238516,-0.5893630895,0.2100241361
C,-5.0792580063,0.8491093612,-0.1735487856
C,-2.9232638477,0.1222131252,-0.9779500372
C,-3.7053978833,-0.5784761183,1.1972531238
C,-4.8825180861,0.1400434138,1.008000871
C,-4.0980984292,0.837290234,-1.1664445749
H,-2.154216964,0.0949807786,-1.7434858415
H,-3.5455269262,-1.133541531,2.1181835048
H,-5.6442340013,0.1463238564,1.7810136066
H,-4.2546213904,1.3871071118,-2.0891860238
H,-5.9966560351,1.4094977193,-0.3241021499
C,1.3109335707,1.8729823693,0.6606321267
C,1.4609718095,4.0057354933,-1.1452882396

C,0.7509435643,1.7564134004,-0.6171284448
C,1.9158129273,3.0795224741,1.0314332495
C,2.0050261023,4.1350212251,0.1307841817
C,0.8272884465,2.8206613155,-1.511312731
H,0.2364613802,0.8407560634,-0.8953214605
H,2.323887072,3.1837459151,2.0336971361
H,2.4889770128,5.0604020241,0.4266555101
H,0.3834492889,2.7245115703,-2.4973665792
H,1.5201640564,4.8310397351,-1.8479305215

IA-*E*,*E*[1,1]^{MeOH} (Intermediate monocoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in MeOH)
E-coord_cydiimph2_EE_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1559979

Zero-point correction= 0.570914 (Hartree/Particle)
Thermal correction to Energy= 0.603263
Thermal correction to Enthalpy= 0.604207
Thermal correction to Gibbs Free Energy= 0.505323
Sum of electronic and ZPE= -1696.585084
Sum of electronic and thermal Energies= -1696.552735
Sum of electronic and thermal Enthalpies= -1696.551791
Sum of electronic and thermal Free Energies= -1696.650675

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.553	130.327	208.121

C,1.2402954659,-2.262922831,1.0735257707
C,1.5548442559,-4.7702872346,1.0136953087
C,-0.4584876179,-3.744713623,-0.1035864096
C,0.0813636177,-4.9638773372,0.6499879598
C,-0.2464961224,-2.4947589761,0.7488351816
C,1.7615841053,-3.4914663885,1.8277919457
H,2.1482248755,-4.7116764132,0.0914354157
H,0.068623585,-3.653348767,-1.0571780746
H,-0.503640772,-5.1145660106,1.5667428025
H,-0.7488708719,-2.6636949938,1.7085560122
H,1.2324921892,-3.5655603775,2.7869393303
H,1.8022826841,-2.1553450877,0.137456891
H,1.9241520585,-5.6327020175,1.5776603923
H,-1.5261333433,-3.8574085771,-0.3201924485
H,-0.0465396928,-5.8603348905,0.0355500077
H,2.822525771,-3.339236384,2.0518346361
N,-0.8805581901,-1.2846930488,0.1601246003

N,1.3565811697,-1.0763180257,1.9072908166
C,2.0733417588,-0.1273290887,1.457342897
C,-1.6730670594,-0.6420382894,0.9466335502
H,-1.7737518257,-1.0124240931,1.9681414996
H,2.5898440018,-0.2014724219,0.4889861016
C,-2.441310622,0.5754194426,0.6574722106
C,-3.7679528507,2.9952596671,0.256524287
C,-3.0902986248,0.8231399426,-0.5583696996
C,-2.5021265866,1.5266579949,1.6877697291
C,-3.1453009396,2.7400841748,1.4791650866
C,-3.7534413136,2.0326033437,-0.7507576897
H,-3.0827302321,0.0729295472,-1.3415483672
H,-2.0150618191,1.3192939919,2.6369456263
H,-3.1648446056,3.4846023946,2.2683882045
H,-4.2552404668,2.2231018812,-1.6940305781
H,-4.2748554324,3.9414373323,0.0938315351
C,2.2754667974,1.1408795719,2.1864974069
C,2.6979963888,3.5669546767,3.5065753253
C,3.1641377158,2.0842210105,1.6629099671
C,1.5857478118,1.4263169461,3.3708433488
C,1.7964730639,2.634202399,4.0258562729
C,3.3805687452,3.2913413292,2.323516731
H,3.6880510315,1.8652125504,0.7356617191
H,0.8903663155,0.6931299392,3.7681091899
H,1.2602509592,2.8517810409,4.944575399
H,4.0764651746,4.0166905277,1.9135738659
H,2.8629117369,4.50760964,4.0231825678
H,2.4090717632,-3.0098384664,-3.3491023394
C,1.3589517627,-2.9265742189,-3.6101849089
C,-1.4009048219,-2.701390693,-4.2552627871
C,0.5071512771,-2.1307677048,-2.8710653749
C,0.8099250961,-3.6194537353,-4.7040841027
C,-0.5392629878,-3.5086775119,-5.0192940688
C,-0.8527996552,-2.0187950623,-3.1878749766
H,1.454516116,-4.2497739099,-5.3084815971
H,-0.9401947535,-4.0538071663,-5.8680119155
H,-2.4561846951,-2.6103706801,-4.4909134056
O,-1.4762707552,-1.1827599799,-2.3161954544
O,0.8018066756,-1.3836661091,-1.7738624158
B,-0.4507660519,-0.7240236341,-1.3412262185
H,0.6710579717,3.8598190846,1.5728313888
C,0.253245593,4.0250618291,0.5843105217
C,-0.8923731046,4.4067762352,-2.0110616782
C,0.0248156162,2.9744714301,-0.2819648171
C,-0.1080170032,5.2973459439,0.1231637148
C,-0.665198933,5.4834032005,-1.1438764969

C,-0.5352852477,3.1574994697,-1.5436232792
H,0.0448031507,6.1562548096,0.7685490759
H,-0.9351071921,6.4843436468,-1.4644490354
H,-1.3353675217,4.5392430653,-2.9920275388
O,-0.6893379422,1.9310972505,-2.1472782396
O,0.2357913619,1.6354004795,-0.0787212906
B,-0.2779480491,0.9824879096,-1.2045590755

IA-*E,Z*[1,1]^{MeOH} (Intermediate monocoordinate *E*-coordinated 1,1-B_2cat_2-*E,Z*-diimine **1** complex in MeOH)
E-coord_cydiimph2_EZ_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1438106

Zero-point correction= 0.571186 (Hartree/Particle)
Thermal correction to Energy= 0.603542
Thermal correction to Enthalpy= 0.604487
Thermal correction to Gibbs Free Energy= 0.504487
Sum of electronic and ZPE= -1696.572624
Sum of electronic and thermal Energies= -1696.540268
Sum of electronic and thermal Enthalpies= -1696.539324
Sum of electronic and thermal Free Energies= -1696.639324

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.729	130.167	210.467

C,0.7536247194,-1.8416011395,1.539131324
C,1.1653540738,-4.341336494,1.4949019718
C,-0.8324510113,-3.3993540206,0.2860629753
C,-0.2870453345,-4.5887473325,1.0820105052
C,-0.699849099,-2.134947071,1.1311378268
C,1.2986157481,-3.0531699849,2.3087786128
H,1.7882263721,-4.2672641898,0.5935847075
H,-0.2652459549,-3.3082792319,-0.642743141
H,-0.9003345566,-4.7436286123,1.9794328917
H,-1.2488265077,-2.3079873732,2.0643130216
H,0.7425750989,-3.1451081247,3.2510187626
H,1.3582341273,-1.6975257309,0.6408818024
H,1.5452505968,-5.1860614134,2.0784145579
H,-1.8850629407,-3.5502657326,0.0236491015
H,-0.3629950277,-5.4986778322,0.4789041111
H,2.3454154714,-2.857124219,2.5653976341
N,-1.3151302268,-0.9307086835,0.5129995219
N,0.7367985769,-0.689516975,2.4339367639
C,1.6825781913,0.1609826496,2.4508202744

C,-2.0831009977,-0.2508433136,1.2921143015
H,-2.2175859899,-0.6227064519,2.3081346302
H,1.6069968633,0.9394323067,3.2180302713
C,-2.7619147183,1.0198442985,1.0073419819
C,-3.881135306,3.545122177,0.6294684477
C,-3.3893669939,1.3304235097,-0.2048666805
C,-2.7407418519,1.9641395992,2.0456048999
C,-3.2789455144,3.2292555992,1.848236225
C,-3.9500656695,2.592661787,-0.3850220907
H,-3.44256702,0.5902846521,-0.9957525952
H,-2.2715077691,1.7068840046,2.9916803601
H,-3.2338068369,3.9664252856,2.6432424613
H,-4.4358715578,2.8324394571,-1.3254469074
H,-4.3064032467,4.5319970216,0.4750073604
C,2.9241139131,0.2484436579,1.6293929944
C,5.3273470716,0.500264808,0.2178824387
C,4.1306965392,0.4472369618,2.3107312015
C,2.9279088562,0.2068099334,0.2304861455
C,4.125805711,0.3333210326,-0.4684173555
C,5.3282605233,0.5581988006,1.6104286281
H,4.1262711137,0.5096902365,3.3960751117
H,1.9966007814,0.0910100729,-0.3144694628
H,4.117889951,0.3055906031,-1.5537696215
H,6.259390733,0.6990191663,2.150506783
H,6.2589847214,0.595960654,-0.3313085326
H,1.8270228358,-2.8444925744,-3.0337866641
C,0.7832783297,-2.6877994523,-3.2868875143
C,-1.9577193212,-2.2644509638,-3.9112621055
C,-0.008287071,-1.846800652,-2.5311567453
C,0.1827278871,-3.3249615159,-4.3873799991
C,-1.1575076225,-3.1171760053,-4.6922954043
C,-1.3590377998,-1.637833691,-2.8363134617
H,0.7794696533,-3.9887171938,-5.0049811912
H,-1.5992570307,-3.6199544855,-5.5468671306
H,-3.0050799736,-2.0965901698,-4.1399263773
O,-1.9177730822,-0.7703695991,-1.9521490632
O,0.345068029,-1.1351237812,-1.4276025405
B,-0.8567051612,-0.3921850798,-0.9790892569
H,0.7027100835,4.214869813,1.7562388784
C,0.2551725532,4.366585215,0.7799550136
C,-0.9428019071,4.7278595927,-1.7922917651
C,-0.0947050754,3.2997434935,-0.0235724567
C,-0.0110761361,5.6433252833,0.2694018076
C,-0.5964586881,5.8195599604,-0.9859882463
C,-0.6759788406,3.4750672369,-1.2766787415
H,0.2411989613,6.5138097596,0.8661353221

H,-0.7909798237,6.8243347265,-1.3465677121
H,-1.4031600924,4.8522025617,-2.7663042585
O,-0.9396048955,2.2423969589,-1.824736774
O,0.013890636,1.9551914784,0.2341910643
B,-0.571392051,1.3009247454,-0.8580288692

IA-*Z,E*[1,1]^{MeOH} (Intermediate monocoordinate *Z*-coordinated 1,1-B_2cat_2-*Z*,*E*-diimine **1** complex in MeOH)
Z-coord_cydiimph2_ZE_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1589768

Zero-point correction= 0.571378 (Hartree/Particle)
Thermal correction to Energy= 0.603524
Thermal correction to Enthalpy= 0.604468
Thermal correction to Gibbs Free Energy= 0.506387
Sum of electronic and ZPE= -1696.587599
Sum of electronic and thermal Energies= -1696.555453
Sum of electronic and thermal Enthalpies= -1696.554509
Sum of electronic and thermal Free Energies= -1696.652590

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.717	130.042	206.429

C,1.2608790525,-1.3550448511,0.2933484786
C,2.1934755154,-3.7190508635,0.1759370656
C,-0.0720306704,-3.2399513067,-0.7942134506
C,0.7908060255,-4.2754943107,-0.072602626
C,-0.1293846184,-1.9548829968,0.0356102359
C,2.1348494277,-2.4182256956,0.9763939439
H,2.6825906474,-3.5314173452,-0.788842525
H,0.3593162977,-3.0273805251,-1.7762206696
H,0.3255173154,-4.5388069341,0.8868698915
H,-0.5273198328,-2.1959780093,1.0255757477
H,1.7179952195,-2.6124910327,1.9735936755
H,1.7331922054,-1.0571594024,-0.6550994434
H,2.8073461491,-4.4508288656,0.7106367256
H,-1.0892230655,-3.6134962635,-0.9559592514
H,0.8419243585,-5.1918776562,-0.6685613449
H,3.1362061739,-1.99856415,1.1199229172
N,-1.0177343001,-0.9407309688,-0.5647192622
N,1.0965991467,-0.2176812674,1.1919076605
C,1.9903410954,0.6874707274,1.167988164
C,-2.1243389175,-0.5843603222,-0.0195104676
H,-2.6285937987,0.252990805,-0.5032782347

H,2.8485446377,0.6461400429,0.4800820937
C,-2.7957156131,-1.1130425006,1.1772374254
C,-4.1721828703,-1.9319630567,3.461137145
C,-3.4190510466,-0.1679597424,2.0034137915
C,-2.8994407204,-2.4770389462,1.4826832125
C,-3.5913948866,-2.8798568677,2.6193344859
C,-4.0855830352,-0.5754022971,3.153272503
H,-3.3650347121,0.8859540797,1.7442604274
H,-2.4718175677,-3.2225960477,0.8198822222
H,-3.6801323612,-3.9372598235,2.8461259548
H,-4.5488817008,0.1628263723,3.7995853361
H,-4.7053073355,-2.2528254386,4.3506173642
C,1.9385188322,1.8560564168,2.0686179692
C,1.8688464598,4.1025061475,3.723765861
C,3.0195015297,2.7408207435,2.0996983539
C,0.8161242185,2.1039371351,2.8697541704
C,0.7838671459,3.2225775469,3.6923992432
C,2.9865674677,3.8603358579,2.9284676307
H,3.8835778804,2.5506093716,1.4675043066
H,-0.0255409285,1.4191547777,2.8268603855
H,-0.0887531864,3.4162305343,4.3088586713
H,3.8280305911,4.5461902591,2.9462473697
H,1.838440758,4.9779020761,4.3654190463
H,0.8023397249,-2.8367659504,-4.6328399519
C,-0.1699471692,-2.3544993153,-4.6236311201
C,-2.7043599227,-1.0661288533,-4.5789081065
C,-0.4675819917,-1.3798841213,-3.6913702325
C,-1.1697463227,-2.6867966859,-5.5533320917
C,-2.4093807429,-2.056176318,-5.5312955115
C,-1.7175745618,-0.7466634237,-3.6666811008
H,-0.9673787403,-3.4498442522,-6.2982908116
H,-3.1657265726,-2.3315802247,-6.259512069
H,-3.6677381263,-0.5674571106,-4.5534954595
O,-1.7599306013,0.1834417347,-2.6717353742
O,0.3376676792,-0.8814888643,-2.7116092104
B,-0.5333702266,-0.044468754,-1.8675610878
H,3.5261404651,3.7509855843,-1.9061809126
C,2.6631322805,3.9886854544,-1.2939264295
C,0.3715483427,4.5837305403,0.3124628173
C,1.6007945069,3.1136589621,-1.175818401
C,2.5608625388,5.1897654077,-0.5818924366
C,1.4416445147,5.4797562234,0.2026834417
C,0.4858300907,3.4026562293,-0.3950202338
H,3.3705475157,5.9097941277,-0.6412071824
H,1.4000172015,6.419344534,0.7443837714
H,-0.4988440737,4.7948712779,0.9241543586

O,-0.3959336853,2.3494205,-0.4665666427
O,1.4323805838,1.8768758279,-1.7551331409
B,0.1890102892,1.4084320833,-1.3216790923

IA-*Z,Z*[1,1]^{MeOH} (Intermediate monocoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in MeOH)
Z-coord_cydiimph2_ZZ_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1477281

Zero-point correction= 0.571986 (Hartree/Particle)
Thermal correction to Energy= 0.603999
Thermal correction to Enthalpy= 0.604943
Thermal correction to Gibbs Free Energy= 0.506545
Sum of electronic and ZPE= -1696.575742
Sum of electronic and thermal Energies= -1696.543729
Sum of electronic and thermal Enthalpies= -1696.542785
Sum of electronic and thermal Free Energies= -1696.641183

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.015	129.755	207.095

C,0.739556113,-0.9657236895,0.7253394913
C,1.763220777,-3.2892217534,0.7104532809
C,-0.4702483469,-2.9189622436,-0.3850679353
C,0.400263653,-3.9065496569,0.3941396092
C,-0.6161292143,-1.6220397939,0.4199459906
C,1.6043049664,-1.9825027727,1.4869757894
H,2.2999109513,-3.092151604,-0.2272714446
H,-0.0082653495,-2.7130681935,-1.3531371166
H,-0.1004395494,-4.1809112486,1.3319646818
H,-1.063162549,-1.8864355832,1.379981009
H,1.1138674447,-2.1798183182,2.4494886448
H,1.2188116793,-0.703295587,-0.2278370408
H,2.3748092635,-3.9881586496,1.2899008534
H,-1.4675241212,-3.3328530432,-0.5701318044
H,0.5212349626,-4.8257036923,-0.1875432953
H,2.5786471203,-1.5372689739,1.7095623844
N,-1.5235125416,-0.6723402796,-0.2589116415
N,0.4803319874,0.2027061239,1.5566485726
C,1.3348187451,1.1126569687,1.818516456
C,-2.6886627583,-0.3913160742,0.1998504114
H,-3.2923781692,0.2514011925,-0.4411173657
H,0.9664068994,1.8901990775,2.4970119573
C,-3.3280845732,-0.8279988243,1.4548980564

C,-4.695621012,-1.5645868985,3.769590269
C,-2.6953369216,-0.73232683,2.7012979495
C,-4.6592334645,-1.2552697101,1.3790784518
C,-5.3326578946,-1.6436084968,2.5322536955
C,-3.3847325735,-1.0971878467,3.8530596584
H,-1.6800029864,-0.3492706233,2.7589761275
H,-5.157007194,-1.2917323548,0.4140040365
H,-6.3577383969,-1.9936261296,2.4666042303
H,-2.8973230026,-1.013022926,4.8190836224
H,-5.2256841738,-1.8544386295,4.6715425788
C,2.7393211782,1.3718837957,1.4121170809
C,5.3629671706,2.1505082243,0.7785370638
C,3.3451780437,2.4639157177,2.0522904479
C,3.4763624657,0.6716736221,0.4425695568
C,4.7727108182,1.066807997,0.1281906068
C,4.6470059543,2.846796371,1.7490258124
H,2.7782281122,3.0225844502,2.7930831709
H,3.0566933469,-0.1776810268,-0.0801942294
H,5.3269196984,0.5208764339,-0.6288951473
H,5.0952950137,3.693555572,2.2593369927
H,6.3767872756,2.4478630412,0.5287718073
H,0.1799628898,-2.7653879799,-4.2703442021
C,-0.7721357368,-2.2443603232,-4.2687847691
C,-3.2526435572,-0.8529247766,-4.2480054075
C,-1.0192145121,-1.2232533708,-3.3722035771
C,-1.7957116028,-2.570961921,-5.1742437593
C,-3.0085150383,-1.8896746279,-5.1645749809
C,-2.2432003756,-0.540386577,-3.3589352142
H,-1.6330864553,-3.3695527259,-5.8911730344
H,-3.7835148733,-2.161611945,-5.8742335383
H,-4.194646426,-0.314509289,-4.2324435923
O,-2.2363721689,0.4276661934,-2.3984474092
O,-0.1830283195,-0.7152409261,-2.4244010905
B,-1.0191368572,0.1713456529,-1.5956156868
H,3.404473688,3.4992338451,-1.6764970745
C,2.5750450924,3.8437830583,-1.0682572591
C,0.3799674607,4.7051777644,0.5528852927
C,1.4142549372,3.1056554527,-0.9494840696
C,2.6253813443,5.0410159033,-0.3447205511
C,1.555941074,5.4587130969,0.4515660077
C,0.3403268704,3.5294824326,-0.1718642676
H,3.5203401761,5.6527249684,-0.3979843092
H,1.6344484818,6.3901651355,1.0026917783
H,-0.4586222725,5.022235167,1.1630042817
O,-0.6720464145,2.6022886784,-0.2614128393
O,1.1032304129,1.8928645087,-1.5149282005

B,-0.1914066555,1.581155451,-1.0855758442

IA-*E*,*E*[1,2]^{MeOH} (Intermediate monocoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in MeOH)
maxstep10_E-coord_cydiimph2_EE_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1570579

Zero-point correction= 0.571338 (Hartree/Particle)
Thermal correction to Energy= 0.603306
Thermal correction to Enthalpy= 0.604250
Thermal correction to Gibbs Free Energy= 0.507496
Sum of electronic and ZPE= -1696.585720
Sum of electronic and thermal Energies= -1696.553752
Sum of electronic and thermal Enthalpies= -1696.552808
Sum of electronic and thermal Free Energies= -1696.649562

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.580	130.247	203.636

C,-0.0845035025,-2.0933833084,-1.1097854102
C,1.4729593125,-3.8994453931,-1.9694065761
C,2.3072078269,-1.5362003686,-1.736124441
C,2.4079179803,-2.8331860288,-2.5430585588
C,0.8587988913,-1.0552277138,-1.7355251404
C,0.0289866184,-3.3993433307,-1.9088500362
H,1.8064004191,-4.162604059,-0.9569392441
H,2.6399821188,-1.7381164463,-0.7127761949
H,2.1403683357,-2.6340322172,-3.5888502239
H,0.5472735926,-0.9422106283,-2.7799842511
H,-0.3500335666,-3.2161633841,-2.9228677665
H,0.2163568934,-2.2929933874,-0.0688591916
H,1.5216869249,-4.8130250246,-2.5702849942
H,2.9559714445,-0.7575181942,-2.1511748001
H,3.4425756387,-3.1889645832,-2.53660854
H,-0.6249040108,-4.1462302182,-1.4464333801
N,-1.4440643132,-1.5782305072,-1.1699725444
N,0.6917736866,0.2762459113,-1.0998986254
C,-0.1011174228,1.0810390708,-1.7212563617
H,-0.6004507203,0.6837782463,-2.6059591375
C,-2.2453559529,-1.9606178737,-0.2605219705
H,-1.936952203,-2.661825806,0.5287634247
B,1.3655369774,0.5492100095,0.362622655
B,1.6075916811,-0.7407244131,1.4320599566
O,2.8689353839,-1.1861580387,1.7559676137

O,0.4542214279,1.438407835,1.1021156544
C,3.8179958212,0.5913506547,0.3651124957
C,6.3313391792,-0.6189434617,0.7418901491
C,3.9443215884,-0.5869029321,1.1307892993
C,4.9738214723,1.1397175833,-0.1949318729
C,6.219567446,0.5480564158,-0.0095724541
C,5.1894928775,-1.1786769736,1.3079043669
H,4.8642372628,2.0466991647,-0.7819590348
H,7.0986948151,0.9996726916,-0.4580244779
H,5.2386160838,-2.084711555,1.9042954816
H,7.2960395165,-1.0921958865,0.8909720922
O,2.6427593312,1.2317578816,0.139254571
C,-0.6311443671,0.8462363635,1.6652194234
C,-2.8791549512,-0.2579080628,2.9336670334
C,-0.5679140736,-0.4319045732,2.2592515312
C,-1.8428488345,1.5386216893,1.6991612311
C,-2.9589125041,0.9961523339,2.3336693976
C,-1.6820162347,-0.970072506,2.8914778948
H,-1.8781806906,2.5215531195,1.2365457087
H,-3.8903234937,1.5535497523,2.3513095915
H,-1.587589779,-1.9491845165,3.3519953755
H,-3.7443096296,-0.6881155212,3.427599725
O,0.6140627813,-1.1412094284,2.3023793379
C,-0.4272945729,2.4772711032,-1.4223897219
C,-1.2007659179,5.1179202652,-0.9803610312
C,0.4849613448,3.3912634608,-0.8782161782
C,-1.7098336003,2.907751945,-1.7877441478
C,-2.1043975423,4.2188711743,-1.5432097599
C,0.0960932407,4.7070858278,-0.6657252182
H,1.4931588177,3.0720575058,-0.6387574742
H,-2.3992193236,2.2063497779,-2.2502624082
H,-3.1068976561,4.5409297581,-1.8051131763
H,0.8051437653,5.4169018832,-0.2522046614
H,-1.4999638232,6.1462422001,-0.8020067926
C,-3.6402554737,-1.4857389981,-0.188513459
C,-6.2555353234,-0.5439316184,0.0640847119
C,-4.5388169566,-2.1256688909,0.6691531446
C,-4.0574893495,-0.3661703951,-0.9170185381
C,-5.3593594595,0.1031170024,-0.789248434
C,-5.8456820164,-1.6607326265,0.7902547863
H,-4.2050515444,-2.9836210072,1.2480619922
H,-3.3445800914,0.1361433462,-1.5640207886
H,-5.6768993826,0.9782146205,-1.3481038767
H,-6.5406590783,-2.1629341591,1.4560230622
H,-7.2710981355,-0.1735005561,0.1655961872

IA-*E*,*Z*[1,2]^{MeOH} (Intermediate monocoordinate *E*-coordinated 1,2-B_2cat_2-*E*,*Z*-diimine **1** complex in MeOH)
E-coord_cydiimph2_EZ_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1478526

Zero-point correction= 0.572175 (Hartree/Particle)
Thermal correction to Energy= 0.603913
Thermal correction to Enthalpy= 0.604858
Thermal correction to Gibbs Free Energy= 0.508682
Sum of electronic and ZPE= -1696.575678
Sum of electronic and thermal Energies= -1696.543939
Sum of electronic and thermal Enthalpies= -1696.542995
Sum of electronic and thermal Free Energies= -1696.639170

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.961	129.897	202.418

C,-1.5609800952,-1.1722612787,0.2720604665
C,-3.1701198155,-1.2598478526,2.2357070819
C,-0.7107398629,-0.9521119906,2.6519935812
C,-2.0113050918,-1.5516763122,3.1895717394
C,-0.4237209323,-1.4987960339,1.2549547615
C,-2.8606559802,-1.7760421004,0.8313476943
H,-3.343483632,-0.1757531642,2.1956362529
H,-0.8259279356,0.1356792597,2.6123938528
H,-1.8961023345,-2.6374154956,3.3027627954
H,-0.3690741019,-2.5907273628,1.3223671192
H,-2.7366649322,-2.8664502734,0.8545198761
H,-1.6530597719,-0.0805986786,0.2030251281
H,-4.0933787306,-1.7194011781,2.6023757688
H,0.1336228179,-1.1722239327,3.313794348
H,-2.218261471,-1.1431373719,4.1832887984
H,-3.6843066574,-1.5653313184,0.1421111165
N,-1.2512734039,-1.7758886953,-1.0111896181
N,0.8881523651,-1.0386108349,0.7343380915
C,1.5856560925,-1.9414906626,0.1352893386
H,1.1185283054,-2.9198909462,0.0190461627
C,-1.7781557903,-1.387794406,-2.104891853
H,-1.4610146018,-1.9544528821,-2.9868623685
B,1.2611033864,0.5496195246,0.8377281118
B,0.0222418809,1.6982398196,0.7459078754
O,-0.3104129331,2.4919675646,1.8197093918
O,2.1107607104,0.8854438866,-0.3166123849
C,1.5081839596,1.4627888371,3.1026515928

C,0.5710353868,2.8916789466,5.3406932324
C,0.3757264107,2.2990249896,3.002900164
C,2.1491143237,1.3687344886,4.3400923343
C,1.6933154898,2.074501756,5.4490493202
C,-0.0803182054,2.9970765255,4.1153294677
H,3.0185043565,0.7212428069,4.4044635701
H,2.2154640438,1.9793585699,6.3957536547
H,-0.9552619782,3.628075187,3.9914589135
H,0.202928157,3.4450857903,6.1980668831
O,2.0190475379,0.7368694795,2.0760709548
C,1.4694326825,1.0489048472,-1.5023036205
C,0.2450238509,1.4355242716,-3.9966910846
C,0.1994312486,1.6586887407,-1.5943557999
C,2.0997730785,0.63469765,-2.6761561155
C,1.4945477131,0.8261473502,-3.9163498877
C,-0.3950237913,1.858016661,-2.833231906
H,3.0790490883,0.1712932589,-2.589222556
H,2.0029832924,0.4973784239,-4.8172480875
H,-1.3680616389,2.3411835588,-2.8656924981
H,-0.2350645741,1.5882822196,-4.9580777181
O,-0.4406035991,2.1492451284,-0.4743778502
C,2.9432084598,-1.8489949462,-0.4076266955
C,5.4904123994,-1.8349510868,-1.5339531365
C,3.9683043755,-1.1078068196,0.1941756093
C,3.2128096143,-2.6155998992,-1.5484943998
C,4.4783638016,-2.5894087085,-2.1247313423
C,5.2380648104,-1.1090890377,-0.3681934286
H,3.7687010804,-0.5464889193,1.1008574189
H,2.4201175879,-3.2134527186,-1.9904218187
H,4.677582774,-3.1655195359,-3.022358429
H,6.0352074125,-0.5420023594,0.1014526546
H,6.4835347395,-1.8239768127,-1.9725521708
C,-2.7213022955,-0.2987426399,-2.4697949922
C,-4.3257635277,1.77873299,-3.4842195668
C,-2.8891102333,-0.116624731,-3.852002952
C,-3.4013311786,0.5708274523,-1.6003167617
C,-4.1905431236,1.5992373423,-2.1089941895
C,-3.6767033991,0.909393537,-4.359021136
H,-2.3719228838,-0.7840605626,-4.5366007713
H,-3.3421764942,0.4635003157,-0.5258569542
H,-4.7052905081,2.2628367227,-1.4213068314
H,-3.7819027396,1.0318830661,-5.4324481066
H,-4.9409150091,2.5854605602,-3.8707881016

IA-*Z*,*E*[1,2]^{MeOH} (Intermediate monocoordinate *Z*-coordinated 1,2-B_2cat_2-*Z*,*E*-diimine **1** complex in MeOH)
Z-coord_cydiimph2_ZE_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.156959

Zero-point correction= 0.571411 (Hartree/Particle)
Thermal correction to Energy= 0.603490
Thermal correction to Enthalpy= 0.604434
Thermal correction to Gibbs Free Energy= 0.506137
Sum of electronic and ZPE= -1696.585548
Sum of electronic and thermal Energies= -1696.553469
Sum of electronic and thermal Enthalpies= -1696.552525
Sum of electronic and thermal Free Energies= -1696.650822

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.696	130.173	206.884

C,-1.5567213401,-0.2354493869,0.1456858385
C,-3.4279349389,-0.0413695197,1.8598438944
C,-1.068160055,0.4268374766,2.5714126186
C,-2.4158422079,-0.15412833,2.999989439
C,-0.5655032667,-0.291419907,1.3202775277
C,-2.9222708984,-0.7622837143,0.6112202736
H,-3.5955273756,1.0191547589,1.6293240498
H,-1.1999981714,1.4951052307,2.3711251199
H,-2.2912609548,-1.2091523124,3.2771815061
H,-0.4522887293,-1.3516357143,1.5541404141
H,-2.8185622399,-1.8352682686,0.8193458482
H,-1.6725391253,0.803283322,-0.2062100364
H,-4.393092067,-0.4611711307,2.1602453198
H,-0.3197900056,0.3322776045,3.366441567
H,-2.7751544326,0.3737763631,3.8884250871
H,-3.6288409902,-0.6601945264,-0.2191426405
N,-1.0499064932,-1.1108003683,-0.9002004118
N,0.7392765215,0.2242454046,0.8639530569
C,1.7406427299,-0.5447331445,0.6360537111
H,2.6034744417,-0.0631670403,0.1725595899
C,-1.2143564689,-0.7598272514,-2.1107845291
H,-1.6947605882,0.19091534,-2.3880071939
B,1.004140809,1.8096270389,0.5216267012
B,-0.2264686556,2.9567070333,0.6197001461
O,-0.3693352194,3.7509384694,1.7361674884
O,1.5400560474,1.8527705871,-0.8421978607
C,1.6702750585,2.7527513966,2.6365114409

C,0.9588998915,3.8147601266,5.1412013921
C,0.4757810705,3.4887327537,2.7968656019
C,2.4890460868,2.5705924309,3.7517636285
C,2.1437417806,3.0985330385,4.9930888952
C,0.1296614595,4.0059781973,4.0387095948
H,3.4053963048,2.0040466084,3.6162569378
H,2.8005098694,2.9422063277,5.8429030145
H,-0.7983873445,4.564018385,4.1175583878
H,0.6782960822,4.2260278974,6.1050844192
O,2.066924095,2.2327752952,1.4447316579
C,0.6629965236,2.0732937425,-1.8557039761
C,-1.0407301758,2.5212809754,-4.0496207298
C,-0.5351363317,2.8062952859,-1.7030216181
C,0.9802820684,1.583431359,-3.1238190544
C,0.1448899248,1.8088648858,-4.2140047194
C,-1.3732923636,3.0176038334,-2.7912651844
H,1.9037361601,1.0216854716,-3.2294876971
H,0.4181628423,1.4150600368,-5.1879696252
H,-2.2820128313,3.5895164536,-2.6293766815
H,-1.7013982424,2.6982230087,-4.892022862
O,-0.8953190872,3.3868032515,-0.5031597147
C,1.8806399621,-1.9864632381,0.8994168027
C,2.2767600485,-4.7149909731,1.2991472409
C,1.5523309958,-2.5673023274,2.1305631119
C,2.4471854437,-2.7690919797,-0.1136932402
C,2.6211704573,-4.1357766911,0.0789237258
C,1.7572800687,-3.9285857856,2.3269547051
H,1.163984218,-1.9512811606,2.9368357117
H,2.7324407333,-2.3047596277,-1.0539828128
H,3.0389780137,-4.7440712503,-0.7168406495
H,1.5125866427,-4.3758593103,3.2848425847
H,2.4258688325,-5.7788475385,1.4550132976
C,-0.787564826,-1.622829993,-3.2322166836
C,-0.0064006216,-3.2271454747,-5.3821811083
C,-1.1595903054,-1.2850846978,-4.5364351631
C,-0.0229875687,-2.7751084832,-3.0105430855
C,0.3675058971,-3.5701161205,-4.0809668015
C,-0.7732535973,-2.0863058667,-5.6084274075
H,-1.7543731427,-0.3911179011,-4.7058961991
H,0.2595235784,-3.0341781483,-1.9945870823
H,0.9649535393,-4.4594402776,-3.9039707929
H,-1.06883144,-1.8192246144,-6.6182882813
H,0.300193884,-3.8499372762,-6.2170674658

IA-*Z,Z*[1,2]^{MeOH} (Intermediate monocoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in MeOH)
Z-coord_cydiimph2_ZZ_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1468077

Zero-point correction= 0.572266 (Hartree/Particle)
Thermal correction to Energy= 0.604005
Thermal correction to Enthalpy= 0.604950
Thermal correction to Gibbs Free Energy= 0.509002
Sum of electronic and ZPE= -1696.574542
Sum of electronic and thermal Energies= -1696.542802
Sum of electronic and thermal Enthalpies= -1696.541858
Sum of electronic and thermal Free Energies= -1696.637806

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.019	129.782	201.940

C,-1.0862819239,-0.8124306646,0.1552275463
C,-2.7323836889,-0.9720045353,2.0796452565
C,-0.3174759384,-0.4498947793,2.5458722993
C,-1.5798611663,-1.1340783116,3.0717717606
C,0.0486396392,-1.0158239583,1.1761979845
C,-2.3454330562,-1.5053597505,0.7008342688
H,-2.9935026484,0.0919710562,1.9976965399
H,-0.5129984816,0.6251593759,2.4604302102
H,-1.3791133456,-2.2022162149,3.2268215413
H,0.1922311821,-2.093876115,1.2629499414
H,-2.134041119,-2.580690185,0.7620501618
H,-1.266723958,0.2657776262,0.0530374782
H,-3.6239182638,-1.4945179251,2.4404201621
H,0.5241735267,-0.5778252098,3.2354265414
H,-1.8479586072,-0.7110582826,4.0445842721
H,-3.1649092597,-1.3825590262,-0.0142684393
N,-0.6845596979,-1.4209781653,-1.100558677
N,1.2888769242,-0.4222802207,0.6448590033
C,2.2224487442,-1.1465197008,0.1444931448
H,3.0299361754,-0.5950254377,-0.3370721045
C,-1.217642088,-1.123198191,-2.2192401465
H,-0.8208858459,-1.6849418903,-3.0718652811
B,1.5059141124,1.1999114557,0.6459285035
B,0.2051428306,2.2523428141,0.4399688294
O,-0.2383129133,3.0653122446,1.456687088
O,2.3968989388,1.4840802486,-0.4943502023
C,1.6022552348,2.2470461866,2.8582092061

C,0.4791742829,3.7253706072,4.9759216604
C,0.4152195746,2.9884818426,2.6719257851
C,2.2011154014,2.2718600405,4.119897243
C,1.6538781209,3.0031406237,5.1693534809
C,-0.1317173946,3.711992842,3.7254972786
H,3.1126047044,1.6964924823,4.2512004206
H,2.145997044,3.0015868308,6.1367011287
H,-1.0451318332,4.2675712867,3.5356717823
H,0.0394873146,4.2970751657,5.7862502997
O,2.2025118781,1.5024627124,1.8951845221
C,1.7782100266,1.5284893966,-1.7076097072
C,0.6051300998,1.6486361751,-4.2553503637
C,0.4830750735,2.0656300485,-1.8798992451
C,2.4536610453,1.0446805983,-2.8278559034
C,1.8760100995,1.1037757242,-4.0943387313
C,-0.0837818903,2.1334974253,-3.1457636105
H,3.4479662349,0.632588157,-2.6819451355
H,2.422548253,0.7226668661,-4.9511084189
H,-1.0789242355,2.5604927926,-3.2396729023
H,0.1445535825,1.6988822481,-5.2368052758
O,-0.2259000314,2.600726928,-0.8235651215
C,2.3464577745,-2.6151597846,0.1359353486
C,2.7284524957,-5.3715958815,0.0133086227
C,2.2332418633,-3.388093158,1.2973085689
C,2.6844667196,-3.2224592567,-1.0783667547
C,2.8541996404,-4.6013014388,-1.1417485801
C,2.4299642582,-4.7635580094,1.2319162895
H,2.015894701,-2.9108690019,2.2488969666
H,2.7974703551,-2.6099846336,-1.969072114
H,3.0964694597,-5.0725465974,-2.0887443589
H,2.3517340721,-5.3607880618,2.1345720085
H,2.874144263,-6.4462651231,-0.0336010305
C,-2.2566959182,-0.1497523542,-2.6461649955
C,-4.0404020989,1.7115105159,-3.7758080782
C,-2.4351078328,-0.0625935232,-4.0364341372
C,-3.0162399405,0.7030467969,-1.8272666693
C,-3.893218605,1.6251849817,-2.3929506472
C,-3.3122661992,0.8555230833,-4.6001609366
H,-1.8560869393,-0.7167833999,-4.68327279
H,-2.9508307287,0.6648443394,-0.7484835807
H,-4.4677559859,2.2783809796,-1.7437326851
H,-3.4249208765,0.9055967898,-5.6785901804
H,-4.725173115,2.4352394701,-4.2069863113

IA-*E*,*E*[1,1]^{DMF} (Intermediate monocoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
E-coord_cydiimph2_EE_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1542304

Zero-point correction= 0.571476 (Hartree/Particle)
Thermal correction to Energy= 0.603768
Thermal correction to Enthalpy= 0.604712
Thermal correction to Gibbs Free Energy= 0.505815
Sum of electronic and ZPE= -1696.582754
Sum of electronic and thermal Energies= -1696.550463
Sum of electronic and thermal Enthalpies= -1696.549518
Sum of electronic and thermal Free Energies= -1696.648415

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.870	130.082	208.146

C,1.2491710205,-2.2226657059,1.0617387658
C,1.6198943449,-4.7248404497,1.0092068557
C,-0.4298577084,-3.7546423988,-0.0879695608
C,0.1456430191,-4.9538925914,0.6708390129
C,-0.233273135,-2.4895471015,0.7452149164
C,1.80796011,-3.4369989714,1.8129666998
H,2.1966008422,-4.6576848959,0.076991544
H,0.0808809005,-3.6635375588,-1.0499422713
H,-0.4212742658,-5.1057820304,1.5986846356
H,-0.7266010533,-2.6512505502,1.7110981482
H,1.2915090471,-3.5174421422,2.7785540268
H,1.7996179782,-2.093114787,0.1213268597
H,2.0184728547,-5.5749054874,1.5718636755
H,-1.4980243118,-3.8915815095,-0.2871384151
H,0.0268690876,-5.8598414406,0.0687258959
H,2.8674206791,-3.2590282936,2.024576075
N,-0.8825537683,-1.2965307574,0.1414487765
N,1.333707659,-1.0392784894,1.9039691028
C,2.0420823766,-0.0746350096,1.4768041
C,-1.6949248996,-0.6639289162,0.9148338936
H,-1.8093437265,-1.040239073,1.9326878759
H,2.5761272726,-0.1278707686,0.5168259238
C,-2.4605260752,0.5554644705,0.6304818714
C,-3.7477415609,3.0037726794,0.269117049
C,-3.0257649954,0.8706707215,-0.6118259217
C,-2.5877145595,1.45322343,1.7017523413
C,-3.2120948336,2.6799942821,1.5159226006

C,-3.6667092716,2.0950665284,-0.7843367327
H,-2.9699557623,0.1629328955,-1.4318183793
H,-2.1672561182,1.1931142994,2.6694197801
H,-3.2841753045,3.3810646744,2.3409514141
H,-4.1013256315,2.3393796519,-1.7482894573
H,-4.2388446026,3.9606721935,0.1220834157
C,2.2115151156,1.1861996688,2.2270606375
C,2.5771205431,3.592427225,3.5995161072
C,3.1103448157,2.1426410191,1.7476775183
C,1.4858303499,1.446408868,3.3953980366
C,1.6670419539,2.644908266,4.0759691019
C,3.2982611064,3.3401634234,2.4343177694
H,3.6641889075,1.9418702203,0.8338186972
H,0.7849239561,0.7005411402,3.7581705249
H,1.1018240839,2.8438180475,4.9813865458
H,4.0020223162,4.0761714307,2.0583246763
H,2.7192206638,4.5255796258,4.1359257805
H,2.3444899051,-3.1017620673,-3.3764977606
C,1.2932058933,-3.0003535617,-3.626223748
C,-1.4676516913,-2.7289689576,-4.2437315223
C,0.4668146414,-2.1785754338,-2.8859331061
C,0.7194533906,-3.6957908088,-4.7066203213
C,-0.6303103401,-3.5619780671,-5.00844054
C,-0.8971181253,-2.0438091266,-3.1889188986
H,1.3452367717,-4.3455362072,-5.3102170984
H,-1.0513672366,-4.108462335,-5.8465249938
H,-2.5232268817,-2.6209519667,-4.4705329045
O,-1.4909539648,-1.1885537664,-2.3248007319
O,0.7880939265,-1.4245990951,-1.8063870597
B,-0.4477119325,-0.7429859487,-1.3658401482
H,0.5884331044,3.8350130206,1.5900938527
C,0.2471046597,4.0024735786,0.5731245175
C,-0.6872154954,4.3929417611,-2.1030311512
C,0.0440894113,2.9486744486,-0.2964333569
C,-0.0297162643,5.2817836839,0.0742474557
C,-0.483653016,5.4719068731,-1.2328129815
C,-0.4149568567,3.1351147978,-1.5997459624
H,0.1086691534,6.1426713513,0.7202441854
H,-0.6893071131,6.4779904348,-1.5835089561
H,-1.0481107195,4.5317925832,-3.1162453642
O,-0.5590699678,1.9139394096,-2.2028835339
O,0.2018960201,1.6095167133,-0.0706803822
B,-0.2474066825,0.9616627937,-1.2260293929

IA-*E*,*Z*[1,1]^{DMF} (Intermediate monocoordinate *E*-coordinated 1,1-B_2cat_2-*E*,*Z*-diimine **1** complex in DMF)
E-coord_cydiimph2_EZ_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1419163

Zero-point correction= 0.571675 (Hartree/Particle)
Thermal correction to Energy= 0.603956
Thermal correction to Enthalpy= 0.604900
Thermal correction to Gibbs Free Energy= 0.505967
Sum of electronic and ZPE= -1696.570241
Sum of electronic and thermal Energies= -1696.537961
Sum of electronic and thermal Enthalpies= -1696.537016
Sum of electronic and thermal Free Energies= -1696.635949

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.988	129.993	208.221

C,0.7658525336,-1.8647022519,1.5360039015
C,1.1418389893,-4.3705107957,1.4633270215
C,-0.8604352264,-3.3909413426,0.2934101858
C,-0.3202949485,-4.5939419874,1.0721107094
C,-0.6966388423,-2.133277006,1.1431263614
C,1.3039959513,-3.0918479449,2.2864780291
H,1.750713457,-4.2959323026,0.5525294923
H,-0.3068488926,-3.3009190168,-0.6434636012
H,-0.9208806272,-4.7455516588,1.978593887
H,-1.2351849196,-2.301616256,2.0833242372
H,0.75831001,-3.1838940385,3.2347911502
H,1.3603144316,-1.7161413284,0.631379117
H,1.5197622212,-5.2256278687,2.0326458376
H,-1.9192226244,-3.5247355052,0.0472871025
H,-0.4196692836,-5.4984666562,0.4644077869
H,2.3564049721,-2.9128232421,2.5318409048
N,-1.3026318853,-0.9202432218,0.5344806837
N,0.7680285439,-0.7281302114,2.4493982957
C,1.7046126356,0.1313044283,2.462766512
C,-2.0747079003,-0.2457527808,1.3139052178
H,-2.2060482257,-0.6209684962,2.329195354
H,1.638997679,0.8926177501,3.2478846976
C,-2.7637246447,1.0193453108,1.0352455912
C,-3.8922076605,3.5448981568,0.6808011025
C,-3.3233844416,1.3665346502,-0.2008320974
C,-2.8198775128,1.9254118661,2.1054306556
C,-3.3644046516,3.1899860042,1.9227180587

C,-3.8853757811,2.6296008395,-0.3698302768
H,-3.3231218365,0.6543895451,-1.0189879418
H,-2.4061141953,1.6392683517,3.0686575833
H,-3.3810542762,3.8965606441,2.745977074
H,-4.315029244,2.8992394602,-1.3292341245
H,-4.3204318248,4.531866502,0.535972019
C,2.9296952047,0.2487128154,1.6203556325
C,5.3072820311,0.5488550312,0.1735893183
C,4.1406580363,0.4827494233,2.2827681036
C,2.9156474514,0.1968028381,0.2217969259
C,4.1005797575,0.347188126,-0.4943502477
C,5.3257045402,0.6180470279,1.5654683132
H,4.149649395,0.5537010715,3.367500624
H,1.9813273932,0.0526663451,-0.3105885856
H,4.0785421768,0.3107061571,-1.5792459115
H,6.2601875458,0.7861790463,2.091572783
H,6.2285595334,0.6628181494,-0.3892582575
H,1.8382541049,-2.8355182982,-3.0182350686
C,0.7926925153,-2.6834319488,-3.266428758
C,-1.952209688,-2.2749877386,-3.8792678532
C,0.0014048739,-1.8448859942,-2.5074225339
C,0.1910782992,-3.3258615195,-4.3642395207
C,-1.1511814721,-3.1252028372,-4.663223399
C,-1.3543133851,-1.6418718074,-2.8068202196
H,0.7886234248,-3.9873696431,-4.9834355986
H,-1.5944525526,-3.6314192683,-5.5149984249
H,-3.001430923,-2.1143350334,-4.104290203
O,-1.9122892313,-0.7816357731,-1.9243887991
O,0.3536243655,-1.1328237699,-1.4076846747
B,-0.8492387692,-0.3895149723,-0.9634538187
H,0.5941484183,4.2494177451,1.78043038
C,0.2004862339,4.3872545462,0.7792151523
C,-0.8525930087,4.7167224803,-1.8584114761
C,-0.1141415618,3.3086462165,-0.0244209127
C,-0.0274399922,5.6581545087,0.2363526983
C,-0.541300726,5.818856825,-1.0519958033
C,-0.6265129325,3.468294648,-1.3112922602
H,0.1991552936,6.5358971459,0.832678801
H,-0.7068905446,6.8191325022,-1.4385581251
H,-1.2561820231,4.8309900384,-2.8584664331
O,-0.8657438644,2.2349890704,-1.853960194
O,-0.0231900323,1.9712575163,0.2553109965
B,-0.5597318678,1.3058197926,-0.8539431873

IA-*Z,E*[1,1]^{DMF} (Intermediate monocoordinate *Z*-coordinated 1,1-B_2cat_2-*Z,E*-diimine **1** complex in DMF)
Z-coord_cydiimph2_ZE_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1579023

Zero-point correction= 0.571120 (Hartree/Particle)
Thermal correction to Energy= 0.603444
Thermal correction to Enthalpy= 0.604388
Thermal correction to Gibbs Free Energy= 0.504877
Sum of electronic and ZPE= -1696.586782
Sum of electronic and thermal Energies= -1696.554459
Sum of electronic and thermal Enthalpies= -1696.553515
Sum of electronic and thermal Free Energies= -1696.653025

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.667	130.131	209.437

C,-0.3621591731,0.391350036,1.9677351304
C,-1.7947014145,0.7206047835,4.0487233824
C,-2.8978645348,0.5823594002,1.8002365218
C,-2.9531593839,1.2236711181,3.186621333
C,-1.5520359591,0.8983830753,1.14054954
C,-0.4505033344,0.9990462837,3.3770077292
H,-1.9063808389,-0.3600783361,4.2061133872
H,-3.0101469512,-0.5012685351,1.8921367142
H,-2.8914976751,2.3161226809,3.0908744819
H,-1.4274672479,1.98454216,1.094632265
H,-0.2963073398,2.0826704813,3.2871597886
H,-0.3892357422,-0.706404421,2.0441370652
H,-1.8159700961,1.1933061775,5.0357295633
H,-3.7105386111,0.9436481519,1.1605094094
H,-3.9121824145,0.994486951,3.6611826139
H,0.3770120126,0.6030601956,3.974911077
N,-1.4789532521,0.3830171181,-0.2398440864
N,0.8619611508,0.8560371322,1.3208869326
C,1.9511623905,0.2744666175,1.6264691558
C,-1.5006379511,1.1549760077,-1.2648668303
H,-1.3504376847,0.6516705575,-2.2200087683
H,1.9872990802,-0.5783189051,2.3213725022
C,-1.668761454,2.6148320813,-1.3444567464
C,-1.8967957193,5.3749395339,-1.6966958259
C,-0.9128567937,3.2685216339,-2.3276643017
C,-2.5710287502,3.3512747783,-0.5641128064
C,-2.6841324823,4.7249840207,-0.7471086258

C,-1.0105792619,4.6458925424,-2.4876292461
H,-0.2413116589,2.6901988233,-2.9562399842
H,-3.2071966778,2.8522030196,0.1593512591
H,-3.3923924387,5.2883937765,-0.1486784752
H,-0.407742107,5.1469905508,-3.237711146
H,-1.9854463052,6.4485292111,-1.8298959647
C,3.2484724262,0.711730457,1.0729947529
C,5.7208735092,1.479939362,0.0289277942
C,4.4248816737,0.1251398032,1.5458017134
C,3.3151813205,1.6890856136,0.0713070835
C,4.5459889528,2.0677632203,-0.4483110467
C,5.659763252,0.5114761176,1.027772264
H,4.3679644548,-0.6400728333,2.3162394023
H,2.3935057454,2.129803727,-0.296231699
H,4.5954642918,2.8200990921,-1.2295546224
H,6.5703553073,0.0505978154,1.3977559469
H,6.6810579927,1.7771843412,-0.3813785646
H,-4.2591471046,-3.1033786475,1.5447839156
C,-4.234501953,-2.889708453,0.4809458249
C,-4.1397037836,-2.3292502772,-2.3042399202
C,-3.1133372944,-2.3312473442,-0.1026862647
C,-5.3296700241,-3.1723431203,-0.3540206727
C,-5.282971036,-2.8983905554,-1.7166089655
C,-3.0675594553,-2.0509623371,-1.4783408839
H,-6.2247681823,-3.6101287579,0.0765432842
H,-6.1419085832,-3.1244535135,-2.3406131405
H,-4.0939636604,-2.1123460826,-3.3664739714
O,-1.8621110329,-1.5245035368,-1.813830824
O,-1.9398115574,-1.9937907089,0.4892974881
B,-1.1940633399,-1.2318778095,-0.5255647518
H,3.3863195716,-3.8858252752,1.1761637637
C,3.5179366951,-3.1901513175,0.3545808343
C,3.8341361174,-1.3482670994,-1.8099642854
C,2.4591279542,-2.4534275518,-0.1425673204
C,4.7608350808,-2.9885320534,-0.2576024936
C,4.9145541732,-2.0885781561,-1.315539037
C,2.6122518888,-1.556470321,-1.1977846178
H,5.6223972598,-3.5433892855,0.0992703783
H,5.8944946879,-1.9542901004,-1.76228241
H,3.9451200295,-0.6425301779,-2.6260019605
O,1.4022824662,-0.9767735491,-1.4699546692
O,1.1492281652,-2.4506428807,0.2585791404
B,0.4920106105,-1.527707507,-0.5611255104

IA-*Z,Z*[1,1]^{DMF} (Intermediate monocoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in DMF)
Z-coord_cydiimph2_ZZ_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1469195

Zero-point correction= 0.572178 (Hartree/Particle)
Thermal correction to Energy= 0.604172
Thermal correction to Enthalpy= 0.605116
Thermal correction to Gibbs Free Energy= 0.507406
Sum of electronic and ZPE= -1696.574742
Sum of electronic and thermal Energies= -1696.542748
Sum of electronic and thermal Enthalpies= -1696.541803
Sum of electronic and thermal Free Energies= -1696.639513

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.124	129.684	205.647

C,0.7507412676,-0.9544908556,0.7008025908
C,1.7900402077,-3.2713721595,0.7001451448
C,-0.4379090104,-2.9155217553,-0.4104823299
C,0.433430375,-3.897904214,0.3742834426
C,-0.6000590819,-1.6217064625,0.3965599302
C,1.6180087166,-1.9628688778,1.4712339356
H,2.3327553742,-3.0732678906,-0.2338365981
H,0.0313272433,-2.6980977486,-1.3725078565
H,-0.0717152808,-4.1755515812,1.308688077
H,-1.0441214283,-1.8911237409,1.3568147868
H,1.1216107324,-2.1591444063,2.4309305373
H,1.227426382,-0.6946750214,-0.2549390903
H,2.401386691,-3.9649974756,1.2860165132
H,-1.4298106713,-3.3369520322,-0.6068449036
H,0.5651333443,-4.8161559224,-0.2063741173
H,2.5884267671,-1.5123894757,1.6989281736
N,-1.5142913902,-0.6802425708,-0.281948738
N,0.4792907525,0.2180457686,1.521882277
C,1.3291643347,1.1246977045,1.8062579245
C,-2.6798225469,-0.4063638953,0.1780652142
H,-3.2890379335,0.2261311736,-0.467970527
H,0.9474124853,1.9036064024,2.4756042454
C,-3.3103280106,-0.8359898397,1.4408993808
C,-4.657963706,-1.5559055003,3.7730750182
C,-2.6693319341,-0.7248436426,2.6820498582
C,-4.6397242646,-1.2706767576,1.3792713792
C,-5.3033317858,-1.650161126,2.5411472327

C,-3.3486964848,-1.0815896159,3.8423754057
H,-1.6553160761,-0.3360330439,2.7279077727
H,-5.1443142667,-1.3190455539,0.4183602826
H,-6.3271601738,-2.0054044047,2.4863641332
H,-2.8549900259,-0.9855611002,4.8039906335
H,-5.1802832924,-1.8390717461,4.6815008464
C,2.7445141545,1.3770439895,1.4336865065
C,5.3867452816,2.1378756148,0.8609354921
C,3.3488463157,2.4523330983,2.1022231455
C,3.4912955432,0.6855330683,0.4658901816
C,4.7975971245,1.0708225761,0.182413146
C,4.6598419402,2.8268949029,1.8285777454
H,2.7732300458,3.0050398962,2.8406833823
H,3.0696462351,-0.1473297096,-0.0809039825
H,5.3599230433,0.5317596482,-0.5735046187
H,5.1073278243,3.6606822583,2.3602464123
H,6.407957957,2.4284085787,0.6348024171
H,0.0955097032,-2.8042021378,-4.2977756971
C,-0.8478757298,-2.2677291968,-4.2833984175
C,-3.3055407335,-0.8393755445,-4.2314169843
C,-1.0622620382,-1.2366319997,-3.3889438947
C,-1.891114907,-2.5856642891,-5.1703663235
C,-3.0927618174,-1.8860421071,-5.1456064147
C,-2.2781979055,-0.5342048534,-3.3596341667
H,-1.7522734226,-3.3916864773,-5.8839998581
H,-3.8836385189,-2.1506809579,-5.8403873117
H,-4.2398858767,-0.2881657249,-4.2050634858
O,-2.2410588087,0.4353781997,-2.4092879709
O,-0.2057324576,-0.737522858,-2.4626178161
B,-1.013359067,0.166134191,-1.6301929704
H,3.4392480549,3.4731977721,-1.6030127623
C,2.5892579396,3.8260825983,-1.0288672103
C,0.342409894,4.712485457,0.5024359253
C,1.4231932528,3.0899331374,-0.942827736
C,2.6196559543,5.031083265,-0.3172840103
C,1.5237567854,5.4613612289,0.435451978
C,0.3220564543,3.5265593459,-0.2084463904
H,3.5182211088,5.639098577,-0.3457865074
H,1.5856169529,6.3987917754,0.9784622255
H,-0.5154279291,5.0417031394,1.0784163478
O,-0.6859941767,2.6070438857,-0.3239344037
O,1.1294085172,1.8774518042,-1.5051333864
B,-0.1780839938,1.5711651953,-1.1140831514

IA-*E*,*E*[1,2]^{DMF} (Intermediate monocoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
E-coord_cydiimph2_EE_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1561642

Zero-point correction= 0.571514 (Hartree/Particle)
Thermal correction to Energy= 0.603474
Thermal correction to Enthalpy= 0.604418
Thermal correction to Gibbs Free Energy= 0.507024
Sum of electronic and ZPE= -1696.584650
Sum of electronic and thermal Energies= -1696.552691
Sum of electronic and thermal Enthalpies= -1696.551747
Sum of electronic and thermal Free Energies= -1696.649140

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.685	130.169	204.983

C,0.026832825,-2.0310333089,-1.1148316986
C,1.6654189578,-3.7681327842,-1.9699319461
C,2.4133002833,-1.3827915366,-1.6852597111
C,2.5721589753,-2.6615425028,-2.5111517315
C,0.9495638772,-0.9502134237,-1.698969953
C,0.2041489059,-3.3195132689,-1.9313663891
H,1.9885468143,-4.0330157439,-0.9545633359
H,2.7383509664,-1.5882749761,-0.6602781498
H,2.3138177958,-2.4546085275,-3.5576727692
H,0.6507546623,-0.8245266481,-2.7458998053
H,-0.1601449609,-3.1310235735,-2.9498037069
H,0.3056049036,-2.2364939855,-0.0686543356
H,1.7575203026,-4.6710638971,-2.5815431175
H,3.0403609925,-0.5750589467,-2.0771489962
H,3.6181839732,-2.981586747,-2.4935043744
H,-0.4328301709,-4.0963294685,-1.4957899429
N,-1.3474087914,-1.5605961191,-1.2084203366
N,0.7279195234,0.3571814871,-1.0337708335
C,-0.0813099554,1.1512100425,-1.6471472463
H,-0.5514210926,0.7615894762,-2.5511700426
C,-2.1801472483,-2.0269433955,-0.36954436
H,-1.8879427833,-2.7594042524,0.3970092855
B,1.3725935534,0.6197254671,0.4494197736
B,1.6746283517,-0.6884256679,1.4824594692
O,2.9566478711,-1.0672202018,1.8076125281
O,0.3984995844,1.4257758537,1.1987363966
C,3.8109225441,0.7875030429,0.4605383548

C,6.3824392963,-0.3139150989,0.7968356152
C,3.9959832851,-0.405408834,1.1952674758
C,4.9394473922,1.4034983882,-0.0869448569
C,6.2127489818,0.8665761097,0.0781180482
C,5.2696985014,-0.9411388003,1.3507748374
H,4.785645413,2.3197911455,-0.6486536097
H,7.0677136957,1.371144179,-0.3605544809
H,5.3652705037,-1.8594362902,1.9220597756
H,7.3686945002,-0.7455159473,0.930199195
O,2.610101292,1.3759649721,0.2598784817
C,-0.6595688959,0.7491616318,1.7031627464
C,-2.873217415,-0.5479457765,2.846505212
C,-0.5296786039,-0.5431025443,2.2594053323
C,-1.9173782407,1.3564539099,1.7133012556
C,-3.0165198284,0.7188249535,2.2855695528
C,-1.628562615,-1.1754625787,2.8293333353
H,-2.0020197764,2.3491131054,1.2792277333
H,-3.9845284307,1.2104472351,2.2835525056
H,-1.4860423912,-2.1614252609,3.2617047373
H,-3.7248193917,-1.0526529402,3.2910710577
O,0.6925533937,-1.1685032038,2.3238479379
C,-0.4686817991,2.5242058349,-1.314054869
C,-1.3619865602,5.1184982375,-0.8221796401
C,0.3795903337,3.4491282636,-0.6899003769
C,-1.7472418375,2.9221102629,-1.7282042511
C,-2.2027488441,4.2085956998,-1.4600578124
C,-0.0686688504,4.7420464043,-0.4544630765
H,1.3831351814,3.1544101459,-0.4049180576
H,-2.3865191803,2.2133645484,-2.2481368439
H,-3.2022480401,4.5038156856,-1.7616371444
H,0.5910255889,5.4614032097,0.0197987202
H,-1.7073817813,6.1286920449,-0.62504703
C,-3.5962343187,-1.6124075614,-0.356745331
C,-6.2612161872,-0.7936635819,-0.2261783229
C,-4.5094704682,-2.3135785976,0.4348304966
C,-4.0238292609,-0.493766537,-1.0807790913
C,-5.3506624559,-0.0860756642,-1.0139994488
C,-5.8406138894,-1.9092617767,0.4956640199
H,-4.1685769488,-3.1714718701,1.0094595235
H,-3.3001187109,0.0543933632,-1.6768017497
H,-5.6774543275,0.7875193056,-1.5696527217
H,-6.5468904658,-2.4583751555,1.1103500493
H,-7.2965275046,-0.4714060106,-0.1723709559

IA-*E*,*Z*[1,2]^{DMF} (Intermediate monocoordinate *E*-coordinated 1,2-B_2cat_2-*E*,*Z*-diimine **1** complex in DMF)
E-coord_cydiimph2_EZ_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1464269

Zero-point correction= 0.572432 (Hartree/Particle)
Thermal correction to Energy= 0.604117
Thermal correction to Enthalpy= 0.605061
Thermal correction to Gibbs Free Energy= 0.509305
Sum of electronic and ZPE= -1696.573995
Sum of electronic and thermal Energies= -1696.542310
Sum of electronic and thermal Enthalpies= -1696.541366
Sum of electronic and thermal Free Energies= -1696.637122

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.089	129.785	201.536

C,0.8324988004,-1.0918133394,1.7101354087
C,0.186308711,-3.384140265,2.5927066112
C,-1.6009180411,-1.8049372629,1.7966007728
C,-1.2572097804,-2.9187929179,2.7872354083
C,-0.6198554683,-0.6453528813,1.9574137723
C,1.1571595748,-2.2107614541,2.7157968469
H,0.2905381596,-3.8396354362,1.5984884903
H,-1.5357256983,-2.2130525471,0.7829293223
H,-1.3858032722,-2.5494004906,3.8127841937
H,-0.6667820482,-0.3037927956,2.9971857779
H,1.0934543058,-1.7778659364,3.7224342962
H,0.9092498824,-1.473738179,0.6827453009
H,0.4428906868,-4.1538095784,3.3272876378
H,-2.6242860631,-1.4437927884,1.9421303826
H,-1.9519837588,-3.7534464004,2.6543408985
H,2.19203391,-2.5376134767,2.5764956624
N,1.7060123921,0.0442577688,1.9385108566
N,-0.982544364,0.5176802905,1.1111902442
C,-0.8694766192,1.6659864917,1.6847690722
H,-0.4595946147,1.6669459866,2.6952785312
C,2.8951843004,0.1145647562,1.4866509434
H,3.4330332936,1.0278997255,1.7627282935
B,-1.3572234638,0.2673490702,-0.4642661992
B,-0.627931046,-1.0120587056,-1.299340212
O,-1.3617797237,-2.0828177904,-1.7561129116
O,-0.9065245976,1.4485913959,-1.2145268859
C,-3.3910716378,-1.0275572225,-0.8798414289

C,-4.7517024788,-3.4135783255,-1.5110108416
C,-2.7027391033,-2.123333069,-1.4486619092
C,-4.7622441496,-1.1636763029,-0.6460744697
C,-5.4410992905,-2.3375884235,-0.9579716691
C,-3.3855529991,-3.2965043115,-1.7516346194
H,-5.2798492462,-0.3155629027,-0.2084015268
H,-6.5065208917,-2.4080235679,-0.7632353538
H,-2.8171566104,-4.1129561923,-2.186511197
H,-5.2670939546,-4.3361467191,-1.7560438407
O,-2.8113619701,0.1471253456,-0.5462534715
C,0.422682847,1.5224100958,-1.4562296187
C,3.1589234503,1.7617824324,-2.0347724285
C,1.1952127132,0.3804153782,-1.7707052808
C,1.050356708,2.7689442792,-1.4321128276
C,2.4081608855,2.8915421356,-1.7205417783
C,2.5464298793,0.5098463167,-2.0653681388
H,0.4410357739,3.6362028373,-1.1923387054
H,2.8752347334,3.8711180352,-1.6976719267
H,3.1087549709,-0.3874659916,-2.3091945787
H,4.2177133709,1.8458588388,-2.2582038318
O,0.6137551367,-0.8607899881,-1.8814628072
C,-1.2315730745,2.991139463,1.1759682929
C,-1.8228799051,5.5878888214,0.3594487235
C,-2.3275357268,3.225670375,0.3351884235
C,-0.4627612356,4.067521339,1.6375130642
C,-0.7425133668,5.3611635566,1.2103437448
C,-2.6219343316,4.5233817437,-0.0624191176
H,-2.9432645931,2.3950124836,0.0078129445
H,0.3653648151,3.8803344261,2.3158289947
H,-0.1299670226,6.1894394048,1.5507568994
H,-3.4756717008,4.7083413115,-0.706222303
H,-2.0542047978,6.5981271169,0.0360278558
C,3.7257025927,-0.7657021595,0.6232953706
C,5.450740177,-2.1261889958,-1.1347274332
C,4.9410854446,-0.1966081579,0.2104394916
C,3.4029759546,-2.0500866237,0.1545600863
C,4.2598910911,-2.7171841303,-0.7171497733
C,5.7948186329,-0.861366804,-0.6611138132
H,5.2046689139,0.7957328423,0.5673578029
H,2.4970129369,-2.5553925455,0.4594564648
H,3.9921825713,-3.7080082408,-1.0702426575
H,6.7240977914,-0.3939492623,-0.9710496876
H,6.1103512389,-2.6524968823,-1.8176326391

IA-*Z*,*E*[1,2]^{DMF} (Intermediate monocoordinate *Z*-coordinated 1,2-B_2cat_2-*Z*,*E*-diimine **1** complex in DMF)
Z-coord_cydiimph2_ZE_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1566691

Zero-point correction= 0.571676 (Hartree/Particle)
Thermal correction to Energy= 0.603690
Thermal correction to Enthalpy= 0.604634
Thermal correction to Gibbs Free Energy= 0.506849
Sum of electronic and ZPE= -1696.584993
Sum of electronic and thermal Energies= -1696.552979
Sum of electronic and thermal Enthalpies= -1696.552035
Sum of electronic and thermal Free Energies= -1696.649820

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.821	130.109	205.805

C,0.2061064972,0.008270096,1.8153146362
C,-1.2927054462,0.1352180793,3.874077928
C,-2.2107897156,0.868477417,1.6636204735
C,-2.2035685529,1.1386150593,3.1677125539
C,-0.7921214792,0.943114221,1.1032576214
C,0.1322876884,0.2314684409,3.3334207036
H,-1.6813582209,-0.8796388139,3.7153389201
H,-2.6310484184,-0.1278900656,1.5004576778
H,-1.8463477073,2.1583782361,3.3615060511
H,-0.4104546076,1.9531165988,1.2615896299
H,0.5386392198,1.2291767656,3.5440869184
H,-0.0344009417,-1.0439461514,1.5839324074
H,-1.2873216348,0.3124211667,4.9540148308
H,-2.8452624181,1.5843353338,1.1291148631
H,-3.2250833086,1.073447991,3.5539110285
H,0.7921565037,-0.4954332311,3.8179012109
N,1.5397463071,0.3766304275,1.3710533699
N,-0.7509569746,0.6382135246,-0.3398157
C,-0.0754900624,1.3431951557,-1.1716728325
H,-0.0047268757,0.9248203259,-2.1764882208
C,2.3498323424,-0.5374349506,1.0189951201
H,2.0690950365,-1.6012208426,1.0053040534
B,-1.5368515437,-0.6637848425,-0.9837293167
B,-2.03172669,-1.9699461423,-0.0360518076
O,-3.3565631749,-2.165366593,0.2777135662
O,-0.6113952275,-1.2243646746,-1.9775357391
C,-3.9219006469,-0.2234654077,-1.0966680748

C,-6.5161997813,-0.3567828632,-0.0044933907
C,-4.2546684035,-1.208491771,-0.1383110602
C,-4.9191234786,0.6736742324,-1.4885843087
C,-6.203383477,0.6108893999,-0.9555762004
C,-5.5364544809,-1.2611051032,0.397301937
H,-4.6537738654,1.4241776317,-2.2267618422
H,-6.9543201085,1.323031756,-1.2826926189
H,-5.7473727122,-2.0329315164,1.1311866039
H,-7.5121494042,-0.4138829262,0.4216689104
O,-2.7022634053,-0.1083090694,-1.6671438806
C,0.3057812904,-2.0992095315,-1.4987607862
C,2.2381080483,-3.9575512566,-0.6443360284
C,0.0242383645,-3.0058532545,-0.449492544
C,1.5717095701,-2.1410154839,-2.0870538552
C,2.528686486,-3.0642141714,-1.6730183494
C,0.9850274315,-3.9217933873,-0.0362651785
H,1.7791287933,-1.4388842655,-2.889247916
H,3.5032544176,-3.0767124211,-2.1510568836
H,0.7246130724,-4.6086976134,0.7631653124
H,2.9778198335,-4.6800657738,-0.3149923192
O,-1.213095892,-3.0627682517,0.1454067554
C,0.629956295,2.6186882173,-0.9554580242
C,2.0475694019,5.0051311083,-0.7052346642
C,0.0350571326,3.7231607399,-0.3330207001
C,1.9198805079,2.7284296914,-1.4872755265
C,2.634818637,3.9132232287,-1.3417208078
C,0.7449629892,4.9130732744,-0.2149626886
H,-0.9865051462,3.6592092078,0.0305578548
H,2.3642763211,1.8767268588,-1.9958158951
H,3.6441330733,3.9857744169,-1.7341792339
H,0.2792498618,5.7711576946,0.2583906699
H,2.5993942985,5.9341866665,-0.6031449238
C,3.7381657523,-0.2218827684,0.6200068992
C,6.366871682,0.3362349152,-0.1473811808
C,4.6279595604,-1.2628065565,0.3403837526
C,4.1797344663,1.1046518567,0.5270103437
C,5.4851542819,1.3808075091,0.1399947949
C,5.9388911856,-0.9850916585,-0.0410721869
H,4.2869196774,-2.2909783312,0.4242031412
H,3.4875473081,1.9073253482,0.7608034575
H,5.8198307576,2.4109922884,0.0638459892
H,6.6241637066,-1.799091273,-0.2556320706
H,7.3867140027,0.5544140815,-0.4490822301

IA-*Z,Z*[1,2]^{DMF} (Intermediate monocoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in DMF)
Z-coord_cydiimph2_ZZ_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.145746

Zero-point correction= 0.572509 (Hartree/Particle)
Thermal correction to Energy= 0.604250
Thermal correction to Enthalpy= 0.605194
Thermal correction to Gibbs Free Energy= 0.508946
Sum of electronic and ZPE= -1696.573237
Sum of electronic and thermal Energies= -1696.541496
Sum of electronic and thermal Enthalpies= -1696.540552
Sum of electronic and thermal Free Energies= -1696.636800

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.173	129.694	202.571

C,-1.0853016496,-0.8044116699,0.1726338613
C,-2.7316267883,-0.9304514789,2.0999297667
C,-0.3173298349,-0.3989525598,2.558823195
C,-1.5796565811,-1.0748058865,3.0953913668
C,0.0500586668,-0.9871414492,1.1990825013
C,-2.3437729721,-1.4889068637,0.7313915103
H,-2.9921008713,0.1319190644,1.9981187311
H,-0.51189512,0.6744158355,2.4558763047
H,-1.3787616883,-2.1400798588,3.2682226129
H,0.1941848988,-2.0637062099,1.304414972
H,-2.1285443797,-2.5621547919,0.8124532797
H,-1.2661972847,0.2718403397,0.0433557548
H,-3.6235388988,-1.445962212,2.4694038341
H,0.5239546186,-0.5150523388,3.2504950899
H,-1.8486869534,-0.6356744196,4.0606817634
H,-3.1636799853,-1.3822963985,0.014530703
N,-0.679847885,-1.4429768884,-1.0660852112
N,1.2879278438,-0.4015900041,0.6551570857
C,2.2036759357,-1.1310546342,0.1318759178
H,3.0084438032,-0.5820586563,-0.3571311794
C,-1.199572937,-1.1744965304,-2.1977284521
H,-0.7949570309,-1.7587263431,-3.0314753009
B,1.5228601434,1.2246612745,0.6655198671
B,0.2268332526,2.2862257449,0.4661474114
O,-0.2006658381,3.1016294688,1.4871237017
O,2.4066581355,1.4993291037,-0.4801265256
C,1.6273089754,2.2471833709,2.879584714

C,0.5160582791,3.7204247488,5.0121359346
C,0.4474244314,3.0058970376,2.6984579383
C,2.2226223132,2.2557937694,4.1445006717
C,1.6822595439,2.9832899079,5.2003689519
C,-0.0917975628,3.7249696574,3.7597910571
H,3.1272263428,1.6692619666,4.2723999733
H,2.1728670618,2.967099161,6.1684016692
H,-0.9984644978,4.2927886012,3.574575808
H,0.0809586146,4.2894284257,5.8268079267
O,2.2185033078,1.5092598745,1.915183227
C,1.7822324133,1.5444752378,-1.6842428289
C,0.5901245121,1.6566489964,-4.2265684342
C,0.485695123,2.0864601004,-1.8498252551
C,2.447487451,1.0562093155,-2.8099370894
C,1.8618668893,1.1118364019,-4.073132445
C,-0.0894993415,2.1465636673,-3.1130123408
H,3.442112937,0.6425648366,-2.6704768673
H,2.4020475335,0.7269297644,-4.9322461501
H,-1.0854031513,2.5721195513,-3.2023620243
H,0.1213794516,1.702180768,-5.2043534121
O,-0.2059263048,2.6353000199,-0.7953905773
C,2.3084384777,-2.6026774528,0.1031635201
C,2.6443504513,-5.3636764671,-0.0551446578
C,2.2310245214,-3.3832608253,1.2618671951
C,2.5851809524,-3.2051138828,-1.1289193185
C,2.7330411722,-4.5857222266,-1.2087520209
C,2.4045616161,-4.7611554273,1.1788738161
H,2.0570815501,-2.9097250215,2.2241681793
H,2.6684618471,-2.5880108312,-2.0196742041
H,2.9286039945,-5.0530419658,-2.1683443853
H,2.3535259994,-5.3640965046,2.0795867894
H,2.7726052764,-6.4397487015,-0.1161497194
C,-2.2307648895,-0.208147468,-2.6594329871
C,-4.0044910203,1.6266804871,-3.8455556433
C,-2.3796885265,-0.1366381994,-4.0538665756
C,-3.0128967564,0.6474438092,-1.8655524301
C,-3.8863486757,1.5554248753,-2.4589989252
C,-3.2509111607,0.7695909148,-4.6456168039
H,-1.7824956236,-0.7937547487,-4.6807428929
H,-2.9674932018,0.6215203467,-0.7853801745
H,-4.480400493,2.2099934138,-1.8291495308
H,-3.3404759783,0.8083718937,-5.726614799
H,-4.6864544852,2.3395371739,-4.2985074303

IA-*E*,*E*[1,1]^{benzene} (Intermediate monocoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in benzene)
E-coord_cydiimph2_EE_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1512803

Zero-point correction= 0.572327 (Hartree/Particle)
Thermal correction to Energy= 0.604352
Thermal correction to Enthalpy= 0.605296
Thermal correction to Gibbs Free Energy= 0.508483
Sum of electronic and ZPE= -1696.578953
Sum of electronic and thermal Energies= -1696.546929
Sum of electronic and thermal Enthalpies= -1696.545985
Sum of electronic and thermal Free Energies= -1696.642798

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.236	129.867	203.760

C,1.2418853962,-2.2136502716,1.0590259292
C,1.6093419376,-4.7168347712,0.9884651002
C,-0.4497283771,-3.7409132878,-0.0861602906
C,0.131660526,-4.9433996912,0.6628737641
C,-0.2417143298,-2.4756771649,0.7446851305
C,1.8048466141,-3.4336138085,1.7978796941
H,2.1757604526,-4.6449188693,0.0505602922
H,0.0478308676,-3.6485373129,-1.0542955308
H,-0.4257825634,-5.1026572259,1.5957606358
H,-0.7306023073,-2.6308012732,1.7153215964
H,1.2985362885,-3.5164999495,2.7685928922
H,1.7853725016,-2.0751797538,0.1157198307
H,2.0140822059,-5.5706749773,1.5407781232
H,-1.5195171706,-3.8752839143,-0.2777536048
H,0.0061499561,-5.8461074044,0.0577766265
H,2.8652381284,-3.2569237285,2.0045428235
N,-0.8836175383,-1.2828596401,0.1380115702
N,1.32509215,-1.0402241242,1.9128848202
C,2.0275583337,-0.0684475221,1.494474676
C,-1.681059886,-0.6319231101,0.9090188539
H,-1.7802156335,-0.989118848,1.9361552306
H,2.5505368762,-0.1061201368,0.5271866036
C,-2.4500205711,0.5809966343,0.60772447
C,-3.7503080375,3.0122346462,0.191226779
C,-3.0305922005,0.8573920206,-0.6363304378
C,-2.5665376096,1.5095943208,1.6528119996
C,-3.197531264,2.7274026315,1.4393629111

C,-3.6790210118,2.0732669938,-0.8346965188
H,-2.9720481356,0.1296448244,-1.4386838383
H,-2.1229540375,1.2855657141,2.6191927924
H,-3.255097257,3.455324813,2.2416133644
H,-4.1198316003,2.2892930695,-1.8022197479
H,-4.2412495594,3.9649455583,0.0207854475
C,2.2008707941,1.1796746332,2.2636119729
C,2.5708314423,3.5562024781,3.6822692076
C,3.0671813064,2.1621826373,1.7800013247
C,1.5111507225,1.3975532023,3.4612482041
C,1.6935398278,2.5816500428,4.1642548007
C,3.2578784164,3.3450466309,2.4896805619
H,3.5905375093,1.9967680806,0.8417039787
H,0.8418834445,0.6238003887,3.8244604022
H,1.1574654738,2.748007206,5.0935624777
H,3.9347238493,4.1026998373,2.1081202893
H,2.7153667459,4.4780339845,4.2370987041
H,2.3452013784,-3.1261013309,-3.3600378306
C,1.2947907239,-3.0265690015,-3.6124958413
C,-1.4621508891,-2.7479794028,-4.2385664628
C,0.4713516839,-2.1912024746,-2.8859106076
C,0.719493427,-3.7318706782,-4.6838236139
C,-0.6285529137,-3.5951175139,-4.9889603826
C,-0.8896390252,-2.0523942883,-3.1930340321
H,1.3422566517,-4.3917324757,-5.2790834553
H,-1.0500568521,-4.1497242535,-5.8211559237
H,-2.5161613064,-2.6347843634,-4.4677586359
O,-1.4800615435,-1.1827618722,-2.3380992372
O,0.7928779434,-1.4270725129,-1.8103409472
B,-0.4375562798,-0.734684107,-1.3902747469
H,0.6162971732,3.8305811067,1.5777693424
C,0.2654137877,4.0029079328,0.565429061
C,-0.6850533408,4.3991105715,-2.10233628
C,0.0592665182,2.9515455854,-0.305369135
C,-0.0168778194,5.2821820222,0.0719992322
C,-0.4782239438,5.4754175546,-1.231229754
C,-0.4091370093,3.1403364836,-1.6046173973
H,0.1253691502,6.1417789731,0.7187746309
H,-0.6853434031,6.4823974365,-1.5783198758
H,-1.0504857338,4.5372242471,-3.1136222449
O,-0.5587201962,1.9222774063,-2.209540777
O,0.221683756,1.6112184615,-0.0854750661
B,-0.233874604,0.9681028707,-1.2422239209

IA-*E*,*Z*[1,1]^{benzene} (Intermediate monocoordinate *E*-coordinated 1,1-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
E-coord_cydiimph2_EZ_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1398021

Zero-point correction= 0.572332 (Hartree/Particle)
Thermal correction to Energy= 0.604714
Thermal correction to Enthalpy= 0.605658
Thermal correction to Gibbs Free Energy= 0.504414
Sum of electronic and ZPE= -1696.567470
Sum of electronic and thermal Energies= -1696.535088
Sum of electronic and thermal Enthalpies= -1696.534144
Sum of electronic and thermal Free Energies= -1696.635389

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.464	129.827	213.088

C,0.740533225,-1.8409345647,1.5140676628
C,1.1872053749,-4.3346737048,1.4207618883
C,-0.8559959867,-3.4069127267,0.2772958484
C,-0.2714212423,-4.5988593242,1.0408926696
C,-0.717246441,-2.149758308,1.1323075657
C,1.3208686458,-3.0568290979,2.2508585547
H,1.7843272845,-4.2365319541,0.5047860381
H,-0.3200878096,-3.2934805419,-0.66678656
H,-0.8578475886,-4.7796729443,1.9518418794
H,-1.2363463022,-2.3372122162,2.0809678804
H,0.7900561602,-3.1676615196,3.2057445922
H,1.3199803998,-1.6694198795,0.6042358416
H,1.5961649295,-5.1827914163,1.9789648304
H,-1.9126298647,-3.5698540954,0.0399535781
H,-0.3496149613,-5.5006979345,0.4265665378
H,2.3698075519,-2.8495302658,2.487127135
N,-1.3637840989,-0.9534257316,0.5378131297
N,0.7085439094,-0.7118939152,2.434111812
C,1.6110929638,0.1819513859,2.4484553943
C,-2.1372362267,-0.2963217013,1.3282037787
H,-2.232881864,-0.6701973991,2.3485447862
H,1.5110755174,0.9362062219,3.2373930743
C,-2.8797318588,0.9388508192,1.0585635135
C,-4.191829421,3.3782270295,0.7437968935
C,-3.4396724789,1.2761754116,-0.1810828353
C,-3.019179395,1.8138394994,2.1463566052
C,-3.6569204317,3.0356074982,1.9850435476

C,-4.0931147866,2.495937171,-0.3289326064
H,-3.3745535019,0.5869984209,-1.0159121174
H,-2.5983855672,1.5381232744,3.1094996256
H,-3.740391908,3.7186248574,2.8236145723
H,-4.5230525895,2.7563799356,-1.2901897269
H,-4.6948221561,4.3314045045,0.6159628195
C,2.8348067918,0.3563384087,1.6143081498
C,5.213284535,0.766004293,0.1964506044
C,4.0194179977,0.6790260671,2.2865142971
C,2.8471163176,0.2703421202,0.2174158619
C,4.0323555648,0.4755773041,-0.4827257833
C,5.2053877505,0.8690817489,1.585355684
H,4.0077351941,0.7749550943,3.3694618397
H,1.9333937485,0.0623463472,-0.3287632478
H,4.028004923,0.4138217065,-1.5663776192
H,6.1189643634,1.1068790537,2.1209726396
H,6.1342838925,0.9233986053,-0.356021786
H,1.7847678588,-2.7849854083,-3.0337232925
C,0.7359310048,-2.6514030439,-3.2771719167
C,-2.0168244542,-2.2846178008,-3.8741173312
C,-0.0630688291,-1.8228873109,-2.5168137604
C,0.1375217714,-3.3048774918,-4.3684306889
C,-1.2087124283,-3.1248720186,-4.6589507978
C,-1.421735549,-1.6399767714,-2.8084425368
H,0.7402884429,-3.9586597391,-4.9903163561
H,-1.6488745153,-3.6397293135,-5.5068766504
H,-3.069063366,-2.1380728196,-4.0921485919
O,-1.9870643638,-0.7863402224,-1.9214017775
O,0.2831697337,-1.1065101907,-1.4150546706
B,-0.9305101702,-0.3897132337,-0.9654785663
H,1.0011117381,4.0871356455,1.7383835395
C,0.5882821889,4.2694837838,0.7525564889
C,-0.4937801922,4.7095668267,-1.8538044708
C,0.0790184819,3.2388547842,-0.0119296254
C,0.5445865312,5.5488847386,0.1866153939
C,0.0150058559,5.7637622575,-1.0863973127
C,-0.4464606443,3.4519637373,-1.2849931689
H,0.9332713326,6.3902992439,0.7506005867
H,-0.0010869182,6.769360787,-1.4934023418
H,-0.9035980867,4.8629777474,-2.8456145965
O,-0.8672046788,2.2571716476,-1.8015533875
O,-0.0110518446,1.9059652441,0.287816223
B,-0.6215794601,1.2977814434,-0.8167692503

IA-*Z*,*E*[1,1]^{benzene} (Intermediate monocoordinate *Z*-coordinated 1,1-B_2cat_2-*Z*,*E*-diimine **1** complex in benzene)
Z-coord_cydiimph2_ZE_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1533605

Zero-point correction= 0.572028 (Hartree/Particle)
Thermal correction to Energy= 0.604234
Thermal correction to Enthalpy= 0.605179
Thermal correction to Gibbs Free Energy= 0.506674
Sum of electronic and ZPE= -1696.581333
Sum of electronic and thermal Energies= -1696.549126
Sum of electronic and thermal Enthalpies= -1696.548182
Sum of electronic and thermal Free Energies= -1696.646687

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.163	129.934	207.321

C,-0.3902313891,0.4286517389,1.9788210095
C,-1.842218909,0.7988819858,4.0400774719
C,-2.9286170197,0.6213917848,1.7855094818
C,-2.9915894155,1.290220693,3.1587516561
C,-1.5757094882,0.9136156694,1.1296497833
C,-0.4913998971,1.0629082721,3.3754037055
H,-1.9590889914,-0.2784508897,4.2142630424
H,-3.0506545351,-0.458933193,1.8952186557
H,-2.9246874843,2.381139569,3.0460499867
H,-1.4431044203,1.9971660079,1.0483177329
H,-0.3310248469,2.1438199091,3.2667562966
H,-0.4140739954,-0.6682433669,2.072822802
H,-1.8723077729,1.2869992578,5.0192750712
H,-3.7359531568,0.9715493664,1.132260608
H,-3.9554124664,1.0755621527,3.6300088733
H,0.3301966568,0.6789847345,3.9891654719
N,-1.4891494382,0.3467957782,-0.2271587107
N,0.8286409154,0.8961631866,1.3303012674
C,1.9215496732,0.3067992323,1.6006320308
C,-1.4488401633,1.0748843774,-1.2805899536
H,-1.2930064863,0.5220451948,-2.2076512239
H,1.9691062656,-0.5666063962,2.2703334946
C,-1.5566350483,2.5376365771,-1.4179169112
C,-1.6741789185,5.2909975537,-1.8570129152
C,-0.7157845078,3.1400415675,-2.361985899
C,-2.4843606613,3.3220837297,-0.7213089885
C,-2.5426291052,4.6924618528,-0.9463662264

C,-0.7601374234,4.5140986188,-2.5649899657
H,-0.0189827861,2.524351556,-2.9239471891
H,-3.1794142496,2.8582782691,-0.0288230531
H,-3.2707286943,5.2936913977,-0.4122402837
H,-0.0920780701,4.9759607294,-3.284165065
H,-1.7197593145,6.3622216436,-2.024551795
C,3.206014139,0.7584136067,1.0302380384
C,5.6449572136,1.5661368933,-0.0548702062
C,4.3946025819,0.1596353671,1.449843423
C,3.2421844006,1.7667553727,0.0589988541
C,4.4567798474,2.1651416985,-0.4805735113
C,5.6130400343,0.5653197593,0.9110779638
H,4.3611974164,-0.6353572575,2.1904813347
H,2.3063007884,2.2130000601,-0.26248154
H,4.4840274629,2.9440456036,-1.2364084935
H,6.533454879,0.0915465291,1.2376010322
H,6.5931367922,1.8798645273,-0.480511133
H,-4.260294852,-3.1062298504,1.7079837521
C,-4.252847853,-2.9228025261,0.638594012
C,-4.1934428699,-2.4506328711,-2.1620305893
C,-3.1432210351,-2.3762736585,0.0246614214
C,-5.3544564309,-3.2382311298,-0.1735438996
C,-5.3249093496,-3.0074019032,-1.5438277545
C,-3.1146962374,-2.1398725718,-1.3580907828
H,-6.2408215457,-3.6700945615,0.2799345156
H,-6.1886536445,-3.2607193199,-2.1501370018
H,-4.1576384706,-2.2692687176,-3.2308362826
O,-1.9160389024,-1.6149141418,-1.7234902114
O,-1.9653448467,-2.0075637904,0.5934761165
B,-1.2299034984,-1.2988644539,-0.457417955
H,3.416851261,-3.8589500024,1.2062539252
C,3.5299479305,-3.1561767554,0.3882970913
C,3.7868685185,-1.304277929,-1.7726069113
C,2.4501205912,-2.445763481,-0.1005913865
C,4.7632416055,-2.9220774182,-0.2297014302
C,4.8878197226,-2.0155930133,-1.2844632838
C,2.5739826109,-1.5451306198,-1.1565448915
H,5.6404951935,-3.4567095054,0.1195901584
H,5.8620505949,-1.8524030462,-1.7336150744
H,3.8748712615,-0.591156959,-2.584185441
O,1.3485229043,-0.9960004756,-1.4196144816
O,1.1450936034,-2.4732506294,0.3121921089
B,0.4586713268,-1.5734223899,-0.5068787477

IA-*Z,Z*[1,1]^{benzene} (Intermediate monocoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in benzene)
Z-coord_cydiimph2_ZZ_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1443686

Zero-point correction= 0.572632 (Hartree/Particle)
Thermal correction to Energy= 0.604717
Thermal correction to Enthalpy= 0.605661
Thermal correction to Gibbs Free Energy= 0.507169
Sum of electronic and ZPE= -1696.571736
Sum of electronic and thermal Energies= -1696.539651
Sum of electronic and thermal Enthalpies= -1696.538707
Sum of electronic and thermal Free Energies= -1696.637200

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.466	129.652	207.295

C,0.7593385777,-0.9469602073,0.6312571369
C,1.7651423783,-3.280610343,0.6390360459
C,-0.5073783233,-2.9211822365,-0.3738850862
C,0.3862153896,-3.8950082321,0.3955281792
C,-0.6135800678,-1.5978114513,0.3940477575
C,1.6477432655,-1.9506256475,1.3834579762
H,2.2633453316,-3.1148433406,-0.3254424544
H,-0.0862713644,-2.7381065256,-1.3649490121
H,-0.0765539582,-4.1412412152,1.3605177551
H,-1.0359056287,-1.8157347249,1.3781883782
H,1.1978846166,-2.1151714703,2.37178006
H,1.1934077472,-0.7131555236,-0.3498349017
H,2.3965925429,-3.9680415908,1.2106659444
H,-1.5129654936,-3.332618972,-0.5115188492
H,0.4759278704,-4.83104284,-0.1640175935
H,2.6338597707,-1.5094780048,1.553194136
N,-1.5204639131,-0.6688131131,-0.3055898894
N,0.5361069971,0.249189703,1.4349880981
C,1.428299279,1.1168196819,1.7089671985
C,-2.6752910764,-0.3555124976,0.1510449563
H,-3.2734547455,0.264486491,-0.5181718268
H,1.0862459498,1.9183094802,2.3733996423
C,-3.290878342,-0.7202771315,1.4423288876
C,-4.5801442864,-1.3135720927,3.8398132119
C,-2.6275064097,-0.5215265327,2.6598045396
C,-4.6120788488,-1.1801155344,1.4339612855
C,-5.2469885802,-1.4949776637,2.630120388

C,-3.2782809892,-0.8166268062,3.8529421824
H,-1.6184809147,-0.1158785009,2.6539281194
H,-5.1339774521,-1.2997711061,0.4886719326
H,-6.2652956113,-1.8692719902,2.6186260173
H,-2.7677959118,-0.6539597325,4.7965732642
H,-5.0804916728,-1.5474049856,4.7741612445
C,2.8542854248,1.2920389113,1.3293380949
C,5.526740131,1.907038783,0.7302523223
C,3.5557860322,2.2576441543,2.0641244169
C,3.5159405556,0.6426314264,0.2764273291
C,4.8385875329,0.9543730555,-0.0194746224
C,4.8818605152,2.5585817852,1.7781048986
H,3.0413453166,2.7895975215,2.8601721857
H,3.0052150352,-0.0873785555,-0.3371200669
H,5.3329329694,0.4512340182,-0.8441903181
H,5.405921111,3.3077482655,2.3627355856
H,6.5597228364,2.1425271276,0.4940929069
H,0.2374564488,-2.8177758386,-4.2905388935
C,-0.720931231,-2.3093024234,-4.3026050558
C,-3.2129841088,-0.9453883748,-4.3224253863
C,-0.9843319332,-1.2795997185,-3.4211275997
C,-1.7322775534,-2.6593513915,-5.2120610188
C,-2.9511371523,-1.9915256976,-5.2220455535
C,-2.2165311949,-0.6088085999,-3.4279958568
H,-1.5548491497,-3.4644923284,-5.9177851189
H,-3.7160335432,-2.2800985479,-5.9358063757
H,-4.1587811302,-0.4142681028,-4.3234889916
O,-2.2296472351,0.3668188526,-2.4821903016
O,-0.1663943832,-0.7564422672,-2.4702639938
B,-1.0091903627,0.1510802844,-1.6879514879
H,3.3500604637,3.5674400325,-1.1338152165
C,2.4239412375,3.900535927,-0.6776655327
C,-0.0172565887,4.7106713542,0.5671235343
C,1.27414411,3.1389268805,-0.755892114
C,2.3353318187,5.0927223304,0.0479038146
C,1.1421225052,5.4885633042,0.6566346562
C,0.0820067407,3.533558295,-0.1514754369
H,3.2161244221,5.7190934065,0.1438870322
H,1.1111303622,6.4203822358,1.2116821246
H,-0.9492344119,5.0074370381,1.0346397211
O,-0.873696892,2.5851707018,-0.386865873
O,1.0839138872,1.9297102362,-1.3681064511
B,-0.2476187024,1.579440555,-1.1298220717

IA-*E*,*E*[1,2]^{benzene} (Intermediate monocoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in benzene)
E-coord_cydiimph2_EE_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1542449

Zero-point correction= 0.572565 (Hartree/Particle)
Thermal correction to Energy= 0.604425
Thermal correction to Enthalpy= 0.605370
Thermal correction to Gibbs Free Energy= 0.509027
Sum of electronic and ZPE= -1696.581680
Sum of electronic and thermal Energies= -1696.549820
Sum of electronic and thermal Enthalpies= -1696.548875
Sum of electronic and thermal Free Energies= -1696.645218

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.283	129.893	202.771

C,-0.0755833508,-2.0789172179,-1.0025351826
C,1.5994976487,-3.8994479264,-1.6337148639
C,2.3702808629,-1.5181562025,-1.5544546783
C,2.506495038,-2.8550250221,-2.2842684986
C,0.9171902016,-1.0500220569,-1.5816572867
C,0.1416575941,-3.4448784975,-1.6723189334
H,1.9139290148,-4.0518492894,-0.5927791664
H,2.7127890609,-1.6630875335,-0.5278946715
H,2.2320742618,-2.7369056939,-3.3409281419
H,0.632179156,-0.9196802908,-2.6324645477
H,-0.1914389881,-3.3573919843,-2.7145260691
H,0.0797210187,-2.1652236518,0.0870473192
H,1.6960919493,-4.8645497045,-2.1404915746
H,3.0067681724,-0.7475708789,-2.0019634278
H,3.551179778,-3.17758291,-2.2571171538
H,-0.5161210931,-4.1736275271,-1.1884174415
N,-1.4135972921,-1.6252416385,-1.33569066
N,0.7161611094,0.257542046,-0.9078602532
C,-0.1494074823,1.0313673334,-1.465811442
H,-0.6452249128,0.6347329598,-2.3538907111
C,-2.2975872071,-1.5525617964,-0.425555679
H,-2.0860296474,-1.7988480195,0.6256740067
B,1.4373991418,0.5521581958,0.5531279979
B,1.9389502975,-0.73284549,1.5369497407
O,3.2711600737,-1.0105643725,1.7263438906
O,0.4408975528,1.2568853615,1.3621623472
C,3.8373672692,0.9104304341,0.3257335345

C,6.4948923609,-0.0161204936,0.3366727459
C,4.1861574707,-0.2737985164,1.0111016922
C,4.8480730327,1.6087220763,-0.3379673432
C,6.1637739416,1.1576060407,-0.3337810002
C,5.5010242637,-0.7238302475,1.0053055404
H,4.5662644734,2.5194191665,-0.856820165
H,6.9262482149,1.7246701584,-0.8578821107
H,5.7213004405,-1.6381361204,1.5470125719
H,7.516727286,-0.3796498989,0.3455194094
O,2.5821066979,1.4154136137,0.2814086985
C,-0.4865667113,0.4878240136,1.9748248103
C,-2.4466873043,-0.9969418893,3.3363934906
C,-0.1863125647,-0.7859669641,2.5109225775
C,-1.7838997654,0.9817143732,2.1224342972
C,-2.7549014959,0.252599309,2.8032069331
C,-1.1606488381,-1.5118161584,3.185605319
H,-1.9981145809,1.9597779244,1.7017546934
H,-3.7541207684,0.6627915937,2.9106435348
H,-0.8811846903,-2.4753474881,3.5998585775
H,-3.1964606523,-1.5678362818,3.874682427
O,1.0810204778,-1.3079509014,2.4480539469
C,-0.6012144366,2.3711103352,-1.0798829105
C,-1.645996814,4.8829917249,-0.4802105074
C,0.2115516802,3.3380109273,-0.4733315857
C,-1.9267367537,2.6832320514,-1.4111522261
C,-2.45547446,3.9280559856,-1.0907203481
C,-0.3141364656,4.5903407886,-0.1856629742
H,1.2434792558,3.1053791961,-0.23737468
H,-2.5487522898,1.9348036974,-1.896001134
H,-3.4896301292,4.1547448303,-1.3270512398
H,0.3165351891,5.34138929,0.2781497807
H,-2.0497764897,5.8619778571,-0.241433484
C,-3.6806812538,-1.1323487375,-0.734849781
C,-6.3026397703,-0.3389392168,-1.2809638433
C,-4.647114507,-1.1489527713,0.2728954608
C,-4.0401944503,-0.7252443155,-2.0259544283
C,-5.3427907105,-0.3264025927,-2.2949064353
C,-5.9546745054,-0.7545806252,0.0008558231
H,-4.3650650018,-1.4697109972,1.271554063
H,-3.285012144,-0.7372305988,-2.8059552235
H,-5.6165743489,-0.0104795355,-3.296732045
H,-6.7005458506,-0.7718258847,0.7891283177
H,-7.3208352597,-0.0287723451,-1.4940586993

IA-*E*,*Z*[1,2]^{benzene} (Intermediate monocoordinate *E*-coordinated 1,2-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
E-coord_cydiimph2_EZ_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1422314

Zero-point correction= 0.573133 (Hartree/Particle)
Thermal correction to Energy= 0.604738
Thermal correction to Enthalpy= 0.605682
Thermal correction to Gibbs Free Energy= 0.510322
Sum of electronic and ZPE= -1696.569098
Sum of electronic and thermal Energies= -1696.537493
Sum of electronic and thermal Enthalpies= -1696.536549
Sum of electronic and thermal Free Energies= -1696.631909

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.479	129.663	200.702

C,0.8200770303,-1.1326130103,1.7314849686
C,0.1368614936,-3.4388529011,2.557465265
C,-1.6278524444,-1.8182556414,1.7966203633
C,-1.2989511612,-2.9551081164,2.7656288323
C,-0.6303506465,-0.6749582042,1.9725094355
C,1.1256025994,-2.2830739214,2.7064783581
H,0.2294821886,-3.8737001844,1.5528306744
H,-1.5754327894,-2.2091675955,0.7764027393
H,-1.4191225905,-2.6067863739,3.7999961484
H,-0.6752109634,-0.3429796962,3.0166546264
H,1.0726923368,-1.874585463,3.7240245022
H,0.9060023169,-1.4785307115,0.6920249837
H,0.3830323464,-4.2309836921,3.2713003579
H,-2.6460586377,-1.4457043773,1.9470482605
H,-2.0070982397,-3.7756587359,2.6190656558
H,2.1564960541,-2.6195164347,2.559816329
N,1.6950974834,-0.0108225218,2.0109987581
N,-0.9705262869,0.4994483415,1.1349214182
C,-0.8103218204,1.6427139979,1.7052670117
H,-0.3685626559,1.6273519926,2.702527086
C,2.8765170294,0.0907555646,1.5491847086
H,3.4083965257,0.9949897148,1.8639897664
B,-1.3644691041,0.2607505193,-0.4505082279
B,-0.6291509903,-1.0170356243,-1.2797961265
O,-1.3565291484,-2.0963821278,-1.7218968059
O,-0.9201642177,1.4451695678,-1.1871579359
C,-3.396004688,-1.0290451284,-0.8753069268

C,-4.7622758061,-3.3935425531,-1.5673386815
C,-2.7048959372,-2.1222440825,-1.4453130184
C,-4.771889346,-1.1577451117,-0.6712929605
C,-5.4535325921,-2.3204040585,-1.0130205175
C,-3.3918689741,-3.2841240405,-1.7787463351
H,-5.2886832668,-0.3091998533,-0.2342975987
H,-6.5233625529,-2.3841436145,-0.8425670522
H,-2.8187685229,-4.0952128716,-2.2165676293
H,-5.2803814583,-4.3072251388,-1.8378625914
O,-2.8155148901,0.1347686595,-0.5034051997
C,0.4049388391,1.5232647868,-1.4534904501
C,3.1295934873,1.7808931587,-2.0694573361
C,1.1853809709,0.3841964257,-1.7554375486
C,1.0186035223,2.7763875017,-1.4627462996
C,2.3700316613,2.9080092387,-1.7700558326
C,2.5315121148,0.5230016521,-2.0670160099
H,0.3998447658,3.639343233,-1.233112124
H,2.8251684473,3.8933832725,-1.7758630342
H,3.0982400891,-0.3738254637,-2.3007194574
H,4.1839818801,1.8714915533,-2.3099141044
O,0.6207931098,-0.8676312858,-1.8388540801
C,-1.1551534963,2.9765254082,1.209813122
C,-1.7230842402,5.5844256616,0.4196025177
C,-2.2587254426,3.2299548607,0.3849721492
C,-0.365236804,4.0392389682,1.6663043506
C,-0.6344739585,5.3387344398,1.254046087
C,-2.5395344587,4.5339471295,-0.0005040433
H,-2.8864960756,2.4086931328,0.0566280979
H,0.4745710239,3.8352195552,2.3252238137
H,-0.0061825834,6.1567078323,1.590115426
H,-3.395470404,4.7325880872,-0.6366893507
H,-1.9447850762,6.5994875548,0.1050558533
C,3.7058875794,-0.7427350179,0.6401962165
C,5.4304291124,-2.0300213826,-1.1715204631
C,4.9036840395,-0.1424189331,0.2236262885
C,3.4006917592,-2.0201571566,0.1442009033
C,4.2560114094,-2.6511388143,-0.7541903716
C,5.7571188848,-0.7706725444,-0.6736608561
H,5.1515993363,0.8475282391,0.5973190718
H,2.5058824871,-2.5451260304,0.4475539723
H,3.9984723951,-3.6357353716,-1.1305447279
H,6.6728360045,-0.2788979242,-0.9857801665
H,6.0897719464,-2.5277233388,-1.8754732559

IA-*Z*,*E*[1,2]^{benzene} (Intermediate monocoordinate *Z*-coordinated 1,2-B_2cat_2-*Z*,*E*-diimine **1** complex in benzene)
Z-coord_cydiimph2_ZE_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1530035

Zero-point correction= 0.572497 (Hartree/Particle)
Thermal correction to Energy= 0.604428
Thermal correction to Enthalpy= 0.605372
Thermal correction to Gibbs Free Energy= 0.508240
Sum of electronic and ZPE= -1696.580507
Sum of electronic and thermal Energies= -1696.548575
Sum of electronic and thermal Enthalpies= -1696.547631
Sum of electronic and thermal Free Energies= -1696.644763

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.284	129.925	204.432

C,0.2315486135,-0.0029516508,1.8157104245
C,-1.2513486943,0.1277671672,3.8875759879
C,-2.185828671,0.8653317879,1.6841901074
C,-2.1657754669,1.1337723834,3.1887730108
C,-0.7709733705,0.935219765,1.111966374
C,0.1696843585,0.2185889938,3.3347620159
H,-1.6458072138,-0.8854879552,3.7340374627
H,-2.6138426593,-0.1271882478,1.5209368853
H,-1.8058444859,2.1528679813,3.3832306302
H,-0.3775564453,1.9426619128,1.2648049585
H,0.586403234,1.2126333643,3.5416085561
H,-0.0148838141,-1.0538389064,1.582846017
H,-1.2373111368,0.3043835053,4.967463537
H,-2.8268799499,1.5797927944,1.1556458099
H,-3.1842684466,1.0711037137,3.5824828415
H,0.8310039469,-0.5102001304,3.8139307943
N,1.5584534604,0.3681573598,1.3610564047
N,-0.7395447618,0.6258532058,-0.328459882
C,-0.0807801267,1.3343542108,-1.1681875359
H,-0.0162515703,0.9080836154,-2.1705355098
C,2.3662289649,-0.5368762615,0.9834673287
H,2.0895699527,-1.6017319989,0.9490137152
B,-1.5168194358,-0.6976330831,-0.9760659515
B,-2.0352466137,-1.9752827851,-0.0047191357
O,-3.3612553572,-2.1336363114,0.3144644746
O,-0.5633230398,-1.2615593045,-1.9339267376
C,-3.8859183009,-0.221427786,-1.1178968605

C,-6.4841200387,-0.2767076595,-0.0338733785
C,-4.2400409671,-1.1737862956,-0.135441389
C,-4.8639177682,0.6827347491,-1.5380788175
C,-6.1499302851,0.658571787,-1.0087239242
C,-5.5240778365,-1.1879019802,0.39549809
H,-4.5799054869,1.4035576838,-2.2980739721
H,-6.8870726258,1.3738537724,-1.359036859
H,-5.7493987161,-1.9387603748,1.1461065498
H,-7.4829716813,-0.3044897898,0.3879669296
O,-2.6603147104,-0.1413234606,-1.6840120684
C,0.3170508253,-2.1657987444,-1.4442426993
C,2.1944216917,-4.0688008835,-0.5620713521
C,0.0091172559,-3.0478719683,-0.3807312136
C,1.5774564933,-2.262593995,-2.0367932983
C,2.506042935,-3.2076965022,-1.6111901691
C,0.9452939387,-3.9820387151,0.0478287598
H,1.8005110152,-1.5840508798,-2.8542580299
H,3.4745160074,-3.262528082,-2.0981968163
H,0.660872339,-4.6467264859,0.8573119532
H,2.9104214596,-4.8107575133,-0.2240211241
O,-1.2255969068,-3.0653788131,0.2192296445
C,0.5997766354,2.6258943091,-0.9601192997
C,1.9412709735,5.0564429911,-0.7240003554
C,-0.0383504702,3.7234807367,-0.3717957949
C,1.8983005864,2.7617276529,-1.460743867
C,2.5736630616,3.9697939013,-1.3236691107
C,0.6326569622,4.9355226744,-0.2594753535
H,-1.06482437,3.63229506,-0.0281273941
H,2.3828014197,1.9125702362,-1.9352031748
H,3.5893422982,4.0632248347,-1.694142162
H,0.1325029162,5.7878599017,0.1880799161
H,2.4633052194,6.0031399121,-0.6292921755
C,3.7475783338,-0.2034956356,0.5762342899
C,6.3623214192,0.3978297537,-0.1980488972
C,4.6348183672,-1.2267405704,0.2357643742
C,4.1829559049,1.1272244078,0.5399154086
C,5.4820604588,1.4243273973,0.1495884391
C,5.9390581841,-0.9274034215,-0.1499122418
H,4.2941434569,-2.2575323272,0.2737188853
H,3.4863826098,1.9101969662,0.8226136334
H,5.8147641966,2.4575551174,0.1208233431
H,6.623750728,-1.7276934152,-0.412202382
H,7.3780291995,0.6327643286,-0.50085762

IA-*Z,Z*[1,2]^{benzene} (Intermediate monocoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in benzene)
Z-coord_cydiimph2_ZZ_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.140699

Zero-point correction= 0.573165 (Hartree/Particle)
Thermal correction to Energy= 0.604861
Thermal correction to Enthalpy= 0.605805
Thermal correction to Gibbs Free Energy= 0.509946
Sum of electronic and ZPE= -1696.567534
Sum of electronic and thermal Energies= -1696.535838
Sum of electronic and thermal Enthalpies= -1696.534894
Sum of electronic and thermal Free Energies= -1696.630753

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.556	129.580	201.753

C,-1.0840843732,-0.8167315566,0.1913927191
C,-2.7171056525,-0.9426041442,2.1321887491
C,-0.2967063732,-0.4202537013,2.5729623655
C,-1.5564969068,-1.0952562883,3.1169259104
C,0.0597752779,-1.0046976966,1.2088161488
C,-2.343679872,-1.4935125355,0.7559429164
H,-2.975438574,0.1214616231,2.0425032954
H,-0.4877306485,0.6538525324,2.4772757133
H,-1.3602169802,-2.1625053299,3.2849847763
H,0.2056245099,-2.0832146138,1.3036332589
H,-2.1385216421,-2.5695616343,0.8237360431
H,-1.2563367695,0.2615752343,0.0663725435
H,-3.6080676759,-1.4557761492,2.5070018219
H,0.5486202324,-0.5332449538,3.2598897714
H,-1.8156901932,-0.659870145,4.0862388842
H,-3.1672171796,-1.3755265586,0.0448215468
N,-0.687005286,-1.4552160045,-1.0477414605
N,1.2878307294,-0.416018594,0.6505808091
C,2.1861317449,-1.144507557,0.1008132326
H,2.982581291,-0.5908330461,-0.3966340587
C,-1.1955509426,-1.1767899698,-2.1801123516
H,-0.7896361002,-1.7636196394,-3.0115953799
B,1.5261629599,1.2216244977,0.666820141
B,0.2148256292,2.2585208269,0.4524140362
O,-0.248036877,3.0527018754,1.472386071
O,2.4189411936,1.4853500964,-0.4685741658
C,1.5985559375,2.2498055408,2.8753594625

C,0.4727522863,3.7484159466,4.9802662464
C,0.409321686,2.9897774567,2.6815341658
C,2.1960321618,2.2913508007,4.1377426822
C,1.6483561784,3.0308642122,5.1799136078
C,-0.1363329731,3.7217388895,3.7300519273
H,3.1099717624,1.7211653456,4.270134087
H,2.1418861345,3.0416713087,6.1463796753
H,-1.0482958321,4.2756562534,3.5313177377
H,0.0329938216,4.3284545135,5.7843606475
O,2.1940381852,1.4900641581,1.9293929005
C,1.8102092624,1.5487360133,-1.6801055777
C,0.6575322234,1.6721781244,-4.2400504815
C,0.5035138919,2.0605454877,-1.8590714014
C,2.5068798599,1.1027851292,-2.8041494611
C,1.9419023107,1.163393006,-4.0751997866
C,-0.0520483493,2.1241139758,-3.1305437037
H,3.5140762564,0.7251921125,-2.6538936436
H,2.5095812263,0.815131066,-4.9321516096
H,-1.0566806001,2.5264971714,-3.2260926475
H,0.2040324062,1.7246420564,-5.2244656917
O,-0.2246461997,2.5765928834,-0.8129360131
C,2.2765644932,-2.6190174632,0.0730460886
C,2.5830062092,-5.3835069892,-0.0571864188
C,2.3182174546,-3.3734607039,1.2490793043
C,2.4116302651,-3.2493505847,-1.1667958253
C,2.5485913651,-4.6311814248,-1.2298103236
C,2.4755512942,-4.7538850984,1.180541147
H,2.2457441995,-2.8756407029,2.2122735198
H,2.3888091982,-2.6525167767,-2.0743647782
H,2.6359608238,-5.121104074,-2.1939184713
H,2.5165461879,-5.336695074,2.0948291321
H,2.701235082,-6.4610589253,-0.1080861844
C,-2.2148366422,-0.1999378405,-2.6464284194
C,-3.9744281337,1.6483983436,-3.8312751688
C,-2.3641769827,-0.1264227765,-4.0398922814
C,-2.9887162958,0.6628056274,-1.853998517
C,-3.8537351416,1.5786564306,-2.4457861889
C,-3.2294656141,0.7845924412,-4.6310282911
H,-1.76921589,-0.7856828053,-4.6662833915
H,-2.9378970213,0.6373313859,-0.7744432926
H,-4.4365099393,2.2423737174,-1.815538975
H,-3.3195369879,0.8239412945,-5.7118405969
H,-4.6499411125,2.3672439885,-4.2839285176

IB-*E*,*E*[1,1]^{MeOH} (Intermediate dicoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in MeOH)
cfc_boat_cydiimph2_EE_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1521442

Zero-point correction= 0.571577 (Hartree/Particle)
Thermal correction to Energy= 0.603169
Thermal correction to Enthalpy= 0.604113
Thermal correction to Gibbs Free Energy= 0.508368
Sum of electronic and ZPE= -1696.580567
Sum of electronic and thermal Energies= -1696.548975
Sum of electronic and thermal Enthalpies= -1696.548031
Sum of electronic and thermal Free Energies= -1696.643776

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.494	129.843	201.512

H,-3.2638233592,2.7291071128,-1.209622292
C,-2.450098532,3.0447672335,-0.5486426649
C,-0.9629431951,4.9754027182,0.1171070301
C,-0.0365982117,2.6609814285,0.0327925456
C,0.2687334879,4.1340705261,-0.2291922205
C,-1.1988359112,2.2232045209,-0.8762855564
C,-2.169995721,4.539297655,-0.7147654339
H,-1.1906866184,4.8619724589,1.1844743213
H,-0.3518570726,2.5623558856,1.0765036956
H,0.5182028124,4.2950509867,-1.285001162
H,-0.8931182414,2.4238264345,-1.9109244464
H,-1.9748603946,4.7538510951,-1.7733988615
H,-2.752251668,2.824664752,0.4815658315
H,-0.7437505389,6.0329904316,-0.0564299512
H,1.1335735949,4.4365289156,0.3705835121
H,-3.0580208205,5.1109332584,-0.4289409903
N,1.112533919,1.7355548829,-0.0909400918
N,-1.4678024918,0.7646015938,-0.7770772658
C,2.1173581388,2.0458362917,-0.8207728479
H,2.0773224839,2.9569437598,-1.4190591916
C,-2.0895573332,0.2420224555,-1.7679485725
H,-2.4203095063,0.9184975778,-2.5619106968
B,0.7948195127,0.2484035762,0.6050803652
B,-0.9261433731,0.0928776091,0.652424134
O,-1.7240087974,0.8317368899,1.6826090213
O,-1.4218568818,-1.2883975071,0.7383822923
O,1.5110939449,0.1355576044,1.901593344

O,1.4142172569,-0.7884062091,-0.2668356927
C,-2.6418263048,-1.210316692,1.3308984619
C,-4.9726613601,-0.6102326006,2.678877761
C,-3.6188381814,-2.1835789956,1.4050158184
C,-2.820500067,0.0573736416,1.905112821
C,-3.9772153226,0.3788530413,2.5884043859
C,-4.79936496,-1.8620032588,2.0975225249
H,-3.4708182607,-3.1549989015,0.9428304124
H,-4.1067097831,1.3601293756,3.0340465743
H,-5.5874712146,-2.6045012802,2.1749308458
H,-5.8940718218,-0.3861932536,3.2073911047
C,2.3698715823,-1.4065868782,0.4698309891
C,4.2148849918,-2.3406647134,2.2980997419
C,3.2241102286,-2.4160685491,0.0749902419
C,2.4266534082,-0.8594184154,1.7610584452
C,3.3403995108,-1.311263768,2.6921818868
C,4.1593716089,-2.880168032,1.0178644314
H,3.1773189362,-2.8208735931,-0.9311218946
H,3.382678934,-0.8765877678,3.6857405
H,4.8452671659,-3.673750094,0.7378880434
H,4.9435293598,-2.7168825573,3.0095560928
C,3.3769732084,1.2788140491,-0.8682633928
C,5.8277118915,-0.0388495356,-0.9536399139
C,3.8472832494,0.7637102948,-2.080231706
C,4.1419860379,1.1524236286,0.2942878476
C,5.375497787,0.5058007066,0.2447945687
C,5.0597747034,0.0839899672,-2.1135834517
H,3.2556994705,0.8813513345,-2.9835270872
H,3.7748048828,1.573063072,1.2257229716
H,5.9719938392,0.4164401954,1.147365195
H,5.4143893041,-0.3390199955,-3.0480786821
H,6.7811786636,-0.5568206869,-0.9886931646
C,-2.4040624257,-1.1812696694,-1.982928618
C,-3.064727824,-3.8306352763,-2.5239654664
C,-1.4255165921,-2.1762444325,-1.884475045
C,-3.7011419358,-1.5097164137,-2.3890510229
C,-4.035950054,-2.8380246517,-2.6366708304
C,-1.7588810912,-3.4967030492,-2.1610934904
H,-0.4147460538,-1.9072393787,-1.5939683729
H,-4.4473009175,-0.7266652948,-2.4932872345
H,-5.049270339,-3.0945428759,-2.9282558222
H,-0.9995223657,-4.2689859076,-2.0906479232
H,-3.3208657522,-4.8653567403,-2.7300746007

IB-*E,Z*[1,1]^{MeOH} (Intermediate dicoordinate 1,1-B_2cat_2-*E,Z*-diimine **1** complex in MeOH)
boat_cydiimph2_EZ_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1475808

Zero-point correction= 0.571633 (Hartree/Particle)
Thermal correction to Energy= 0.603420
Thermal correction to Enthalpy= 0.604364
Thermal correction to Gibbs Free Energy= 0.506600
Sum of electronic and ZPE= -1696.575948
Sum of electronic and thermal Energies= -1696.544161
Sum of electronic and thermal Enthalpies= -1696.543217
Sum of electronic and thermal Free Energies= -1696.640981

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.652	129.665	205.762

H,1.1116469277,-3.3335963829,1.4768276114
C,0.3604615605,-2.6460035006,1.8798092915
C,-1.8820975458,-2.4887334772,3.0554813736
C,-1.3033192832,-0.86757401,1.2753570874
C,-2.4486536377,-1.6729959433,1.8869988604
C,-0.2286265185,-1.824951865,0.7307289866
C,-0.7590735168,-3.4183203621,2.5856751552
H,-1.4963150208,-1.8061085913,3.8232977953
H,-0.8558328176,-0.2850566768,2.0892614105
H,-2.8870909658,-2.3558751692,1.1536724974
H,-0.7251512804,-2.5081688148,0.0322723835
H,-1.1750139677,-4.1615925555,1.8930158561
H,0.8617976086,-1.9721958929,2.5818816037
H,-2.6852002763,-3.0717664325,3.5158840938
H,-3.2348710428,-0.9904961635,2.2254109206
H,-0.3421263597,-3.9686487112,3.43444725
N,-1.6109655044,0.1500223637,0.2524069623
N,0.7957158348,-1.0793387332,-0.0466188123
C,-2.5131145274,0.1019771404,-0.6489258685
H,-2.5566251624,0.9727183081,-1.3056413745
C,1.3699037339,-1.7385068604,-0.9836211223
H,1.1229503601,-2.8013945718,-1.0682565732
B,-0.4622904958,1.3455208326,0.3187902708
B,1.0439268865,0.5057552606,0.4870429791
O,1.5032336244,0.2842486975,1.8926365883
O,2.22321185,1.0388525867,-0.2006658099
O,-0.83929237,2.1859041401,1.4894832582

O,-0.6655859385,2.210110627,-0.8611164508
C,3.2912657574,0.6665781143,0.5544283316
C,5.1269743706,-0.1597727562,2.4388910129
C,4.6290881808,0.6957124178,0.213735154
C,2.8602902277,0.2203402108,1.8128850832
C,3.7618929877,-0.1947449958,2.7737963366
C,5.5514098192,0.2728948731,1.1867978895
H,4.9446754467,1.0325659384,-0.7691462907
H,3.422686302,-0.5344079192,3.7473272412
H,6.6112074621,0.2822925065,0.9520539891
H,5.8594001757,-0.4825156281,3.1722475137
C,-1.372033374,3.2909907806,-0.421864575
C,-2.7094482817,5.3102522096,0.9005979856
C,-1.9228476195,4.3094234167,-1.1740839417
C,-1.4801530211,3.2689852707,0.9767632924
C,-2.1459360654,4.2696512609,1.6586957524
C,-2.6005111026,5.3304432761,-0.4856225272
H,-1.82991956,4.3143601534,-2.2553727683
H,-2.2241855675,4.2460471122,2.7408250402
H,-3.0448414783,6.144742484,-1.0492857887
H,-3.238391328,6.1094961468,1.4103593426
C,-3.4613887272,-1.0043883203,-0.9163544227
C,-5.2461848232,-3.0729327329,-1.4420896017
C,-4.8059528003,-0.8665029535,-0.5650268228
C,-3.0147265958,-2.159907862,-1.5632173723
C,-3.9111273228,-3.1933820304,-1.8230875735
C,-5.6926495512,-1.9090808151,-0.8177295872
H,-5.1471181931,0.0427449765,-0.0789536593
H,-1.9735479602,-2.243266875,-1.8632532525
H,-3.565015905,-4.0923925483,-2.3229572221
H,-6.7341028212,-1.8111005368,-0.5283399838
H,-5.9414199948,-3.8827069821,-1.6397623493
C,2.3083125428,-1.2287703726,-1.9970902538
C,4.0658054517,-0.4126073146,-3.9955960322
C,2.0381479119,-0.068600885,-2.7314748548
C,3.438988924,-1.9972631094,-2.2910291065
C,4.3290037228,-1.5755241653,-3.2746396685
C,2.9148472205,0.332059417,-3.7320000604
H,1.1439527682,0.5081449465,-2.5155366864
H,3.6249279322,-2.9141402351,-1.738368549
H,5.2182870482,-2.1604324977,-3.4858212911
H,2.7026731535,1.2278675535,-4.3066552457
H,4.751216532,-0.0906297726,-4.7735127023

IB-*Z*,*E*[1,1]^{MeOH} (Intermediate dicoordinate 1,1-B_2cat_2-*Z*,*E*-diimine **1** complex in MeOH)
boat_cydiimph2_ZE_b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1538641

Zero-point correction= 0.571943 (Hartree/Particle)
Thermal correction to Energy= 0.603434
Thermal correction to Enthalpy= 0.604378
Thermal correction to Gibbs Free Energy= 0.508560
Sum of electronic and ZPE= -1696.581921
Sum of electronic and thermal Energies= -1696.550431
Sum of electronic and thermal Enthalpies= -1696.549486
Sum of electronic and thermal Free Energies= -1696.645304

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.660	129.527	201.666

H,-2.8947410489,1.6623527876,-2.0300681195
C,-2.6257991281,1.9054929764,-0.9966673919
C,-2.2212793952,3.7793519504,0.6509296465
C,-0.7827487364,1.7459413263,0.7108978441
C,-0.7981938886,3.2621965092,0.8835919142
C,-1.2025640682,1.4023160899,-0.7292741091
C,-2.7133040668,3.4123300589,-0.7504032688
H,-2.8919770632,3.3442474828,1.4025028747
H,-1.5147637215,1.3170054434,1.4029101065
H,-0.1286977696,3.7410379356,0.1584061723
H,-0.5074092175,1.9129742361,-1.4012141988
H,-2.1000355544,3.9340485665,-1.4963606537
H,-3.3158537653,1.367162079,-0.3360959363
H,-2.2423812876,4.8643943769,0.7881774136
H,-0.4447912405,3.5176369683,1.8880070813
H,-3.7455999408,3.7458881688,-0.8921947866
N,0.4887464713,1.0648045199,1.044056937
N,-1.1359551714,-0.0514721891,-0.9697047218
C,1.5958491492,1.7044905999,0.9841516631
H,1.5926976961,2.7355791921,0.6282947724
C,-0.9139638394,-0.5435133167,-2.1302002193
H,-0.9630362104,-1.6308449002,-2.1943650859
B,0.2935986391,-0.5925971327,1.1937256092
B,-1.1846532622,-0.9932779922,0.3800126152
O,-2.4993489704,-0.7350318531,1.0330693539
O,-1.2594479466,-2.3974538628,-0.0814208401
O,0.401287489,-0.9956299692,2.6174925412

O,1.4611520816,-1.2256210639,0.5221037964
C,-2.5746749259,-2.7462300726,-0.015888847
C,-5.2909451214,-3.0537806722,0.3729353922
C,-3.1749716785,-3.8978125067,-0.4857992754
C,-3.3125546409,-1.7535610129,0.6453318988
C,-4.6725935366,-1.8851140305,0.8496024603
C,-4.5581710691,-4.039019192,-0.2800905392
H,-2.5930234275,-4.6605837202,-0.9931085902
H,-5.2343707534,-1.111228823,1.3629129927
H,-5.0583961932,-4.9327621868,-0.6396927603
H,-6.3586961652,-3.184715434,0.5184343182
C,2.1395747891,-1.9110483492,1.4751144185
C,3.2090280605,-3.1193346007,3.7160509652
C,3.3068784798,-2.633885548,1.3316439422
C,1.5070555201,-1.7803998338,2.7215011359
C,2.0208833893,-2.3783795884,3.8546779441
C,3.8394735212,-3.2422478404,2.4830187445
H,3.7945359929,-2.7142597463,0.3652617227
H,1.5277379131,-2.2659302574,4.8149264384
H,4.756483337,-3.817747546,2.4020580586
H,3.6370974442,-3.600949531,4.5897789252
C,2.8981073773,1.1566568899,1.408885473
C,5.3887985416,0.2380807889,2.2459898478
C,3.9559501818,1.0859950958,0.4965484075
C,3.0925749213,0.7878689157,2.7422459219
C,4.3451023326,0.3429002642,3.1611377258
C,5.1914481078,0.6026334891,0.9125161623
H,3.8020566944,1.3915593287,-0.5345713468
H,2.2688011152,0.8638062585,3.4457831392
H,4.4969989006,0.0654996384,4.1995532895
H,6.0061415893,0.5224737066,0.19995577
H,6.3598562715,-0.1236280132,2.5698150196
C,-0.5928136899,0.2063783128,-3.3633514776
C,0.0299879516,1.5190298202,-5.7395796473
C,0.5630607552,0.9909055995,-3.4456157634
C,-1.4207417681,0.0583488398,-4.4799631334
C,-1.1152555405,0.7286972685,-5.6609357233
C,0.8724855563,1.6417222019,-4.6356584876
H,1.2240298165,1.0690259102,-2.586057823
H,-2.3028027235,-0.5724645774,-4.4166881658
H,-1.7669886743,0.6253639293,-6.5225116614
H,1.7740565788,2.2422381115,-4.7015153568
H,0.2720085361,2.0320897452,-6.6650125455

IB-*Z*,*Z*[1,1]^{MeOH} (Intermediate dicoordinate 1,1-B_2cat_2-*Z*,*Z*-diimine **1** complex in MeOH)
boat_cydiimph2_ZZ_b2cat2_meoh

M062X/6-31G(d,p)
E(RM062X) = -1697.1491688

Zero-point correction= 0.572515 (Hartree/Particle)
Thermal correction to Energy= 0.604074
Thermal correction to Enthalpy= 0.605018
Thermal correction to Gibbs Free Energy= 0.507728
Sum of electronic and ZPE= -1696.576654
Sum of electronic and thermal Energies= -1696.545095
Sum of electronic and thermal Enthalpies= -1696.544151
Sum of electronic and thermal Free Energies= -1696.641441

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.062	129.238	204.765

H,2.481344816,1.9668404814,-1.6818111144
C,1.6211563299,1.3989011294,-2.0519837845
C,-0.3647870215,1.434700241,-3.6257137294
C,-0.5786593329,0.3871699485,-1.3910256151
C,-1.3159394644,1.2081497266,-2.4451276377
C,0.6620358911,1.1411641298,-0.8840428049
C,0.9032974166,2.1608782934,-3.1690371466
H,-0.0952740553,0.4688473181,-4.0715918894
H,-0.2239760825,-0.5173443034,-1.9018232125
H,-1.6251350931,2.1797595652,-2.0545640478
H,0.3385205787,2.0997983722,-0.4731634381
H,0.6337887991,3.16136586,-2.806084729
H,1.9889712304,0.4349915264,-2.4215810177
H,-0.8755007898,2.016739816,-4.3985081792
H,-2.2165402042,0.6694644356,-2.7570517815
H,1.5882021132,2.2986569376,-4.0110922796
N,-1.3282813653,-0.1511268371,-0.2441496703
N,1.3372792113,0.3700728641,0.181158537
C,-2.3611039774,0.3130967923,0.3518394426
H,-2.7394008776,-0.3332289329,1.1456151634
C,2.0260610757,0.9467162059,1.0913558111
H,2.5363558278,0.283923608,1.7902780012
B,-0.5987536609,-1.5676270437,0.2318786498
B,1.1123495302,-1.277929812,0.1652234261
O,1.7743073189,-1.736992482,-1.0917184393
O,1.9486638723,-1.8194973527,1.2549357986
O,-1.0732198632,-2.5818403908,-0.7565488155
O,-1.206792149,-1.9697537919,1.5155269376
C,3.1240398263,-2.1962777592,0.6734658913
C,5.2696168676,-2.9004943711,-0.9136475761

C,4.2886432664,-2.6025129683,1.2943728448
C,3.0185896841,-2.1405660854,-0.7241978672
C,4.080462492,-2.4871298342,-1.5378967348
C,5.3719656569,-2.9574481516,0.472229514
H,4.3566100249,-2.6430753751,2.3767803333
H,3.9894747089,-2.4415077028,-2.6184551849
H,6.301805484,-3.2788520671,0.9308563648
H,6.1208134164,-3.1778711716,-1.5276249818
C,-2.1452484288,-2.9129722896,1.2166968436
C,-3.8594159683,-4.810168487,0.1789410087
C,-3.067220787,-3.4923071036,2.0658287967
C,-2.0694464096,-3.2672772656,-0.1385820446
C,-2.9186965718,-4.2145237123,-0.6787034742
C,-3.9325307742,-4.4574215155,1.5221123539
H,-3.1140982286,-3.2086496132,3.1123449199
H,-2.8530170383,-4.4843221247,-1.7277993573
H,-4.668365417,-4.9310001042,2.1644125386
H,-4.5388784797,-5.5575838728,-0.2187454948
C,-3.1352236704,1.5528623855,0.1522588468
C,-4.7627481893,3.8089969072,-0.0744742457
C,-4.5300079109,1.4215539597,0.1597220028
C,-2.5618121803,2.8267070725,0.0737091123
C,-3.3766037777,3.9490991563,-0.0348122435
C,-5.3392354856,2.5435437043,0.0215008343
H,-4.9730738782,0.4347974798,0.2622980253
H,-1.4847812951,2.9479823958,0.1174928292
H,-2.9260670772,4.9350776859,-0.0853316313
H,-6.4184063874,2.431428107,0.00497335
H,-5.3939193695,4.687440259,-0.1651692527
C,2.173643799,2.4069394208,1.284992821
C,2.4853913879,5.1395350333,1.7169671046
C,1.0735081529,3.1833604166,1.6632433647
C,3.434634034,2.9931349306,1.1488586062
C,3.5834763859,4.3624803788,1.3528385188
C,1.2332131495,4.5484908845,1.8797214634
H,0.1041597534,2.7115015769,1.8022109189
H,4.2887707773,2.3800602203,0.8758887018
H,4.559990063,4.8207323008,1.2336122606
H,0.379370857,5.1489077465,2.1774134552
H,2.6068974632,6.2053972478,1.8824530284

IB-*E*,*E*[1,2]^{MeOH} (Intermediate dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in MeOH)
boat_cydiimph2_EE_1-2-b2cat2_meoh
M062X/6-31G(d,p)

E(RM062X) = -1697.1660253

Zero-point correction= 0.572346 (Hartree/Particle)
Thermal correction to Energy= 0.603503
Thermal correction to Enthalpy= 0.604447
Thermal correction to Gibbs Free Energy= 0.509582
Sum of electronic and ZPE= -1696.593679
Sum of electronic and thermal Energies= -1696.562523
Sum of electronic and thermal Enthalpies= -1696.561578
Sum of electronic and thermal Free Energies= -1696.656443

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.704	129.177	199.660

H,-2.530952109,2.1557629639,-2.3876436777
C,-2.3039257145,2.4133157052,-1.3480891299
C,-1.9152791179,4.3197498305,0.2674511949
C,-0.5945250532,2.2141860069,0.4623058285
C,-0.5421904064,3.7345350201,0.6051727331
C,-0.9314941448,1.8358174917,-0.9802575491
C,-2.3331372625,3.9298467757,-1.1508441601
H,-2.6551945553,3.9441107744,0.9855515201
H,-1.3963406534,1.8459319732,1.1123304314
H,0.2022858114,4.1625237617,-0.076511585
H,-0.1610942765,2.2691270958,-1.6328126065
H,-1.6478024314,4.3971857976,-1.8697999326
H,-3.0582562233,1.9277998623,-0.7155278857
H,-1.8874648287,5.4084527778,0.3707131082
H,-0.2439442886,3.9855508868,1.6279806685
H,-3.3363325035,4.3063510754,-1.3721169678
N,0.6133997668,1.4961199752,0.9155573541
N,-0.9396499504,0.3664914716,-1.2023687921
C,1.7753671031,1.9948937461,0.6894888418
H,1.84021945,2.9032158874,0.0887002121
C,-0.8025035714,0.0164302667,-2.4351374392
H,-0.5037624008,0.7967144481,-3.1409227802
B,0.1650481166,-0.0058504939,1.3344345389
B,-0.9511887344,-0.5885241937,0.12866752
O,-2.3477827639,-0.5720887587,0.5753916933
O,-0.4623909065,0.1518652681,2.6556964548
O,-0.5880216287,-1.9598711552,-0.2478507086
O,1.3322190619,-0.8665193994,1.4792641343
C,-1.6788934093,-0.3920132268,2.9125417847
C,-4.2001384073,-1.4202284283,3.6048728278
C,-2.0427252529,-0.5693828564,4.2484149416

C,-2.6016290593,-0.7439608758,1.9016495832
C,-3.8468556891,-1.254634671,2.2676166887
C,-3.29094064,-1.0767105061,4.601262784
H,-1.3156967258,-0.2902203967,5.0058046678
H,-4.5355831004,-1.5145021267,1.4685906829
H,-3.5454434673,-1.2007256449,5.6491594985
H,-5.1774647764,-1.817590782,3.8598017608
C,1.7001106731,-1.6582217549,0.443228547
C,2.4917058375,-3.4312128902,-1.5718358021
C,3.0475104468,-1.966210747,0.2615995648
C,0.7339145242,-2.2306554855,-0.4107017157
C,1.1421302897,-3.1177071555,-1.4052580257
C,3.4459164467,-2.8492873177,-0.7422790557
H,3.7710016884,-1.5118099302,0.9344563756
H,0.3790729218,-3.5625322905,-2.0389363578
H,4.4989261063,-3.0819571963,-0.8672801446
H,2.7894748575,-4.1261681085,-2.3508783471
C,3.0490161743,1.4749325704,1.1962661007
C,5.5283511913,0.608380259,2.1223051366
C,3.169138058,0.9593104829,2.4930234408
C,4.1812549277,1.58767915,0.380791402
C,5.414553903,1.1328636149,0.8352738142
C,4.4095794072,0.5348059108,2.953828335
H,2.2938291451,0.9090244973,3.1332314471
H,4.0853133558,2.0176082848,-0.6126317843
H,6.2870531644,1.2004503029,0.1936083793
H,4.5058124354,0.1447547641,3.9619572938
H,6.4939356469,0.2692473349,2.4848767928
C,-1.0638001222,-1.2917721809,-3.0314823918
C,-1.5534685953,-3.7148800784,-4.3106832964
C,-0.3209597489,-1.6515494849,-4.1634237879
C,-2.0870413336,-2.1301594818,-2.5697761804
C,-2.3298949785,-3.3370627534,-3.2137168281
C,-0.5500817399,-2.8717602453,-4.7880348463
H,0.4468100446,-0.9785296631,-4.5356890041
H,-2.6902257623,-1.8233980247,-1.7214565696
H,-3.1263142871,-3.9851411572,-2.8626094747
H,0.0416159912,-3.1598952857,-5.6507262887
H,-1.7441759463,-4.6623012569,-4.8055849486

IB-*E,Z*[1,2]^{MeOH} (Intermediate dicoordinate 1,2-B_2cat_2-*E,Z*-diimine **1** complex in MeOH)
boat_cydiimph2_EZ_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1602787

Zero-point correction= 0.572651 (Hartree/Particle)
Thermal correction to Energy= 0.603856
Thermal correction to Enthalpy= 0.604800
Thermal correction to Gibbs Free Energy= 0.509437
Sum of electronic and ZPE= -1696.587627
Sum of electronic and thermal Energies= -1696.556422
Sum of electronic and thermal Enthalpies= -1696.555478
Sum of electronic and thermal Free Energies= -1696.650842

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.925	129.073	200.710

H,-2.0884633226,1.5943666894,-2.3190711984
C,-1.9362296645,1.8775064694,-1.2724086812
C,-1.6354451202,3.830821963,0.3156974639
C,-0.3632023414,1.7327207458,0.6582025432
C,-0.2862856779,3.2559223839,0.7588203336
C,-0.5940006232,1.3081942039,-0.7969812618
C,-1.9633547138,3.4001215192,-1.1155942436
H,-2.4226900628,3.4803932573,0.995390586
H,-1.2436705364,1.4254728818,1.2352690714
H,0.5026425763,3.6556440035,0.1150645554
H,0.2114164509,1.7318496975,-1.4094457233
H,-1.2278550316,3.8420576386,-1.8002727862
H,-2.7378469145,1.4150067467,-0.6832218125
H,-1.6096216256,4.9222596075,0.3854695191
H,-0.0546332565,3.5382083457,1.7908587115
H,-2.9461610558,3.7781284751,-1.4128797983
N,0.7249365673,0.9335390328,1.2434215143
N,-0.5772323435,-0.1659418749,-0.9869033044
C,1.9671179683,1.223865834,1.3075094728
H,2.5843723095,0.4735398523,1.8042137652
C,-0.2190511043,-0.5494941259,-2.1630949361
H,0.213794576,0.2069597033,-2.8241477747
B,0.1252242584,-0.5100495876,1.6603029002
B,-0.8438095769,-1.090371412,0.3525778282
O,-2.2864168257,-0.9749939867,0.5782592351
O,-0.6486760733,-0.2546262447,2.8832321849
O,-0.5145613892,-2.4877624343,0.0700963605
O,1.2565992836,-1.3683157821,2.0078964734
C,-1.9629176441,-0.5809068214,2.9669734986
C,-4.6928160385,-1.1540614673,3.3130505578
C,-2.5566030332,-0.5354981943,4.2303135414
C,-2.7595633435,-0.9288741078,1.8523008301
C,-4.1126983623,-1.2089144443,2.0484662752

C,-3.907974405,-0.8165060534,4.412173012
H,-1.9217306211,-0.2658819139,5.0696011441
H,-4.6996959573,-1.4707129868,1.1725539232
H,-4.3390331264,-0.7704034069,5.4072909962
H,-5.7484716564,-1.3761115997,3.4327279982
C,1.6648036107,-2.3100783284,1.1189191021
C,2.5622896265,-4.350647288,-0.5803436577
C,2.9799001226,-2.7685658794,1.1873978087
C,0.7841792578,-2.8756106471,0.17049498
C,1.2485545235,-3.8918894502,-0.6644002436
C,3.4327200894,-3.7834614319,0.3458559574
H,3.635149476,-2.3193314384,1.9286826361
H,0.5495294577,-4.3177724524,-1.3797160913
H,4.4597850184,-4.1268530292,0.4207475668
H,2.898356865,-5.1444811546,-1.240150903
C,2.641636291,2.4267921915,0.7689109798
C,3.940719065,4.6758742777,-0.2319616595
C,2.853468804,2.5532954514,-0.6066820041
C,3.1115889978,3.4063266998,1.6472111246
C,3.7484706411,4.5358259534,1.1417669509
C,3.50266972,3.6805683424,-1.1034414186
H,2.5179777063,1.7686235875,-1.2789388621
H,2.9592940091,3.2907992644,2.7163281956
H,4.0972246284,5.3062130651,1.8221199587
H,3.665881192,3.7801961447,-2.1717991985
H,4.4405859563,5.556735308,-0.6223987096
C,-0.3886431258,-1.8761463875,-2.7563733382
C,-0.7029331763,-4.3256389588,-4.0405932015
C,0.5705827756,-2.313474361,-3.678022678
C,-1.5288544126,-2.6516629481,-2.5103772925
C,-1.6844008961,-3.8712996071,-3.1580268054
C,0.4250875853,-3.5477167795,-4.3009884874
H,1.4354273082,-1.6897577777,-3.8878498825
H,-2.2889589025,-2.2858924437,-1.8272918399
H,-2.5713613487,-4.4695427301,-2.9761862217
H,1.1805475366,-3.8963501618,-4.9974905563
H,-0.8266709753,-5.2822296374,-4.5391149444

IB-*Z,E*[1,2]^{MeOH} (Intermediate dicoordinate 1,2-B_2cat_2-*Z,E*-diimine **1** complex in MeOH)
boat_cydiimph2_ZE_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1646192

Zero-point correction= 0.572628 (Hartree/Particle)

Thermal correction to Energy= 0.603875
Thermal correction to Enthalpy= 0.604819
Thermal correction to Gibbs Free Energy= 0.508678
Sum of electronic and ZPE= -1696.591991
Sum of electronic and thermal Energies= -1696.560744
Sum of electronic and thermal Enthalpies= -1696.559800
Sum of electronic and thermal Free Energies= -1696.655941

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.937	129.052	202.347

H,-2.4764056813,1.9733951558,-2.0487643278
C,-2.144443033,2.19139699,-1.0284957811
C,-1.3210562619,4.0066553,0.5344028564
C,-0.389436399,1.7041978132,0.691151489
C,-0.057014082,3.1886781289,0.8162170197
C,-0.8664766962,1.39977771,-0.7327705886
C,-1.8863444395,3.6896026152,-0.8520223874
H,-2.074987735,3.7764298887,1.2979147134
H,-1.2080827491,1.4883753647,1.3862187916
H,0.7216351468,3.4733080509,0.0986404444
H,-0.075865557,1.7179478605,-1.4176445109
H,-1.1730304577,4.0202148726,-1.6182081071
H,-2.9293804639,1.849960169,-0.3424369504
H,-1.0944214227,5.0737673034,0.6161003271
H,0.32525552,3.3870347895,1.8224408014
H,-2.815932751,4.2418346466,-1.0191296534
N,0.6916489879,0.7727696136,1.0787051432
N,-1.1006190594,-0.0500303308,-0.907792236
C,1.899820827,1.0269983767,0.7239062579
H,2.0800349705,1.8888087198,0.078441764
C,-1.1424538967,-0.5830425777,-2.0724807634
H,-1.4269970982,-1.6344752418,-2.0969235052
B,-0.0045106708,-0.6219761064,1.5744975995
B,-1.2661624,-0.9574674205,0.4378969442
O,-2.6059245057,-0.6350074728,0.929324026
O,-0.5003744271,-0.3364825671,2.9261932322
O,-1.2386698314,-2.3631099526,0.0063788691
O,0.9768193412,-1.6949936102,1.6534369988
C,-1.8092221596,-0.5192543477,3.2369045249
C,-4.4832183998,-0.8099676181,4.05299881
C,-2.1546002886,-0.5303504041,4.5898781731
C,-2.8324060097,-0.6627723373,2.2717460382
C,-4.1524489381,-0.8064387105,2.7004031894
C,-3.4761876453,-0.6724910969,5.0042181581

H,-1.3496444302,-0.4182414999,5.3107086433
H,-4.916421224,-0.9129390698,1.9353937061
H,-3.7114691992,-0.6752719665,6.063848751
H,-5.5195887946,-0.92231145,4.3552030484
C,1.0998991407,-2.5506332504,0.6086749931
C,1.4066819908,-4.4391495521,-1.4402960281
C,2.3401857919,-3.1384899034,0.3617124749
C,-0.0047973279,-2.9053969471,-0.1966992405
C,0.1653979976,-3.8456053577,-1.2112161072
C,2.4976950667,-4.0803958434,-0.6544692072
H,3.17493798,-2.8471839108,0.9948853139
H,-0.7017204247,-4.1089800819,-1.8109607157
H,3.4711597729,-4.5292454718,-0.8256100951
H,1.5148483398,-5.1729214666,-2.2327304963
C,3.0864335846,0.274775467,1.140270351
C,5.4137882598,-1.0553931513,1.8933203122
C,4.1407149718,0.1361062723,0.2299559024
C,3.2145076459,-0.2262111796,2.4418821739
C,4.3808832874,-0.8826113496,2.8161633961
C,5.2933435818,-0.5485981423,0.5996357249
H,4.0445349852,0.5534141784,-0.7689442258
H,2.4073668407,-0.0819140986,3.1535158138
H,4.4861550964,-1.2613760209,3.8276936274
H,6.1011394497,-0.6747890603,-0.1138630265
H,6.3207129703,-1.5742537412,2.1883691617
C,-0.8642310119,0.073596636,-3.3665013418
C,-0.3806681131,1.207393474,-5.8652619272
C,0.3715969515,0.6731204707,-3.6343620834
C,-1.8432891907,0.0127958641,-4.3637199126
C,-1.6058454676,0.5961846258,-5.6044340153
C,0.6098890043,1.2343875181,-4.8848730042
H,1.1504168044,0.6727564391,-2.8767581671
H,-2.7891300162,-0.4808771404,-4.1593242402
H,-2.3735820561,0.5631076656,-6.3706775061
H,1.5724131253,1.6896240158,-5.094464973
H,-0.1928571769,1.6522334243,-6.8374143812

IB-*Z,Z*[1,2]^{MeOH} (Intermediate dicoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in MeOH)
boat_cydiimph2_ZZ_1-2-b2cat2_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1625792

Zero-point correction= 0.573653 (Hartree/Particle)
Thermal correction to Energy= 0.604659
Thermal correction to Enthalpy= 0.605603
Thermal correction to Gibbs Free Energy= 0.510652

Sum of electronic and ZPE= -1696.588926
Sum of electronic and thermal Energies= -1696.557920
Sum of electronic and thermal Enthalpies= -1696.556976
Sum of electronic and thermal Free Energies= -1696.651928

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.429	128.591	199.842

H,-0.9035642668,-1.6250572535,-3.0388388074
C,-0.6043937748,-2.0877336214,-2.0934305326
C,-1.1566725311,-3.8826077926,-0.3862030247
C,-0.1640697047,-1.7324696078,0.3277480096
C,-1.1505652309,-2.8285240592,0.7289741437
C,-0.6569371282,-1.054629299,-0.9631487595
C,-1.5196173357,-3.2644649294,-1.740770051
H,-0.1628729752,-4.3435970423,-0.4515405303
H,0.7844474366,-2.2328321787,0.1029049224
H,-2.1604488402,-2.4252954283,0.8515183335
H,-1.6954310248,-0.7544003792,-0.7913680213
H,-2.5585302971,-2.9089305944,-1.7089739948
H,0.4318634043,-2.4251171032,-2.2117683929
H,-1.8651568259,-4.6771117764,-0.1339966496
H,-0.8437199899,-3.2678350283,1.6835497626
H,-1.4635178556,-4.0216448877,-2.5284558877
N,0.215774613,-0.7113633163,1.3204315563
N,0.1253960199,0.1547725164,-1.2616473772
C,-0.5452565718,-0.14743898,2.178171767
H,-0.053201043,0.5879884152,2.8167136144
C,-0.4247906367,1.2166796169,-1.7346701034
H,0.2554541956,2.0539450513,-1.8759415116
B,1.7068590896,-0.1753468376,0.9572021224
B,1.676201133,0.1880817148,-0.7269604942
O,2.3742189245,-0.7842419045,-1.5654261744
O,2.6180936203,-1.2667931772,1.3131765228
O,2.200679472,1.5301938126,-1.004421956
O,1.9914011592,0.9684321493,1.8199438307
C,3.4290637974,-1.8286875807,0.3799634501
C,5.1560239161,-3.1356749641,-1.4123632166
C,4.4159174342,-2.7057459822,0.8353466061
C,3.3107589747,-1.5990774391,-1.0104434126
C,4.1794372462,-2.2609079165,-1.8803356394
C,5.2764491156,-3.3578136129,-0.0433382916
H,4.4847839738,-2.863532321,1.9079792263
H,4.0633180525,-2.0662133408,-2.9428393693
H,6.0322038645,-4.0336672515,0.3441532633

H,5.8158186349,-3.6343050986,-2.1152573141
C,1.8715860518,2.2215576422,1.3093852511
C,1.7051556929,4.8704261282,0.3931329008
C,1.6708848154,3.2779402222,2.1985201245
C,1.989019082,2.4999780353,-0.0711075572
C,1.898791288,3.8229833435,-0.5056752506
C,1.58894289,4.5952804318,1.7524907583
H,1.5900105675,3.0375445368,3.2550025314
H,1.9958929747,4.0094095968,-1.5720203598
H,1.435478086,5.3974751592,2.4673295922
H,1.6446717311,5.8905188717,0.0275053782
C,-2.0018712098,-0.3574076026,2.3444325472
C,-4.743781667,-0.7395469552,2.6332779318
C,-2.4900919356,-1.087478979,3.4302456625
C,-2.8857411597,0.2161391367,1.4254481887
C,-4.2565879371,0.0194032872,1.5708838115
C,-3.861240051,-1.2857065212,3.5644740587
H,-1.7977422226,-1.5143681214,4.1498084545
H,-2.5013252587,0.8197153147,0.6066427156
H,-4.9406336206,0.4608195365,0.8526837881
H,-4.2407287795,-1.8680090157,4.3980480268
H,-5.8121493217,-0.8974539508,2.7420335123
C,-1.8339429613,1.5186038014,-2.0218958059
C,-4.4756048026,2.3670116433,-2.3726866047
C,-2.1899521535,2.8592469425,-1.7998194962
C,-2.8131405098,0.6145232347,-2.4625887805
C,-4.1238654528,1.0441265216,-2.6384707188
C,-3.5058936314,3.2768214763,-1.9556783703
H,-1.4262907639,3.5651040536,-1.4829384292
H,-2.5599575841,-0.410994186,-2.7027910583
H,-4.8729740371,0.3416937034,-2.9888691078
H,-3.7716524593,4.310711862,-1.76172894
H,-5.503075726,2.6910223381,-2.5056213936

IB-*E*,*E*[1,1]^{DMF} (Intermediate dicoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
boat_cydiimph2_EE_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1481842

Zero-point correction= 0.571932 (Hartree/Particle)
Thermal correction to Energy= 0.603457
Thermal correction to Enthalpy= 0.604401
Thermal correction to Gibbs Free Energy= 0.509201
Sum of electronic and ZPE= -1696.576253
Sum of electronic and thermal Energies= -1696.544727

Sum of electronic and thermal Enthalpies= -1696.543783
Sum of electronic and thermal Free Energies= -1696.638984

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.675	129.734	200.367

H,3.1516077004,2.7580833848,1.3565894505
C,2.3437818835,3.0736632954,0.6880926538
C,0.8110291143,4.9825956567,0.059173354
C,-0.0461327434,2.6416324668,0.0414927522
C,-0.4021756919,4.09426834,0.3502835333
C,1.1104168443,2.2068136941,0.9601438083
C,2.0148947675,4.5528107251,0.8996346175
H,1.0627166251,4.9129524012,-1.0066235398
H,0.2978618504,2.5897126785,-0.9956203556
H,-0.6761012263,4.2100106959,1.4058758873
H,0.777825736,2.3650278943,1.9941564723
H,1.7919981535,4.7241900959,1.9606656234
H,2.6706772705,2.8950390524,-0.3421769095
H,0.5581033236,6.0269278527,0.2642127884
H,-1.2642179621,4.3933139227,-0.25516626
H,2.8898537293,5.1613530322,0.6523412136
N,-1.1613111772,1.6718413105,0.1106454965
N,1.4178781845,0.7619020233,0.8142553975
C,-2.1750165754,1.9137287452,0.8528800176
H,-2.1675772899,2.7988350196,1.4908687092
C,1.9831808453,0.2063927296,1.8209101249
H,2.250900728,0.854281619,2.661385922
B,-0.7757871957,0.2054129197,-0.6396697667
B,0.9539963493,0.14554754,-0.6830233655
O,1.7294544979,1.0045220309,-1.6299965108
O,1.5504506533,-1.1866944314,-0.833033633
O,-1.4989863904,0.0939238194,-1.9261483753
O,-1.3464433125,-0.8656303403,0.220168813
C,2.76930707,-0.9902633291,-1.3848706204
C,5.0856071141,-0.148020543,-2.6339742255
C,3.8109186469,-1.8899119037,-1.5060994031
C,2.8753273909,0.3250190884,-1.8710770285
C,4.0236575174,0.7655072009,-2.5011791096
C,4.982747308,-1.4457525022,-2.1454335148
H,3.7194780293,-2.8996992905,-1.1178417735
H,4.0974038275,1.7809251917,-2.8778910317
H,5.8188259913,-2.1295558328,-2.2546000825
H,6.000917592,0.1717989656,-3.1223651321
C,-2.2744478946,-1.5098312023,-0.5194253291

C,-4.0826877545,-2.4961109871,-2.3620578399
C,-3.0813559636,-2.5652521493,-0.1435554861
C,-2.3615815364,-0.938859976,-1.8027984599
C,-3.2574174307,-1.4191241722,-2.7384473254
C,-3.9986642978,-3.0556645148,-1.0925346772
H,-3.0133987415,-2.9871510615,0.854339834
H,-3.3247743094,-0.9697366137,-3.7241002516
H,-4.6457911199,-3.8855000362,-0.8254516213
H,-4.7948961522,-2.8928066055,-3.0791497035
C,-3.4070070857,1.1030763189,0.8713968143
C,-5.8164586273,-0.2923374349,0.9126980741
C,-3.8820840201,0.5699126034,2.0737983354
C,-4.1501084652,0.9580288322,-0.3029497765
C,-5.363002723,0.2724624649,-0.2759555279
C,-5.0719124993,-0.1490797046,2.0856583279
H,-3.3107281148,0.7044860058,2.9876478387
H,-3.7795755092,1.3927916948,-1.2261376463
H,-5.9422195578,0.1684686066,-1.1880966099
H,-5.4284162446,-0.5860837157,3.0128720971
H,-6.7532846783,-0.8405117317,0.9304493485
C,2.3105864059,-1.2170931336,2.0044534986
C,2.9871713706,-3.868346227,2.5212891104
C,1.4019280572,-2.2381397733,1.7017094498
C,3.5378463729,-1.5246555106,2.6022127956
C,3.8854537592,-2.8512452575,2.8381065978
C,1.7434860473,-3.5589937778,1.9683718375
H,0.4387764345,-1.9859210312,1.2685938674
H,4.2215443965,-0.7228155684,2.8676672888
H,4.8474681874,-3.0883394022,3.2805775259
H,1.0379599916,-4.3524340903,1.7429405085
H,3.249338523,-4.9033190686,2.7182841068

IB-*E,Z*[1,1]^{DMF} (Intermediate dicoordinate 1,1-B_2cat_2-*E,Z*-diimine **1** complex in DMF)
boat_cydiimph2_EZ_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1438619

Zero-point correction= 0.572080 (Hartree/Particle)
Thermal correction to Energy= 0.603742
Thermal correction to Enthalpy= 0.604686
Thermal correction to Gibbs Free Energy= 0.507984
Sum of electronic and ZPE= -1696.571782
Sum of electronic and thermal Energies= -1696.540120
Sum of electronic and thermal Enthalpies= -1696.539175
Sum of electronic and thermal Free Energies= -1696.635878

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.854	129.518	203.527

H,1.1656256939,-3.3441177094,1.5188356728
C,0.4162166187,-2.6538752268,1.9207213967
C,-1.8294235468,-2.4877833669,3.0909402491
C,-1.2498532871,-0.8749471433,1.3052669645
C,-2.3963397962,-1.6776397852,1.9180038787
C,-0.1730738049,-1.8381536418,0.7693971328
C,-0.7068160172,-3.4217319791,2.6268635747
H,-1.4423478344,-1.801022427,3.8545073612
H,-0.8008051613,-0.2864506145,2.113332172
H,-2.8331716828,-2.3652934398,1.1881270767
H,-0.6706722266,-2.5270036264,0.0762701101
H,-1.1239159101,-4.1660945113,1.9360600969
H,0.9169212289,-1.9770120161,2.619156696
H,-2.6326016006,-3.0673879456,3.5554859148
H,-3.1845829317,-0.9957553046,2.2530096716
H,-0.2941536281,-3.9703594239,3.4787975885
N,-1.5406768699,0.1308645335,0.2676555329
N,0.8363876218,-1.0826858603,-0.0122220133
C,-2.4304420124,0.0709183044,-0.6437398972
H,-2.4543265268,0.9259180687,-1.3214065684
C,1.3238749951,-1.6844768702,-1.0330719795
H,1.0532699392,-2.7357404801,-1.1712289169
B,-0.3802185069,1.3451729946,0.3269844733
B,1.1141209102,0.4953092157,0.5735567606
O,1.4917689297,0.2310203925,1.9908882034
O,2.3466424267,0.9832083561,-0.0495697391
O,-0.816638039,2.2295807028,1.4346463834
O,-0.5558845903,2.1407409919,-0.9039805036
C,3.3559601995,0.5858844292,0.760014673
C,5.0636647514,-0.2910558005,2.7459898993
C,4.7136266059,0.5962185908,0.5052547463
C,2.842433647,0.1377247428,1.9897139427
C,3.6794545186,-0.302576976,2.997528298
C,5.5696390333,0.1469066129,1.5270028068
H,5.095861896,0.9381057862,-0.4516237098
H,3.2777283449,-0.6428462022,3.9468402987
H,6.6416616327,0.1405743035,1.3560469928
H,5.7446179693,-0.6347842466,3.5184565333
C,-1.2788075051,3.2333980264,-0.5464794516
C,-2.6756374554,5.3073455838,0.6275712712
C,-1.8070570144,4.2125367846,-1.3650234952
C,-1.439387375,3.276396819,0.8500617869

C,-2.1359825756,4.3065318043,1.4549648193
C,-2.5153776763,5.2621570058,-0.7526197447
H,-1.6745646435,4.1674164645,-2.4412867904
H,-2.2560030523,4.3354982743,2.533147927
H,-2.9418003586,6.0457412763,-1.371062042
H,-3.2265746282,6.1267011047,1.0788849432
C,-3.3856199359,-1.0345071716,-0.8974010634
C,-5.1727695455,-3.1113558312,-1.3877052757
C,-4.7270572516,-0.8967063816,-0.5338152828
C,-2.9444028976,-2.1950058283,-1.5386778043
C,-3.8411215984,-3.2328750189,-1.7801091341
C,-5.6149241486,-1.9423874131,-0.7698673257
H,-5.0651510812,0.0151791872,-0.050715613
H,-1.9063168243,-2.2799534478,-1.8484640954
H,-3.4980452251,-4.1358460527,-2.2747949806
H,-6.653671303,-1.8431843359,-0.4715853363
H,-5.8683218019,-3.9240889717,-1.5710880561
C,2.1756915363,-1.1123636983,-2.086627791
C,3.7301149527,-0.1799905737,-4.2002248321
C,1.9183426084,0.1494046309,-2.6372668277
C,3.1861054749,-1.9176171307,-2.6228431291
C,3.9788184823,-1.4412360286,-3.6626519972
C,2.6923871084,0.6063359445,-3.6967363426
H,1.1121893946,0.7591987367,-2.2392174954
H,3.3544027781,-2.9102635204,-2.214194489
H,4.7770583348,-2.0584688621,-4.0616580514
H,2.4887109553,1.5796845088,-4.1314133038
H,4.3363932821,0.1872776871,-5.0225447707

IB-*Z,E*[1,1]^{DMF} (Intermediate dicoordinate 1,1-B_2cat_2-*Z,E*-diimine **1** complex in DMF)
boat_cydiimph2_ZE_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1496584

Zero-point correction= 0.572055 (Hartree/Particle)
Thermal correction to Energy= 0.603585
Thermal correction to Enthalpy= 0.604529
Thermal correction to Gibbs Free Energy= 0.508156
Sum of electronic and ZPE= -1696.577603
Sum of electronic and thermal Energies= -1696.546073
Sum of electronic and thermal Enthalpies= -1696.545129
Sum of electronic and thermal Free Energies= -1696.641502

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K

Total	378.755	129.510	202.834

H,-2.8979781815,1.615475118,-2.0164573544
C,-2.6302637018,1.8582746224,-0.9826096413
C,-2.2461248915,3.7330389746,0.669979584
C,-0.7842844433,1.7169047094,0.7224592849
C,-0.8160524257,3.2328384673,0.8979299642
C,-1.1998330432,1.3733731811,-0.7195813617
C,-2.7377854851,3.3629933276,-0.7308839811
H,-2.9090812879,3.2871272128,1.4221221973
H,-1.5156084583,1.2774248458,1.4079761588
H,-0.1538837161,3.7210263865,0.1722196166
H,-0.5118806395,1.895386212,-1.3906069697
H,-2.1335871964,3.8955164926,-1.4765951685
H,-3.3073262596,1.3047878326,-0.3212522689
H,-2.2814434681,4.8173348052,0.8100133211
H,-0.4632815129,3.4913290797,1.9017579137
H,-3.7747209698,3.6836597209,-0.868454029
N,0.4905450151,1.0446332477,1.0544028561
N,-1.1176392093,-0.0773515934,-0.9609715952
C,1.5916546823,1.6923094004,0.9848100906
H,1.5784815694,2.7212811228,0.6222802392
C,-0.8847847979,-0.5707801136,-2.1176545717
H,-0.9246018947,-1.659043753,-2.1738444742
B,0.3068351039,-0.6325551069,1.205403726
B,-1.1800746007,-1.0249082348,0.3969166893
O,-2.4907369412,-0.7244194272,1.0384016548
O,-1.2978386867,-2.4190514003,-0.0770247339
O,0.4272714024,-1.0268800857,2.6263212396
O,1.4832064247,-1.232973802,0.5305311997
C,-2.6184357524,-2.7205590399,-0.0268593821
C,-5.3521067282,-2.9370013868,0.3291901942
C,-3.256363653,-3.8462443413,-0.5118422311
C,-3.3306662373,-1.7057782824,0.636530801
C,-4.6975437353,-1.7943212001,0.8229803442
C,-4.6468871275,-3.9416836682,-0.3235809512
H,-2.6969372683,-4.6253368884,-1.0198535672
H,-5.2394173755,-1.0062942174,1.3363184824
H,-5.1736679125,-4.8142598071,-0.697187196
H,-6.4255328107,-3.0312723165,0.4612628097
C,2.1683113183,-1.9121757651,1.4719145039
C,3.2557856852,-3.1258810522,3.706982317
C,3.3429827219,-2.6236014417,1.3255025009
C,1.5350913273,-1.7947962786,2.7240891187
C,2.0596447349,-2.3966750197,3.8512479697
C,3.884828328,-3.2348611133,2.4725511695

H,3.8314035518,-2.6939310068,0.3586827795
H,1.5681456155,-2.2963143197,4.8137659824
H,4.8073281034,-3.800898535,2.3859489914
H,3.689703842,-3.6090282617,4.5771142728
C,2.9024639651,1.1630257543,1.4076016626
C,5.4133356643,0.297243713,2.2469426974
C,3.9699679026,1.1402930969,0.5039740965
C,3.0987026894,0.7738963917,2.7348301371
C,4.3602100473,0.3562033504,3.1554590535
C,5.2153516817,0.682551836,0.9193468402
H,3.8165538156,1.463613612,-0.5217329299
H,2.2666268204,0.8109515086,3.4312113813
H,4.5118911727,0.0631597673,4.1895785069
H,6.037286769,0.639913058,0.2119658936
H,6.3917517452,-0.0430769466,2.5714946884
C,-0.5683406654,0.1763237045,-3.3548274245
C,0.03594276,1.4877730988,-5.7384515377
C,0.5712914999,0.9841576709,-3.4393437556
C,-1.3884536727,0.0052865452,-4.4742643486
C,-1.0927626964,0.6741406664,-5.6586112102
C,0.871513087,1.6343524883,-4.6321944698
H,1.2277768195,1.0820094877,-2.5787093891
H,-2.2576653546,-0.6429879625,-4.410727704
H,-1.7392666634,0.5519550448,-6.5215595237
H,1.7605235736,2.2531081601,-4.6983147998
H,0.2704500248,2.0002686739,-6.6660163808

IB-*Z,Z*[1,1]^{DMF} (Intermediate dicoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in DMF)
boat_cydiimph2_ZZ_b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1456299

Zero-point correction= 0.572661 (Hartree/Particle)
Thermal correction to Energy= 0.604183
Thermal correction to Enthalpy= 0.605127
Thermal correction to Gibbs Free Energy= 0.508523
Sum of electronic and ZPE= -1696.572969
Sum of electronic and thermal Energies= -1696.541447
Sum of electronic and thermal Enthalpies= -1696.540503
Sum of electronic and thermal Free Energies= -1696.637107

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.131	129.238	203.321

H,2.4980266462,1.9456870717,-1.6400926021

C,1.6458703997,1.3721173137,-2.0201730323
C,-0.3166873959,1.3907334837,-3.6232020424
C,-0.5623690949,0.3572184922,-1.3852227929
C,-1.2857361835,1.1688726611,-2.4561637567
C,0.6702399908,1.1172669073,-0.8656822248
C,0.9416964993,2.1251023256,-3.1518963811
H,-0.0359581158,0.4225444726,-4.0569901422
H,-0.1971851223,-0.5524998249,-1.8784894277
H,-1.604416601,2.1421719853,-2.0775166796
H,0.3384686639,2.0764596376,-0.4616104878
H,0.6617968577,3.126211949,-2.7986924667
H,2.0205445277,0.4054626317,-2.3746539462
H,-0.8167170563,1.9647004378,-4.4088384437
H,-2.1798031431,0.625676016,-2.7790008606
H,1.6378098453,2.2615676027,-3.984905547
N,-1.3198218367,-0.1673545688,-0.2392031502
N,1.3288197062,0.345100888,0.2065885658
C,-2.3528231347,0.3067502441,0.3458322806
H,-2.7332491594,-0.3263318225,1.1491562351
C,1.9976543171,0.914886864,1.1343900474
H,2.4955850615,0.2429962186,1.8339503061
B,-0.5989143971,-1.6038028925,0.2566880161
B,1.1153435909,-1.3209448309,0.1653911971
O,1.7607055841,-1.7261993917,-1.114944562
O,1.9902859885,-1.8572085237,1.222728933
O,-1.1078876205,-2.6095248,-0.7149066838
O,-1.2184986274,-1.9607230067,1.5458981311
C,3.1572817352,-2.1821526813,0.61000375
C,5.2909546244,-2.7815083131,-1.0418961135
C,4.3492852008,-2.5673630069,1.1927388551
C,3.0186840128,-2.0967035047,-0.7867508289
C,4.0748166052,-2.3904771204,-1.6294881659
C,5.425750385,-2.8687615484,0.3392252449
H,4.4444804942,-2.6318882908,2.2720009169
H,3.9599286484,-2.3220860708,-2.7066397659
H,6.3749495412,-3.1718420242,0.7699471585
H,6.136436222,-3.0167864245,-1.6809578865
C,-2.1722674463,-2.883909804,1.267303748
C,-3.9322709413,-4.7637362186,0.2641763966
C,-3.1038788618,-3.4337831344,2.1267490776
C,-2.1098970346,-3.2603122831,-0.0867094296
C,-2.982806954,-4.1988116461,-0.6061443215
C,-3.9920591452,-4.390052011,1.6017929893
H,-3.1415918376,-3.1348142641,3.1694229944
H,-2.9290694828,-4.4862243307,-1.6512773895
H,-4.7341580846,-4.8389696607,2.2546183816

H,-4.6283622264,-5.5031005442,-0.1198231891
C,-3.1251659159,1.5452011608,0.1207073222
C,-4.7429828853,3.8027659359,-0.1612224316
C,-4.5198827907,1.4170584917,0.102165946
C,-2.5477619454,2.8168862144,0.0391907189
C,-3.3574566787,3.9401937883,-0.0970691054
C,-5.3238737281,2.539524989,-0.0627007715
H,-4.9673032757,0.4325079884,0.2062373723
H,-1.4708462252,2.9336320144,0.0997999102
H,-2.9034947208,4.9243402923,-0.1508280125
H,-6.4027182145,2.4295121874,-0.0988966326
H,-5.3700928608,4.6814381167,-0.2739493883
C,2.1430395093,2.3743127489,1.3423720284
C,2.453940661,5.1057471272,1.7910948338
C,1.0378639085,3.1539048475,1.6989924916
C,3.4081351156,2.9580300368,1.2362870593
C,3.5572338163,4.3261402974,1.4488839016
C,1.1966779898,4.5179582557,1.9234661109
H,0.0637821942,2.6857516602,1.813720273
H,4.2662902199,2.3436470524,0.9796223464
H,4.5377053153,4.7811983715,1.3530683984
H,0.3381158419,5.1199583251,2.2035539048
H,2.5750590245,6.1705994394,1.9627218189

IB-*E*,*E*[1,2]^{DMF} (Intermediate dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
boat_cydiimph2_EE_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1614746

Zero-point correction= 0.572521 (Hartree/Particle)
Thermal correction to Energy= 0.603611
Thermal correction to Enthalpy= 0.604555
Thermal correction to Gibbs Free Energy= 0.510016
Sum of electronic and ZPE= -1696.588953
Sum of electronic and thermal Energies= -1696.557863
Sum of electronic and thermal Enthalpies= -1696.556919
Sum of electronic and thermal Free Energies= -1696.651459

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.772	129.096	198.975

H,-2.5160804997,2.1619130393,-2.3916830264
C,-2.2935335807,2.4115871385,-1.3493489756
C,-1.9179372466,4.3052989612,0.2837150339

C,-0.591166016,2.2018712008,0.4661285697
C,-0.5453932322,3.7209489783,0.6245781536
C,-0.9219817462,1.8328520032,-0.9799835184
C,-2.3259596187,3.9264572665,-1.1404885534
H,-2.6609919168,3.9202156992,0.9935134441
H,-1.3931936223,1.8218559899,1.1088191061
H,0.2030947729,4.157680729,-0.0471607981
H,-0.1502263458,2.2700409182,-1.6285788382
H,-1.6357840885,4.4001810628,-1.8505298065
H,-3.0480905688,1.918864061,-0.7230778059
H,-1.894791861,5.3930542001,0.3970770808
H,-0.2547903704,3.9623899319,1.6518226063
H,-3.3278333538,4.3041290561,-1.3654982397
N,0.6177532507,1.4862524998,0.9158897962
N,-0.9295119138,0.3653427613,-1.2043509057
C,1.7783444664,1.9792117263,0.6701997185
H,1.8402393704,2.8777379546,0.0541741909
C,-0.7963232437,0.0154635413,-2.4371872682
H,-0.4991001898,0.7938722103,-3.1459387047
B,0.168408721,-0.017756458,1.3447321005
B,-0.9435904293,-0.5984042031,0.1286089547
O,-2.3396976586,-0.5760137804,0.564015142
O,-0.4705208612,0.1501332291,2.6539873537
O,-0.5705841939,-1.9601793623,-0.257947357
O,1.3377111995,-0.8702847639,1.4873463584
C,-1.6847857211,-0.3860917912,2.9019986727
C,-4.2200652845,-1.4009484724,3.5804541627
C,-2.0640989997,-0.5556967311,4.2355405038
C,-2.6032245598,-0.7407832376,1.8831866047
C,-3.8535293619,-1.2437325275,2.2448839513
C,-3.3177642538,-1.0558468265,4.5822167138
H,-1.3425810179,-0.2750476297,4.997398029
H,-4.5367734368,-1.5045943564,1.4416929608
H,-3.5811216974,-1.1724684437,5.6288713119
H,-5.2013465697,-1.7927561961,3.8290366208
C,1.709694255,-1.6528278392,0.4530209232
C,2.518605342,-3.4157691899,-1.5696108799
C,3.0587583652,-1.9584320502,0.2743310335
C,0.7479752215,-2.2240137086,-0.4116494877
C,1.1671263154,-3.1048597144,-1.4084379669
C,3.4664344639,-2.8358581466,-0.7316248482
H,3.776608745,-1.5032851194,0.9523852702
H,0.4082006146,-3.5457912433,-2.0497178338
H,4.5209574945,-3.0646143627,-0.8516764885
H,2.8224107387,-4.1055454914,-2.351009644
C,3.0530510978,1.4644390685,1.178692745

C,5.5325550718,0.6159465221,2.1227949162
C,3.1647612973,0.9319247662,2.4692959611
C,4.1933029297,1.5997756014,0.3776533926
C,5.4269372164,1.1544536978,0.8405945572
C,4.4051752045,0.5180897308,2.9398797529
H,2.2814728353,0.8604184005,3.0951548138
H,4.1035888463,2.0412828529,-0.6112383357
H,6.3058297128,1.2405720283,0.210133176
H,4.4949427534,0.1164993694,3.9440494791
H,6.4981792315,0.2849067787,2.4924904409
C,-1.0669013193,-1.2936178338,-3.027854394
C,-1.5825302884,-3.7185081473,-4.293776218
C,-0.3586649433,-1.6479998301,-4.1834387485
C,-2.0677482053,-2.1400595085,-2.5322125339
C,-2.3242927034,-3.3471017782,-3.1709014957
C,-0.6002131755,-2.8687334242,-4.8025193659
H,0.391695235,-0.9692231554,-4.5799682708
H,-2.6378186748,-1.8390780864,-1.6595257398
H,-3.1038802739,-4.0016656636,-2.7948626695
H,-0.0355672023,-3.1518845021,-5.6846693255
H,-1.7838245418,-4.6661893698,-4.7838955383

IB-*E,Z*[1,2]^{DMF} (Intermediate dicoordinate 1,2-B_2cat_2-*E,Z*-diimine **1** complex in DMF)
boat_cydiimph2_EZ_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.156283

Zero-point correction= 0.572719 (Hartree/Particle)
Thermal correction to Energy= 0.603927
Thermal correction to Enthalpy= 0.604871
Thermal correction to Gibbs Free Energy= 0.509409
Sum of electronic and ZPE= -1696.583564
Sum of electronic and thermal Energies= -1696.552356
Sum of electronic and thermal Enthalpies= -1696.551412
Sum of electronic and thermal Free Energies= -1696.646874

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.970	129.069	200.918

H,-2.0972077208,1.5815627093,-2.2960108402
C,-1.9417161631,1.8597035218,-1.2485626571
C,-1.6468955275,3.8091596643,0.3474026902
C,-0.3608054053,1.7180086298,0.6736002732
C,-0.291501294,3.2411484191,0.7806855116
C,-0.5918661189,1.3000003608,-0.7837055074

C,-1.981177079,3.3813508863,-1.0835060179
H,-2.4271939008,3.4501608257,1.0306084762
H,-1.2393744242,1.4029208873,1.2488937292
H,0.491977045,3.6476883801,0.1343335324
H,0.2073464728,1.736114677,-1.3958773968
H,-1.2538059947,3.8325754854,-1.7707693391
H,-2.7322571364,1.3826003073,-0.656413575
H,-1.6287226269,4.9004398275,0.421054276
H,-0.0558613857,3.5210009481,1.8124766548
H,-2.9688593275,3.7530848178,-1.3723371504
N,0.7294151384,0.9202087601,1.2526547529
N,-0.5634850146,-0.1709365409,-0.9811405718
C,1.971599474,1.2103433156,1.3071726106
H,2.5904374269,0.4575262536,1.7981898319
C,-0.2026702472,-0.5474770486,-2.1582486145
H,0.2281699227,0.2121711022,-2.8169831417
B,0.1303912753,-0.5295430233,1.6734099671
B,-0.8345819041,-1.1063415466,0.3574301948
O,-2.2747500947,-0.9827119846,0.5703592145
O,-0.6504711562,-0.2713418865,2.8861784373
O,-0.4944196651,-2.495158762,0.0632980835
O,1.2690433492,-1.3765487736,2.0127223416
C,-1.9643566742,-0.5725769492,2.9563318937
C,-4.7123581899,-1.095189258,3.2780157078
C,-2.5748300026,-0.5072610133,4.2119584694
C,-2.7575531554,-0.9172222716,1.8334438101
C,-4.1181312547,-1.1698629146,2.0202381584
C,-3.9333668036,-0.7630344795,4.3826884422
H,-1.9447515033,-0.2414991015,5.055870654
H,-4.7000114308,-1.4274389795,1.1398519442
H,-4.3736938742,-0.7010835501,5.3729784987
H,-5.773229285,-1.2972249588,3.3873556519
C,1.6769464313,-2.31238823,1.1267874921
C,2.58707416,-4.3485388744,-0.5784633225
C,2.9921497256,-2.7734046163,1.1978543463
C,0.8000382827,-2.876853244,0.1697317824
C,1.2732181223,-3.8890422846,-0.666573797
C,3.4516640488,-3.7851006152,0.3551736226
H,3.6432783448,-2.3264447003,1.9440762117
H,0.5780984625,-4.3103142486,-1.38827415
H,4.4786368119,-4.1278698076,0.4349052736
H,2.9270336907,-5.138974845,-1.2404236719
C,2.641730084,2.4139480339,0.7621403592
C,3.9285867439,4.6658242813,-0.2519684503
C,2.8463070872,2.5384825364,-0.6150241561
C,3.1130221751,3.398236663,1.6345468216

C,3.7440806682,4.5284231715,1.1230523042
C,3.4887953077,3.6668036171,-1.1183320585
H,2.5099848056,1.7513839128,-1.2840111817
H,2.9668344482,3.2858979281,2.7047475656
H,4.093941767,5.3014645593,1.7996822582
H,3.645569177,3.7642363019,-2.1877560043
H,4.4235068292,5.5471784107,-0.6472928307
C,-0.3749634551,-1.8720382197,-2.7556349317
C,-0.7069653333,-4.3135671708,-4.0508205804
C,0.5595973938,-2.293556615,-3.709528267
C,-1.4993050391,-2.6609490552,-2.4795226766
C,-1.6644201788,-3.8756403615,-3.1342524115
C,0.406276416,-3.5238666807,-4.3385402543
H,1.4113525472,-1.6597509187,-3.9412695582
H,-2.2355325286,-2.3085694796,-1.7645699697
H,-2.5397623664,-4.4839679471,-2.930823772
H,1.1426912911,-3.8597683758,-5.061040082
H,-0.8379416944,-5.2665898628,-4.5542248673

IB-*Z,E*[1,2]^{DMF} (Intermediate dicoordinate 1,2-B_2cat_2-*Z,E*-diimine **1** complex in DMF)
boat_cydiimph2_ZE_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.160457

Zero-point correction= 0.572560 (Hartree/Particle)
Thermal correction to Energy= 0.603839
Thermal correction to Enthalpy= 0.604783
Thermal correction to Gibbs Free Energy= 0.508755
Sum of electronic and ZPE= -1696.587897
Sum of electronic and thermal Energies= -1696.556618
Sum of electronic and thermal Enthalpies= -1696.555674
Sum of electronic and thermal Free Energies= -1696.651702

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.914	129.143	202.107

H,-2.4970510271,1.9346041501,-2.015495093
C,-2.1642472913,2.1426154471,-0.9934075348
C,-1.3587583479,3.9480967149,0.5918604632
C,-0.3960836561,1.6576825847,0.7122140996
C,-0.0816122497,3.1443283776,0.8561412259
C,-0.872899814,1.3670980842,-0.7151155136
C,-1.9276945114,3.6418383607,-0.7957657246
H,-2.1048757129,3.6958787316,1.3561151833

H,-1.2124078192,1.423097983,1.4037061255
H,0.6895780606,3.4486067958,0.1384705827
H,-0.0897861905,1.7095471342,-1.3971050124
H,-1.2234183182,3.9939378561,-1.5606431258
H,-2.9385914575,1.7759388244,-0.3086446337
H,-1.1479229266,5.0172675257,0.6869383784
H,0.3029827901,3.3347314491,1.8629693455
H,-2.8658965957,4.1832309874,-0.9494985417
N,0.6929047942,0.7323047568,1.0868596863
N,-1.0828755735,-0.0820421666,-0.9080593536
C,1.8971351226,0.9967256342,0.727026168
H,2.0698695547,1.8627711383,0.0850258152
C,-1.1111490108,-0.604154582,-2.0771561645
H,-1.3743825998,-1.6610940775,-2.1080929579
B,0.0024639932,-0.6759372748,1.5811658345
B,-1.2545632844,-1.0085838859,0.4352221246
O,-2.5931388535,-0.6840007943,0.9145073388
O,-0.4954481497,-0.3968415212,2.9277432488
O,-1.2101961737,-2.4023739505,-0.0197844931
O,0.9960794786,-1.7332038641,1.6460750845
C,-1.8093912005,-0.4984029947,3.2217609246
C,-4.5080883021,-0.6250827184,4.0149425239
C,-2.1753819281,-0.4320711649,4.5690116872
C,-2.8296733008,-0.6371294569,2.2471351767
C,-4.1598553298,-0.6967636348,2.6681175534
C,-3.5068588845,-0.493391448,4.9729371916
H,-1.3743444269,-0.3255978328,5.2948376666
H,-4.918755903,-0.8005369408,1.8979013834
H,-3.7535442834,-0.4375712005,6.0285845757
H,-5.5524157197,-0.6742246557,4.3067334836
C,1.1259367585,-2.5742055275,0.5976340233
C,1.4556055352,-4.4447364391,-1.4692384702
C,2.371349052,-3.1511428335,0.3462186107
C,0.0238357582,-2.9306560774,-0.2161961475
C,0.2090019238,-3.8621383174,-1.2376109535
C,2.5413480585,-4.0832907377,-0.6776681715
H,3.2008245308,-2.855823942,0.9840389756
H,-0.6536003083,-4.1273649539,-1.843117576
H,3.5195170848,-4.521476455,-0.8500051097
H,1.5714022651,-5.1704770966,-2.2680442571
C,3.0908740194,0.2500428601,1.1342172355
C,5.4350083739,-1.0569517313,1.8793285114
C,4.1581814037,0.1544566443,0.2332291501
C,3.2130891093,-0.286191843,2.4222264826
C,4.3879846643,-0.9292136294,2.793372988
C,5.3194065013,-0.5184799794,0.5978833237

H,4.0663581799,0.5968534315,-0.7551691163
H,2.3925283749,-0.1803020119,3.124093883
H,4.488726613,-1.3336596431,3.7953706399
H,6.1374678504,-0.6099951279,-0.1090306193
H,6.348530331,-1.5656633629,2.1714833267
C,-0.8504385112,0.069209291,-3.367368169
C,-0.4097077694,1.235196218,-5.8610478972
C,0.3649536944,0.7092211772,-3.6354248205
C,-1.8296997701,-0.0140086105,-4.3631729999
C,-1.6143923053,0.5843757142,-5.6008490563
C,0.581961464,1.2863813381,-4.8827267221
H,1.146112456,0.7288189303,-2.8807986085
H,-2.7592899888,-0.5380730559,-4.1601568929
H,-2.3830663884,0.5323348006,-6.3649868799
H,1.5289239326,1.7734180511,-5.0912540113
H,-0.2384379052,1.6922445177,-6.8304653344

IB-*Z*,*Z*[1,2]^{DMF} (Intermediate dicoordinate 1,2-B_2cat_2-*Z*,*Z*-diimine **1** complex in DMF)
boat_cydiimph2_ZZ_1-2-b2cat2_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1591111

Zero-point correction= 0.573555 (Hartree/Particle)
Thermal correction to Energy= 0.604638
Thermal correction to Enthalpy= 0.605582
Thermal correction to Gibbs Free Energy= 0.509999
Sum of electronic and ZPE= -1696.585557
Sum of electronic and thermal Energies= -1696.554473
Sum of electronic and thermal Enthalpies= -1696.553529
Sum of electronic and thermal Free Energies= -1696.649112

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.416	128.677	201.172

H,-0.8751389861,-1.5948205545,-3.04351464
C,-0.5685527558,-2.0566360332,-2.0999840854
C,-1.09407612,-3.869789809,-0.4028702555
C,-0.144154339,-1.7062864629,0.3249930349
C,-1.1132993606,-2.8208546286,0.7169047591
C,-0.6430071313,-1.0296724617,-0.9652075933
C,-1.4626314988,-3.2520787091,-1.7562001332
H,-0.0906738608,-4.3099000192,-0.4658735315
H,0.8124101263,-2.1900806106,0.0994819864
H,-2.1306362685,-2.4358028778,0.835713624
H,-1.6869343694,-0.746704129,-0.7959658794

H,-2.5080501758,-2.9160863278,-1.726506092
H,0.4756049978,-2.3687971194,-2.2161623119
H,-1.7875734537,-4.6796289904,-0.1582158173
H,-0.8040493033,-3.2586679499,1.6713818222
H,-1.3897328044,-4.0046534011,-2.5468876443
N,0.2181452319,-0.6846235906,1.3214779863
N,0.1254110597,0.189759712,-1.2532328099
C,-0.5482256662,-0.1437278237,2.1882348438
H,-0.0641170554,0.5958515261,2.8282206442
C,-0.4305610874,1.2491294936,-1.7222291036
H,0.2450854128,2.0924307666,-1.8502577828
B,1.7121906658,-0.1276176315,0.9669602282
B,1.6851648759,0.2279790466,-0.7202928373
O,2.3675950834,-0.7562670055,-1.5523266573
O,2.6271169257,-1.2091979046,1.3290532344
O,2.1973115528,1.5688954991,-1.0052696785
O,1.9601413939,1.0213854698,1.8283782468
C,3.3929407383,-1.8174783938,0.3979237475
C,5.0374145111,-3.2301504285,-1.3990531987
C,4.3467954204,-2.7334982923,0.8503496822
C,3.2667527308,-1.6020229848,-0.9979788152
C,4.0938265838,-2.3185163362,-1.8665434961
C,5.1666466702,-3.4369145315,-0.0285835679
H,4.4222379027,-2.8789591173,1.9241118496
H,3.9718249858,-2.1344058273,-2.930132129
H,5.8963015028,-4.1404425917,0.359961947
H,5.6640851482,-3.7684411225,-2.1031210418
C,1.8679813524,2.2660760576,1.3080073417
C,1.7511186695,4.9179236657,0.378399573
C,1.6791525914,3.3333507999,2.1884860347
C,1.9992962578,2.5368880135,-0.0764348526
C,1.9329869922,3.861759607,-0.5133323807
C,1.6214897586,4.6508447927,1.7379210789
H,1.5865134287,3.0988872927,3.2452575286
H,2.0391810405,4.0419291616,-1.5798047546
H,1.4764020083,5.4580562884,2.4489549512
H,1.7095961974,5.9369777398,0.0071072652
C,-1.9998269055,-0.3844893994,2.3621909521
C,-4.7318882836,-0.8307493569,2.6639891101
C,-2.4670088525,-1.1231107245,3.4516931628
C,-2.9016625887,0.1648342654,1.4458235344
C,-4.2669261511,-0.0635360841,1.5974449209
C,-3.8325745043,-1.3533669697,3.5926040719
H,-1.762170002,-1.5319094061,4.1695518428
H,-2.5346312522,0.7736011872,0.6230831342
H,-4.9641243096,0.3592156014,0.8808271701

H,-4.1945297889,-1.9425258448,4.4290653709
H,-5.7956684539,-1.0136222482,2.7775386822
C,-1.8403606536,1.5408397902,-2.021862349
C,-4.4841257807,2.3678972993,-2.413246292
C,-2.21034294,2.8792742829,-1.8101165503
C,-2.8070718476,0.6279443412,-2.4718743153
C,-4.1187372688,1.0465421438,-2.6674829033
C,-3.5268862375,3.2866274858,-1.986909806
H,-1.4562758365,3.5920865893,-1.4863845053
H,-2.5426468146,-0.3966148897,-2.7037340423
H,-4.8575880201,0.3367753435,-3.0245614032
H,-3.8027823726,4.3193864063,-1.8016853838
H,-5.5118707364,2.6836229805,-2.5621637418

IB-*E,E*[1,1]^{benzene} (Intermediate dicoordinate 1,1-B_2cat_2-*E,E*-diimine **1** complex in benzene)
boat_cydiimph2_EE_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1372708

Zero-point correction= 0.572215 (Hartree/Particle)
Thermal correction to Energy= 0.603828
Thermal correction to Enthalpy= 0.604772
Thermal correction to Gibbs Free Energy= 0.509608
Sum of electronic and ZPE= -1696.565056
Sum of electronic and thermal Energies= -1696.533443
Sum of electronic and thermal Enthalpies= -1696.532498
Sum of electronic and thermal Free Energies= -1696.627663

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.908	129.808	200.290

H,3.1669486304,2.7616489388,1.3260843874
C,2.3525236294,3.0673110673,0.6606400033
C,0.8148184216,4.9695817426,0.0161851653
C,-0.0405987352,2.6258842634,0.0274665027
C,-0.3968593175,4.0829220648,0.3207146309
C,1.1211987787,2.2014602067,0.9469817133
C,2.0236248862,4.5492747625,0.8551782764
H,1.0614459172,4.8881656864,-1.0495139567
H,0.3056220609,2.5627808717,-1.0080202855
H,-0.6699503157,4.2158373749,1.3755472281
H,0.7910505217,2.3769464888,1.9814649712
H,1.8084871321,4.7384971935,1.9154602775

H,2.6748717615,2.8721690391,-0.367123524
H,0.5638422936,6.0166635068,0.2089223459
H,-1.2608433851,4.3753356181,-0.2851286407
H,2.8961965051,5.1556466028,0.5955750988
N,-1.1505857656,1.6552444893,0.1084509208
N,1.4179194275,0.7585094326,0.8154753317
C,-2.1310382269,1.8720933087,0.9009955098
H,-2.0923896114,2.7368953435,1.5678977987
C,1.9538235819,0.1956820414,1.8330728782
H,2.2156452035,0.8432071539,2.6783741412
B,-0.7574063103,0.1652187306,-0.6896633063
B,0.9738634669,0.135082778,-0.7309435825
O,1.7400609635,1.0241620296,-1.6398521962
O,1.6006337194,-1.1725830449,-0.8619429575
O,-1.482271035,0.0950896498,-1.9643617579
O,-1.326818082,-0.9024197997,0.1568900776
C,2.814040591,-0.9546589862,-1.4229223739
C,5.1065607382,-0.0664587801,-2.677124312
C,3.8680535776,-1.8365490077,-1.5552024465
C,2.8967856995,0.3628092324,-1.8991788272
C,4.0319906518,0.8276838309,-2.5330965825
C,5.0268669942,-1.3684246226,-2.1966104599
H,3.7912789826,-2.8486984256,-1.1719347962
H,4.0827800745,1.8450063937,-2.9075084672
H,5.8730360109,-2.0375075372,-2.3169772768
H,6.0129259944,0.2695179333,-3.1708622492
C,-2.2692740272,-1.5280576904,-0.5888528249
C,-4.1090788194,-2.4442063889,-2.4297058447
C,-3.087912134,-2.5764880293,-0.2247911464
C,-2.3576082261,-0.9322987348,-1.8574895712
C,-3.2728741168,-1.3737513941,-2.7925099074
C,-4.0199757228,-3.0317889783,-1.1732801396
H,-3.0187209099,-3.0147946246,0.7652583176
H,-3.3370023878,-0.9040160919,-3.768295536
H,-4.6766413886,-3.8575982412,-0.9180795543
H,-4.8328783053,-2.8174010812,-3.147591198
C,-3.3640287866,1.0702462946,0.9488828418
C,-5.766191585,-0.3295444523,1.045293293
C,-3.852839235,0.6082150255,2.1750813753
C,-4.0958702548,0.8576047517,-0.2224792306
C,-5.3023536668,0.1656213173,-0.1691309398
C,-5.0398851958,-0.1116294543,2.2168423012
H,-3.291482164,0.793004337,3.0865844561
H,-3.7159629329,1.2410211078,-1.1640096995
H,-5.8634181238,-0.0045779498,-1.0818124896
H,-5.4057285752,-0.495195858,3.1636131036

H,-6.698144845,-0.8845163141,1.08294244
C,2.2532706616,-1.2292527527,2.0345507307
C,2.8724101764,-3.8855003414,2.5853367453
C,1.364767629,-2.2422321321,1.6546046552
C,3.4281763458,-1.5489805291,2.7248265758
C,3.7487219319,-2.8769241374,2.9799618433
C,1.6795631238,-3.5657655141,1.9378661933
H,0.4372875722,-1.984595888,1.1532953147
H,4.0983467628,-0.7549295812,3.0436731322
H,4.672062821,-3.1230593446,3.4936428902
H,0.9905686533,-4.3520289595,1.6475768814
H,3.1133762943,-4.9232269422,2.7941787315

IB-*E,Z*[1,1]^{benzene} (Intermediate dicoordinate 1,1-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
boat_cydiimph2_EZ_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1350779

Zero-point correction= 0.572155 (Hartree/Particle)
Thermal correction to Energy= 0.604031
Thermal correction to Enthalpy= 0.604976
Thermal correction to Gibbs Free Energy= 0.507754
Sum of electronic and ZPE= -1696.562923
Sum of electronic and thermal Energies= -1696.531046
Sum of electronic and thermal Enthalpies= -1696.530102
Sum of electronic and thermal Free Energies= -1696.627324

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.035	129.791	204.621

H,1.1829000809,-3.3723162139,1.456230347
C,0.4408379742,-2.6822193436,1.8723649421
C,-1.7805709854,-2.5131632424,3.0864685965
C,-1.2245501981,-0.8861021939,1.3031028563
C,-2.3638382977,-1.688182343,1.9317444636
C,-0.1596682091,-1.8485431187,0.7388760266
C,-0.6728582616,-3.4497110178,2.5931857362
H,-1.3748435559,-1.836578323,3.8488888494
H,-0.7555575987,-0.3056789891,2.1053648678
H,-2.8258282852,-2.3638651033,1.2055114178
H,-0.6766459301,-2.5263362943,0.0448355361
H,-1.1083786076,-4.1889886176,1.9074808518
H,0.9591680788,-2.0120118128,2.5635727833
H,-2.5780897063,-3.091394297,3.5621799937

H,-3.1396412651,-1.0041726363,2.2902507474
H,-0.2474419354,-4.0077453382,3.4324405535
N,-1.52309353,0.1239172147,0.2751793165
N,0.8415228798,-1.0883668421,-0.0395874363
C,-2.4278901364,0.0797683182,-0.6199526053
H,-2.4430657066,0.9362236992,-1.2966423857
C,1.344956729,-1.6771031805,-1.0576708099
H,1.0915833409,-2.733745309,-1.2076314259
B,-0.3503640277,1.3720815,0.3306592077
B,1.1420792025,0.5382392816,0.6081709094
O,1.4917113834,0.2089984862,2.0036763279
O,2.3756735121,0.9927388171,-0.0047857087
O,-0.8276577735,2.2567819614,1.4061505838
O,-0.5299276636,2.118826472,-0.9224129923
C,3.3756881396,0.5727585613,0.8089476278
C,5.0483262057,-0.3592539302,2.7944369858
C,4.7347505124,0.5722313815,0.5672493384
C,2.8454201166,0.1075007926,2.0214567053
C,3.6634685482,-0.3600242919,3.0310657727
C,5.5718421682,0.0945170228,1.5889374354
H,5.1273431849,0.9278996169,-0.3795751368
H,3.2456584346,-0.7070947887,3.9704753946
H,6.6456672875,0.0807185447,1.4314740326
H,5.717969184,-0.7209278585,3.5682910489
C,-1.2795627305,3.2086835043,-0.6020333927
C,-2.7491848618,5.2667120236,0.4989493171
C,-1.8197795911,4.1520622566,-1.4525004747
C,-1.4640566713,3.2785478286,0.7886658392
C,-2.1977200631,4.3019369366,1.3580458436
C,-2.5651388794,5.1945931053,-0.8765499009
H,-1.6638830392,4.0858602882,-2.5241865584
H,-2.3319066975,4.3521379612,2.4332225866
H,-3.000188275,5.9535458436,-1.518849468
H,-3.3272725057,6.0825398348,0.9212770218
C,-3.4106356446,-1.00754464,-0.85528742
C,-5.2425235756,-3.0559134037,-1.3047008549
C,-4.7343027143,-0.8616580746,-0.4357335951
C,-3.0131187209,-2.1631482399,-1.5317969675
C,-3.9302710707,-3.1868904764,-1.7525574043
C,-5.6438762416,-1.8919961754,-0.6522677485
H,-5.0417008143,0.0463634196,0.0742669915
H,-1.9910642773,-2.2540206781,-1.8892467993
H,-3.6198339474,-4.0852612234,-2.2760814398
H,-6.6683394799,-1.7847315392,-0.3113107791
H,-5.9550915258,-3.8567734442,-1.472722458
C,2.196258476,-1.0860827778,-2.0994340477

C,3.7622432978,-0.1036883971,-4.1789278135
C,1.9650825557,0.2028953447,-2.5955409486
C,3.1865282891,-1.8902559355,-2.6737327855
C,3.9836857367,-1.3919565175,-3.6974762804
C,2.7473786237,0.6845831283,-3.6371862565
H,1.1766613421,0.8172311345,-2.1709101342
H,3.3412272911,-2.9000660639,-2.302926839
H,4.7667608119,-2.0092492785,-4.1248547891
H,2.5674288774,1.6819608267,-4.0240545166
H,4.3746947357,0.2842138441,-4.986900682

IB-*Z*,*E*[1,1]^{benzene} (Intermediate dicoordinate 1,1-B_2cat_2-*Z*,*E*-diimine **1** complex in benzene)
boat_cydiimph2_ZE_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1391098

Zero-point correction= 0.572705 (Hartree/Particle)
Thermal correction to Energy= 0.604232
Thermal correction to Enthalpy= 0.605176
Thermal correction to Gibbs Free Energy= 0.509874
Sum of electronic and ZPE= -1696.566405
Sum of electronic and thermal Energies= -1696.534878
Sum of electronic and thermal Enthalpies= -1696.533934
Sum of electronic and thermal Free Energies= -1696.629235

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.161	129.441	200.579

H,-2.9092119804,1.5572842941,-2.0595732779
C,-2.6569543735,1.8200780752,-1.0268838449
C,-2.3074047995,3.7287592371,0.5950220681
C,-0.8288933689,1.7218531776,0.7053472685
C,-0.8767138558,3.2423224542,0.8478097154
C,-1.2297259839,1.3412062153,-0.7339714064
C,-2.7785381914,3.3284816686,-0.80457561
H,-2.9754776389,3.2921635337,1.3475235596
H,-1.5656698807,1.2904062768,1.3893022419
H,-0.2127412497,3.7264533429,0.1198577567
H,-0.5310765252,1.8384111093,-1.4175995872
H,-2.1722408037,3.8547738798,-1.5536001517
H,-3.3391767685,1.272397844,-0.3666105021
H,-2.3538184364,4.8149527538,0.715624641
H,-0.5348974779,3.5258654605,1.8487119415

H,-3.8158039696,3.6386841624,-0.9606816378
N,0.4463761876,1.068023687,1.0628495253
N,-1.1526059334,-0.1126493477,-0.9285221175
C,1.5433876352,1.716975763,0.9461185183
H,1.5178390406,2.7264870256,0.5293526256
C,-0.854035016,-0.6450147822,-2.0505016811
H,-0.8840359905,-1.7353085673,-2.063360836
B,0.2659978956,-0.6590461498,1.2284097469
B,-1.2514634404,-1.0314845605,0.4674054474
O,-2.5433408749,-0.6693998433,1.0951723392
O,-1.4051410019,-2.4205680455,0.0161935426
O,0.4413690085,-1.05878729,2.6274063511
O,1.4160573743,-1.2200742255,0.495774283
C,-2.7324840121,-2.6929379838,0.0937837337
C,-5.463136732,-2.8348698252,0.4868993508
C,-3.4008630157,-3.8161179131,-0.3517899179
C,-3.4126795939,-1.6456965652,0.7351592936
C,-4.7774609834,-1.6957379466,0.9406221298
C,-4.7891793309,-3.8729114649,-0.1450700979
H,-2.8626921895,-4.6228128958,-0.8381699458
H,-5.2917829481,-0.8825469242,1.4421186172
H,-5.3405038847,-4.7440235355,-0.48455463
H,-6.536117266,-2.9022996611,0.6361241083
C,2.1414815941,-1.9201885211,1.3976194576
C,3.316759638,-3.1601709083,3.5677659609
C,3.3165185664,-2.6145787702,1.1956019084
C,1.5533090888,-1.8324607466,2.6704460651
C,2.1226011435,-2.4453095259,3.7685924981
C,3.9022901695,-3.2398867298,2.309939078
H,3.7694408055,-2.6600830578,0.2109963473
H,1.6599187004,-2.3684350553,4.7469010043
H,4.8245759026,-3.7976793078,2.1808187689
H,3.7839917983,-3.6589699932,4.4112224222
C,2.8665948124,1.2270679239,1.3583590133
C,5.4030012486,0.396850736,2.1438898482
C,3.9503402585,1.3689152029,0.4842657625
C,3.0640331325,0.7051709814,2.6391155992
C,4.3360554396,0.2985646086,3.0312341476
C,5.2105749048,0.9309383864,0.8691531895
H,3.7979577619,1.8018595863,-0.5008595861
H,2.2205162287,0.6257116924,3.3168976695
H,4.4839729889,-0.1157393232,4.0227515242
H,6.0456244717,1.0137149233,0.1812873165
H,6.3902758421,0.0622716529,2.445947031
C,-0.4571653513,0.0805446966,-3.2812144605
C,0.3212182652,1.3888123867,-5.6149013557

C,0.7835598867,0.7230357375,-3.3429877018
C,-1.2974497677,0.0766763175,-4.3969048994
C,-0.9097534888,0.7401499533,-5.5576540246
C,1.1697874994,1.3741176151,-4.5098047554
H,1.4452347047,0.687246522,-2.4816699644
H,-2.2519463477,-0.4396362571,-4.3518476484
H,-1.5684161464,0.7442345784,-6.4198802189
H,2.1363051562,1.865061385,-4.5585363231
H,0.6236314683,1.8989008969,-6.5236672552

IB-*Z*,*Z*[1,1]^{benzene} (Intermediate dicoordinate 1,1-B_2cat_2-*Z*,*Z*-diimine **1** complex in benzene)
cfc_boat_cydiimph2_ZZ_b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1408086

Zero-point correction= 0.573038 (Hartree/Particle)
Thermal correction to Energy= 0.604620
Thermal correction to Enthalpy= 0.605564
Thermal correction to Gibbs Free Energy= 0.508721
Sum of electronic and ZPE= -1696.567771
Sum of electronic and thermal Energies= -1696.536188
Sum of electronic and thermal Enthalpies= -1696.535244
Sum of electronic and thermal Free Energies= -1696.632087

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.405	129.188	203.824

H,0.0862549861,3.0039678612,1.9437282432
C,0.0976351272,1.9507323823,2.2430930392
C,1.1518107642,0.2312461897,3.7795254356
C,0.4365700738,-0.4082758861,1.4946189367
C,1.4950069828,-0.6480221058,2.5701026657
C,0.4804736864,1.0682741309,1.0503285077
C,1.0842628382,1.7121261191,3.3905043899
H,0.1839781076,-0.0803194667,4.1915596228
H,-0.5442516399,-0.5926739438,1.9492016315
H,2.4941935448,-0.3884101088,2.2068836127
H,1.5126844864,1.2835185598,0.7503769498
H,2.0843777778,2.0495918246,3.0845112949
H,-0.9227066896,1.6926680208,2.5444003864
H,1.8981574017,0.0820746019,4.5652175596
H,1.5050484798,-1.7074214066,2.8454469588
H,0.7953545038,2.3171740454,4.2548439272
N,0.4226917692,-1.2553751075,0.2947685167

N,-0.4020235041,1.2589511188,-0.1036179503
C,1.4222640765,-1.7057128379,-0.3541458118
H,1.1615524686,-2.2937408847,-1.2365292096
C,-0.07622473,1.9477066926,-1.1323237276
H,-0.8126180382,1.9175240902,-1.9368176413
B,-1.1815182528,-1.3848490074,-0.2628501762
B,-1.7967141977,0.2435933871,-0.1587345257
O,-2.5177055763,0.5891907688,1.0814751913
O,-2.5969154163,0.7859785006,-1.2569134699
O,-1.7970984441,-2.3515452892,0.6653163671
O,-1.0848894798,-2.0662889686,-1.5573846329
C,-3.4777156541,1.6450864634,-0.6776985986
C,-5.1197034503,3.1934468577,0.9121592231
C,-4.3443402193,2.5248429848,-1.2948049662
C,-3.4257908545,1.528315229,0.7204394086
C,-4.2383359123,2.2941089635,1.5339021799
C,-5.1720804416,3.3065526695,-0.4721812218
H,-4.3803271143,2.599571973,-2.3765385129
H,-4.1949257322,2.1915354945,2.6131848666
H,-5.8635636358,4.0075816566,-0.9286247126
H,-5.770765981,3.8074713777,1.5263299893
C,-1.3449616099,-3.3764837033,-1.3044297087
C,-1.984588695,-5.8872583821,-0.3534094734
C,-1.2445768342,-4.4480370959,-2.1692533118
C,-1.7605009202,-3.5435877726,0.0270871368
C,-2.0850583355,-4.7926116613,0.5211824076
C,-1.5732781929,-5.7197606095,-1.6702355868
H,-0.9280024924,-4.3024894502,-3.1968088569
H,-2.409814046,-4.9117099461,1.5493202698
H,-1.5053688781,-6.5812386015,-2.3269392683
H,-2.2349305209,-6.8792956608,0.009164372
C,2.8601665648,-1.474367995,-0.0642122874
C,5.5547787017,-1.0169103903,0.4739294653
C,3.6293432228,-2.4730730038,0.5367404333
C,3.4496924219,-0.2609588679,-0.4294805776
C,4.7953950719,-0.0335577753,-0.1552962857
C,4.9724039583,-2.2367219214,0.8132129259
H,3.1711603684,-3.4207391625,0.8034578135
H,2.8585694038,0.5002552989,-0.9324610388
H,5.2460556706,0.9127683513,-0.4370246439
H,5.565407067,-3.0074692303,1.2945585844
H,6.6027233311,-0.8375849275,0.6912799905
C,1.1691445342,2.6827268424,-1.4184112588
C,3.5545573074,3.9288356535,-2.1765842384
C,1.5881928576,2.6660914401,-2.7566449613
C,1.9409194305,3.368716974,-0.4696225584

C,3.1246534804,3.9894438216,-0.8520883791
C,2.7828625153,3.2695424384,-3.1306283049
H,0.9762798524,2.1606963498,-3.4985862144
H,1.6068885994,3.4452767009,0.5588666415
H,3.7104451654,4.5270197194,-0.1139159021
H,3.1052934072,3.2343339161,-4.1657377209
H,4.4825054823,4.4104577005,-2.4676442097

IB-*E*,*E*[1,2]^{benzene} (Intermediate dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in benzene)
boat_cydiimph2_EE_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1513138

Zero-point correction= 0.572968 (Hartree/Particle)
Thermal correction to Energy= 0.604065
Thermal correction to Enthalpy= 0.605010
Thermal correction to Gibbs Free Energy= 0.510628
Sum of electronic and ZPE= -1696.578346
Sum of electronic and thermal Energies= -1696.547248
Sum of electronic and thermal Enthalpies= -1696.546304
Sum of electronic and thermal Free Energies= -1696.640686

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.057	129.061	198.644

H,-2.5299161258,2.107469694,-2.383557495
C,-2.2977270024,2.3525872288,-1.3419587449
C,-1.9395545038,4.2408013836,0.3024855015
C,-0.572172241,2.1581834567,0.4542944286
C,-0.5525496882,3.6774609356,0.6198373286
C,-0.912292007,1.7909241937,-0.9922109879
C,-2.3609212743,3.8645498326,-1.1185671757
H,-2.6645502035,3.8377073933,1.02018795
H,-1.3655333357,1.7614324235,1.0980762371
H,0.1784566999,4.1349172576,-0.0591712669
H,-0.1528324945,2.2451727471,-1.6473656434
H,-1.6949922849,4.363043434,-1.8357020335
H,-3.0329431242,1.8333982405,-0.7146990988
H,-1.9362921835,5.327740724,0.4245248322
H,-0.2513797838,3.9198215247,1.643633711
H,-3.3738167308,4.2219729324,-1.3254089987
N,0.6438962584,1.4595012564,0.900280771
N,-0.9091602232,0.3303291791,-1.2252444661

C,1.8001246103,1.9833390051,0.705240069
H,1.8613512478,2.8998038836,0.114289547
C,-0.7786593922,-0.0215539207,-2.4574336353
H,-0.4681206112,0.7534329807,-3.1660030425
B,0.2149004013,-0.0707942629,1.316258995
B,-0.9145982489,-0.6498319405,0.1149355771
O,-2.3030250082,-0.6081073486,0.5522672838
O,-0.3994966947,0.0869277837,2.6305844612
O,-0.5419769012,-1.9951011677,-0.2910175426
O,1.398456195,-0.8949079505,1.4143789881
C,-1.6437307384,-0.378053812,2.8876663538
C,-4.227203122,-1.2359775262,3.5858555582
C,-2.033116259,-0.484615228,4.2236215491
C,-2.5753178773,-0.716654211,1.8791603201
C,-3.8508549067,-1.1406739938,2.2492335316
C,-3.3104543508,-0.9072491537,4.5793396565
H,-1.2963405198,-0.2208131175,4.9760957971
H,-4.5408260272,-1.3928667568,1.4495937062
H,-3.5819494344,-0.9792246169,5.6277236913
H,-5.2272546484,-1.569644969,3.8434755571
C,1.7527112153,-1.673259995,0.368846708
C,2.5292001033,-3.4165865118,-1.6774299836
C,3.099812002,-1.959125533,0.1554329708
C,0.7771637988,-2.251588084,-0.4718874664
C,1.1796280883,-3.1242563817,-1.4811349495
C,3.49078183,-2.8267931008,-0.8635671357
H,3.8264413077,-1.4955217043,0.8177428462
H,0.4090346197,-3.5734756901,-2.101683236
H,4.5442021918,-3.0438416209,-1.0108432762
H,2.8210266006,-4.1025009025,-2.4665423915
C,3.0667323135,1.4903886999,1.248945684
C,5.5264604914,0.6712767182,2.2637552599
C,3.1342702727,0.878907374,2.5076770762
C,4.2398747521,1.7183438071,0.5200809929
C,5.4651280153,1.2913054427,1.0166111919
C,4.3651561877,0.4777339319,3.0114287924
H,2.2248330405,0.7310459622,3.0801182998
H,4.1846450601,2.2141524427,-0.4453214574
H,6.3699744829,1.4493820542,0.4394456004
H,4.4184027465,0.0075919233,3.9875751255
H,6.4840787602,0.3484935681,2.6601833003
C,-1.0809335504,-1.3216957134,-3.0468890363
C,-1.6698461393,-3.7344159269,-4.2996457503
C,-0.4143960909,-1.6837577834,-4.2246273442
C,-2.0759286286,-2.1560697594,-2.5191096979
C,-2.3666634265,-3.3582821463,-3.1514739365

C,-0.6941225745,-2.8967464637,-4.8396359713
H,0.3399150632,-1.0205908882,-4.6396254835
H,-2.610626615,-1.8522333302,-1.625324738
H,-3.1359024553,-4.0064648795,-2.74560212
H,-0.160920995,-3.1867788721,-5.7386791221
H,-1.8977599539,-4.6790841223,-4.783522003

IB-*E*,*Z*[1,2]^{benzene} (Intermediate dicoordinate 1,2-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
boat_cydiimph2_EZ_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1466478

Zero-point correction= 0.573229 (Hartree/Particle)
Thermal correction to Energy= 0.604404
Thermal correction to Enthalpy= 0.605348
Thermal correction to Gibbs Free Energy= 0.510165
Sum of electronic and ZPE= -1696.573418
Sum of electronic and thermal Energies= -1696.542244
Sum of electronic and thermal Enthalpies= -1696.541300
Sum of electronic and thermal Free Energies= -1696.636482

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.269	128.991	200.328

H,-2.0590984552,1.5803404459,-2.3040067483
C,-1.9135868259,1.8486255388,-1.252237168
C,-1.6493814243,3.7830730556,0.3674207523
C,-0.3512161352,1.696107006,0.6852893982
C,-0.2941639914,3.2189945488,0.8068023845
C,-0.5670091277,1.2867293583,-0.7772445934
C,-1.9678060012,3.3680164797,-1.0709396745
H,-2.4332902021,3.4121538367,1.0394552013
H,-1.2320923551,1.3659891176,1.2480980475
H,0.4956932353,3.63962146,0.1764290383
H,0.2412590136,1.728121268,-1.3777200653
H,-1.240474428,3.8361550977,-1.7475921405
H,-2.7054266283,1.3542720858,-0.6766200132
H,-1.6409849526,4.8734506424,0.4530968138
H,-0.072078467,3.4900592376,1.8437364302
H,-2.955868076,3.7343763226,-1.3644291119
N,0.7376565714,0.9015863819,1.2659897192
N,-0.5434589687,-0.1795969423,-0.9796460076
C,1.9794300636,1.1895352448,1.3221299389
H,2.5916940838,0.4295451713,1.8110499326

C,-0.1948570496,-0.5609681564,-2.1583848337
H,0.2466427143,0.1938429443,-2.8183127162
B,0.1370327415,-0.5574616491,1.6942484413
B,-0.8169360389,-1.1372681195,0.3692504784
O,-2.2532954378,-1.0123918031,0.5620969021
O,-0.6531796633,-0.2818328638,2.8871554625
O,-0.4522243065,-2.504531345,0.0523442561
O,1.2795779831,-1.388440913,2.032598201
C,-1.9730048536,-0.5705100397,2.9462080154
C,-4.7265585439,-1.0577489477,3.2382784414
C,-2.5973746123,-0.4744594557,4.1914797901
C,-2.7539690459,-0.9248969849,1.821234251
C,-4.1180886513,-1.1611637054,1.9911418448
C,-3.9591339799,-0.7134715251,4.3466908584
H,-1.9720481771,-0.2042088284,5.036806904
H,-4.6870386769,-1.4315574325,1.1066694695
H,-4.4124285629,-0.6314639419,5.3294201993
H,-5.7900398398,-1.2495039273,3.3384117663
C,1.7077197726,-2.3077312825,1.1364135667
C,2.6670892636,-4.2840322879,-0.6072032447
C,3.0285502775,-2.7486808834,1.2106639115
C,0.8496638952,-2.8669582752,0.1616319072
C,1.3464799252,-3.8481682635,-0.6956204902
C,3.5122518931,-3.7304356648,0.3484656169
H,3.6609571263,-2.3134246377,1.9791816226
H,0.6629944121,-4.2661748068,-1.4296504799
H,4.5428890783,-4.0605748986,0.4319698185
H,3.0267072543,-5.0531592093,-1.2833421485
C,2.6474317563,2.3961108255,0.7769256204
C,3.9117789321,4.6563151963,-0.2510294603
C,2.8971920146,2.4946679577,-0.5944397619
C,3.0646842909,3.4141439908,1.6373641643
C,3.6854365595,4.5462894462,1.1193809335
C,3.5263708573,3.6263992347,-1.1055355944
H,2.6098826036,1.6798610206,-1.2532596684
H,2.8843195384,3.3256860095,2.7045058534
H,3.9942092955,5.3432252138,1.7878490402
H,3.7192100722,3.7010218556,-2.1707707314
H,4.3983691839,5.5397377512,-0.6512547838
C,-0.4016430464,-1.8763285817,-2.7598447001
C,-0.8037637952,-4.3094152588,-4.0470228423
C,0.4874547479,-2.3002098077,-3.7554216335
C,-1.5168694069,-2.6604944204,-2.4353822153
C,-1.7145936454,-3.8721753671,-3.085438987
C,0.2986540688,-3.5243402591,-4.3834593656
H,1.3377642894,-1.676370753,-4.0175897432

H,-2.2162570938,-2.3102444573,-1.6834493278
H,-2.5782543144,-4.4800374014,-2.837918258
H,1.0009701273,-3.8625685398,-5.1377928478
H,-0.9605228917,-5.2610521091,-4.5453255971

IB-*Z*,*E*[1,2]^{benzene} (Intermediate dicoordinate 1,2-B_2cat_2-*Z*,*E*-diimine **1** complex in benzene)
boat_cydiimph2_ZE_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1510071

Zero-point correction= 0.573341 (Hartree/Particle)
Thermal correction to Energy= 0.604663
Thermal correction to Enthalpy= 0.605607
Thermal correction to Gibbs Free Energy= 0.508941
Sum of electronic and ZPE= -1696.577666
Sum of electronic and thermal Energies= -1696.546344
Sum of electronic and thermal Enthalpies= -1696.545400
Sum of electronic and thermal Free Energies= -1696.642066

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.432	128.980	203.452

H,-2.6400122365,1.8187779876,-2.0236935469
C,-2.2904385562,2.0294950626,-1.0077619136
C,-1.5286275479,3.8508265337,0.5766643828
C,-0.4391778814,1.6110874605,0.6338582544
C,-0.2000380296,3.1131302223,0.7744228019
C,-0.953205001,1.3126880669,-0.7831189909
C,-2.1320669816,3.5360211299,-0.793715702
H,-2.2276373975,3.5451783327,1.3649426662
H,-1.224690015,1.3364156971,1.3460562004
H,0.5164314789,3.4679333816,0.0223203267
H,-0.2143511688,1.6983190939,-1.4936441725
H,-1.480617295,3.9435593001,-1.5781670908
H,-3.0206688115,1.6051252604,-0.3089464896
H,-1.3726053248,4.9280006859,0.6852678801
H,0.2222490884,3.3224328995,1.7624557362
H,-3.1042076183,4.0255026784,-0.9023044013
N,0.6914122398,0.7282999629,0.9794309752
N,-1.1200567504,-0.1344493863,-1.000833966
C,1.8979158052,1.1454621957,0.8528623947
H,2.0624589667,2.1196302792,0.3867875181
C,-1.0863686151,-0.6446626305,-2.1738490939

H,-1.3136229496,-1.7093561041,-2.2223939676
B,0.0883892823,-0.7846876207,1.3528161594
B,-1.2719703928,-1.0719039084,0.3387517902
O,-2.5453923849,-0.6647874333,0.913059901
O,-0.2751572356,-0.6753996059,2.7635583788
O,-1.3351926221,-2.4490306077,-0.1268980857
O,1.1543842517,-1.7451424245,1.174480713
C,-1.5678963202,-0.5894560175,3.1544024052
C,-4.1878660658,-0.3540614165,4.1495219105
C,-1.8166730517,-0.4791972877,4.5243719644
C,-2.6680794707,-0.5885012554,2.2623049249
C,-3.9574352352,-0.4660538675,2.7821407855
C,-3.1081781834,-0.3638209381,5.0274580629
H,-0.953962987,-0.4876142135,5.1835452198
H,-4.7776796513,-0.4690310751,2.0705865634
H,-3.2645419362,-0.2819739302,6.0983387986
H,-5.2036102081,-0.2649101141,4.5210870911
C,1.0492469896,-2.7432312785,0.2707998384
C,0.9734257181,-4.9120087375,-1.5121930437
C,2.2025037699,-3.4695402336,-0.0295029155
C,-0.1688512061,-3.1066407537,-0.3483725993
C,-0.1822041697,-4.1882906899,-1.2298579328
C,2.1739466987,-4.5457592332,-0.9119228075
H,3.1215748917,-3.164339386,0.4625602754
H,-1.1358549789,-4.4521923355,-1.678560051
H,3.0861468048,-5.0951091842,-1.1219840142
H,0.9307812098,-5.7524111492,-2.1974817063
C,3.1063127362,0.4649698541,1.3223767374
C,5.4798791915,-0.6868176775,2.209298497
C,4.3068638248,0.7174995239,0.6479372321
C,3.1048085122,-0.3392361463,2.4699384313
C,4.293859418,-0.9068392721,2.9093378359
C,5.4883284576,0.1264181659,1.0775525242
H,4.3071793068,1.367709621,-0.2231198368
H,2.1787477342,-0.502612904,3.011240112
H,4.2953368889,-1.5256121705,3.8003419212
H,6.4133942623,0.3073070216,0.5405667903
H,6.4035506153,-1.1398352836,2.5556760634
C,-0.7737342981,0.0657813832,-3.4355372346
C,-0.1978178795,1.3237314454,-5.8554879369
C,0.4941628946,0.6145758378,-3.6557031785
C,-1.7422802854,0.1259896423,-4.44127719
C,-1.4564921511,0.7667898485,-5.6429247022
C,0.7786980734,1.2391755328,-4.865302283
H,1.2583184664,0.5263380495,-2.8880306615
H,-2.7180732167,-0.3218866551,-4.2760888917

H,-2.2153553426,0.8229377063,-6.4163228255
H,1.7662561215,1.6546647533,-5.0372052507
H,0.026127694,1.814628281,-6.7969175214

IB-*Z,Z*[1,2]^{benzene} (Intermediate dicoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in benzene)
boat_cydiimph2_ZZ_1-2-b2cat2_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.150696

Zero-point correction= 0.573982 (Hartree/Particle)
Thermal correction to Energy= 0.605063
Thermal correction to Enthalpy= 0.606007
Thermal correction to Gibbs Free Energy= 0.511117
Sum of electronic and ZPE= -1696.576714
Sum of electronic and thermal Energies= -1696.545633
Sum of electronic and thermal Enthalpies= -1696.544689
Sum of electronic and thermal Free Energies= -1696.639579

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	379.683	128.684	199.714

H,-0.8243832973,-1.5831768375,-3.0736109073
C,-0.5134760477,-2.0369319669,-2.127084203
C,-1.0087633176,-3.8624753064,-0.4323427266
C,-0.1189806907,-1.6773384821,0.3034429816
C,-1.0667772686,-2.813193867,0.6861338132
C,-0.6171156684,-1.0107306823,-0.9932654684
C,-1.3797448098,-3.2550503447,-1.7897976269
H,0.0062453152,-4.2757610619,-0.4851364687
H,0.8497492448,-2.1391089517,0.0867300873
H,-2.0944578779,-2.4539153266,0.7992932427
H,-1.6683651434,-0.7434045979,-0.8371966594
H,-2.4356012717,-2.9505967618,-1.77024104
H,0.5391920613,-2.3183999503,-2.2404912307
H,-1.6818968706,-4.69138984,-0.1952455222
H,-0.7558032031,-3.2443851921,1.6428983172
H,-1.2802204989,-4.0059954045,-2.578879821
N,0.2119174109,-0.6445858171,1.2960397675
N,0.1397987471,0.2157240397,-1.2735448363
C,-0.5693606436,-0.1153141944,2.1550698836
H,-0.0981107436,0.6407952561,2.7859692426
C,-0.4230066019,1.2836174721,-1.7092148796
H,0.2528310325,2.128132807,-1.8291917364
B,1.7186126366,-0.064929192,0.9579420995

B,1.7173522796,0.2598830804,-0.7364995148
O,2.3827887712,-0.7454893535,-1.5427424747
O,2.6276429126,-1.1300492811,1.3505248081
O,2.2121006465,1.5935967955,-1.0437686227
O,1.9090770471,1.0987163,1.8043419857
C,3.3576398936,-1.8062787319,0.434124543
C,4.9102396026,-3.3574292924,-1.3243791238
C,4.2576450789,-2.7616538904,0.9113403229
C,3.239736928,-1.6236693402,-0.964886413
C,4.0196818309,-2.4083333241,-1.8159298503
C,5.0317599243,-3.5330038846,0.0506662954
H,4.3281126159,-2.8760914958,1.9886716334
H,3.9057258601,-2.2407778623,-2.8827487453
H,5.7232711936,-4.2644449472,0.4565401786
H,5.5049815011,-3.9483887865,-2.0134631479
C,1.8597546723,2.334350465,1.2559678437
C,1.809627538,4.9699142675,0.2777810933
C,1.6714929134,3.4205740404,2.1119382558
C,2.0254287533,2.577881355,-0.128973767
C,1.9945206805,3.8956704206,-0.5896658052
C,1.6449932137,4.7292847884,1.637681228
H,1.5601526904,3.2047940014,3.1705763588
H,2.1389970189,4.0515423255,-1.6552957848
H,1.5022054077,5.5514996597,2.3314788335
H,1.7999867847,5.9830474901,-0.1110386827
C,-2.0160464006,-0.3924155473,2.3302745974
C,-4.7360131466,-0.9134850096,2.6354035212
C,-2.4626974287,-1.1552375853,3.4114785101
C,-2.936313968,0.1415963469,1.4234632204
C,-4.2942416538,-0.1238941154,1.576461666
C,-3.8206238202,-1.4223346281,3.5546694947
H,-1.745927299,-1.5540020473,4.1231232189
H,-2.592079231,0.7720797986,0.6071489722
H,-5.0036632664,0.2905656109,0.8674405887
H,-4.1642959593,-2.0290299396,4.3860999704
H,-5.794314354,-1.1237907591,2.7507258774
C,-1.8445695998,1.571623305,-1.9671014602
C,-4.5130762023,2.3477466777,-2.2730706137
C,-2.2514948699,2.8729300165,-1.6343389949
C,-2.7853694317,0.6747019262,-2.4929067954
C,-4.1103280766,1.0670337906,-2.6471001803
C,-3.5814355393,3.2523766647,-1.7684861514
H,-1.516574945,3.5760593973,-1.2505416524
H,-2.483504101,-0.3161464535,-2.812302183
H,-4.8293876637,0.3707710792,-3.0657290885
H,-3.8874911525,4.2549774059,-1.4896411672

H,-5.5501421634,2.6452675285,-2.3904981274

TS-*E,E*[1,1]^{MeOH} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E,E*-diimine **1** complex in MeOH)
cydiimph2_EE_b2cat2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1304131

Zero-point correction= 0.571244 (Hartree/Particle)
Thermal correction to Energy= 0.602192
Thermal correction to Enthalpy= 0.603136
Thermal correction to Gibbs Free Energy= 0.509323
Sum of electronic and ZPE= -1696.559169
Sum of electronic and thermal Energies= -1696.528221
Sum of electronic and thermal Enthalpies= -1696.527277
Sum of electronic and thermal Free Energies= -1696.621090

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.881	128.071	197.446

H,1.1386244956,4.4554925418,0.6706319889
C,1.1815692631,3.9508477261,-0.2993146081
C,0.8606348326,4.2751177356,-2.8157967252
C,0.1686114662,2.1643194194,-1.7447514692
C,-0.1725738519,3.1373428082,-2.8651652934
C,0.0767271374,2.9055326409,-0.3917450875
C,0.9366124189,4.9529886876,-1.4401481417
H,1.8453968948,3.8601569364,-3.0657403405
H,1.2004278301,1.8351297068,-1.891659093
H,-1.1851825309,3.5375035726,-2.7343921732
H,-0.8699453049,3.4520163053,-0.3811028082
H,-0.0046276766,5.4839667394,-1.2476254255
H,2.1655936041,3.4865245049,-0.4014263897
H,0.6242354707,5.0190543968,-3.582390472
H,-0.1335992082,2.6244508554,-3.8308165852
H,1.7314796796,5.7047487321,-1.4434635003
N,-0.6377738453,0.9226733632,-1.6504661543
N,-0.0343989479,1.8823812052,0.6884881474
C,-1.9249763679,1.0798962591,-1.407877429
H,-2.3095435655,2.0973036098,-1.3677654564
C,-1.2268261447,1.8648063301,1.246750563
H,-1.8331704972,2.7491934849,1.0665551322
B,0.2469871114,-0.1798777707,-1.0964840294
B,0.9539065861,0.7553212575,0.5267930861
O,2.3089671796,1.2017811332,0.1900138099

O,1.0985692728,-0.2584380067,1.5592293574
O,1.4483516081,-0.5044970103,-1.8654423321
O,-0.3261117171,-1.4355194927,-0.6626247521
C,2.4120192873,-0.6280695898,1.517428105
C,5.1052288111,-1.0209086929,1.0924245932
C,3.0087451554,-1.7157042434,2.12151986
C,3.1348409298,0.2497767751,0.7001170361
C,4.4858291847,0.0782766806,0.4737256359
C,4.3835661272,-1.899258808,1.8947271709
H,2.431428203,-2.3995056909,2.73497375
H,5.0356578424,0.7606064563,-0.1659318236
H,4.8858139495,-2.7463049423,2.3510397208
H,6.1655211307,-1.1886578992,0.9320234309
C,0.6583674245,-2.3629147137,-0.8395269733
C,2.9216589769,-3.844430984,-1.3536229766
C,0.6954198301,-3.6633667775,-0.3798209294
C,1.7237122685,-1.8018583236,-1.5549838771
C,2.8731959051,-2.5198979982,-1.8193552676
C,1.8571399766,-4.404442202,-0.6530697353
H,-0.1356514396,-4.082039105,0.1782599948
H,3.7023832265,-2.0691197933,-2.3544831879
H,1.9255415097,-5.4290492307,-0.3017914936
H,3.8114718541,-4.4371851383,-1.5406422663
C,-2.8952322399,0.0009820717,-1.2729446423
C,-4.8261555583,-2.0004979845,-0.9549282205
C,-4.0125225824,0.2111985387,-0.4469655769
C,-2.7749230389,-1.2161052617,-1.9620949866
C,-3.7366407537,-2.2072685947,-1.8005266821
C,-4.9650612956,-0.7859804094,-0.281842893
H,-4.1119856692,1.1562933926,0.0813792544
H,-1.9402302802,-1.3686676513,-2.6383138493
H,-3.6384320409,-3.1431477668,-2.3417298992
H,-5.8149155455,-0.6180379171,0.3722716404
H,-5.5711094942,-2.780094967,-0.8290913294
C,-1.8339390883,0.9081113754,2.1727321529
C,-3.2908813868,-0.7532505761,3.8966967369
C,-1.7254562627,-0.4871364498,2.0706563542
C,-2.7171907799,1.4540773523,3.1211366972
C,-3.4244367965,0.6321110864,3.9885880072
C,-2.4510615985,-1.3049638453,2.9311145673
H,-1.1049917402,-0.9314118412,1.3039735232
H,-2.836310641,2.5329041781,3.1765461604
H,-4.0883243347,1.0706146058,4.7268246558
H,-2.3667826617,-2.3832092516,2.8362835587
H,-3.8521555577,-1.3996285357,4.5643321848

TS-*E,Z*[1,1]^{MeOH} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E,Z*-diimine **1** complex in MeOH)
cydiimph2_EZ_b2cat2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1175902

Zero-point correction= 0.571909 (Hartree/Particle)
Thermal correction to Energy= 0.602537
Thermal correction to Enthalpy= 0.603481
Thermal correction to Gibbs Free Energy= 0.511737
Sum of electronic and ZPE= -1696.545681
Sum of electronic and thermal Energies= -1696.515053
Sum of electronic and thermal Enthalpies= -1696.514109
Sum of electronic and thermal Free Energies= -1696.605854

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.098	127.740	193.093

H,-1.3152231982,-1.8397423458,-3.4496683989
C,-1.1331851885,-2.3321189577,-2.4894888725
C,-1.9312758258,-4.1705781234,-0.9226464968
C,-1.1733034966,-2.0222835379,0.0170314351
C,-2.1874950343,-3.1485994906,0.1951175287
C,-1.4037634616,-1.3475589031,-1.3559166666
C,-2.0693075811,-3.5355986828,-2.3110566003
H,-0.9222542191,-4.5872252413,-0.8090352556
H,-0.1881531128,-2.4970225576,0.0062107396
H,-3.2105512007,-2.7762114855,0.1058399354
H,-2.4623796748,-1.0732911826,-1.4009675738
H,-3.1075141057,-3.2087043765,-2.4535474948
H,-0.0915777762,-2.6603421588,-2.467585366
H,-2.6357793176,-5.0013622532,-0.8201940096
H,-2.0718382917,-3.6100935454,1.1803895921
H,-1.8582504234,-4.2778140643,-3.0866531525
N,-1.032282902,-0.9173882996,1.0114146092
N,-0.6396908761,-0.0645790034,-1.3964272648
C,-1.9598194719,-0.003316112,1.226150223
H,-1.5949792373,0.9081905797,1.6978624285
C,-1.4276367128,0.9939182755,-1.3520130538
H,-2.4739822727,0.7955278387,-1.5627876034
B,0.4063933459,-0.4838126859,1.031306682
B,0.7706893167,-0.1990772822,-0.901954556
O,1.490477775,-1.3835302326,-1.3758810733
O,1.7070093073,0.9106556785,-0.9748026854
O,1.4230191261,-1.461223685,1.4203038068

O,0.6962413894,0.741869911,1.7538697426
C,2.9380260902,0.3278983278,-1.0613421244
C,5.1714906977,-1.2733526416,-1.2319494336
C,4.1706607067,0.9202644564,-0.8814383281
C,2.806470396,-1.0449696836,-1.3048422582
C,3.909735466,-1.86913336,-1.40074018
C,5.2994520655,0.0881532499,-0.9746531892
H,4.254094062,1.9802899897,-0.6650995476
H,3.7983145966,-2.9329991059,-1.5819708232
H,6.2862187976,0.5180110238,-0.8346701485
H,6.0602010084,-1.8933375521,-1.2947640596
C,1.9922247612,0.6055361493,2.1644417612
C,4.5850348899,-0.1145511236,2.7523978554
C,2.8339642443,1.5775375258,2.6639774862
C,2.4255339303,-0.7116422521,1.9608535441
C,3.7213371944,-1.0972904426,2.2406698039
C,4.152010157,1.191556141,2.9610256019
H,2.4885793508,2.5963854005,2.8063737701
H,4.0527087896,-2.1140852312,2.0574004568
H,4.8439879646,1.9309209033,3.3513556577
H,5.6121674342,-0.3817733789,2.9800411103
C,-3.4255901239,-0.1543907234,1.1580404487
C,-6.2232805431,-0.2914701931,1.2467040346
C,-4.0658719779,-1.2250343097,1.7974343001
C,-4.2076432693,0.8759147344,0.6140780287
C,-5.5949827487,0.8001840209,0.6471759486
C,-5.4558347116,-1.2960408525,1.8311328556
H,-3.471832645,-1.986142675,2.2929653223
H,-3.7209922579,1.7361106169,0.1616637672
H,-6.1871872862,1.5968520166,0.2081591957
H,-5.9373810915,-2.1322525223,2.3281801125
H,-7.3069294542,-0.3485134753,1.2736584148
C,-1.0885212035,2.422712602,-1.2963691449
C,-0.7194398348,5.2026892428,-1.2692117112
C,-1.8568469616,3.2586472431,-2.1253448674
C,-0.162518133,3.0059000108,-0.4189853706
C,0.0175433378,4.3851950102,-0.4136322783
C,-1.6627695739,4.6347588118,-2.1237769148
H,-2.6006042007,2.8161924291,-2.782866395
H,0.3939170732,2.3855541527,0.2712921411
H,0.7334589723,4.8249561004,0.2740828082
H,-2.2531508681,5.2629799088,-2.7832988323
H,-0.5704196107,6.277942629,-1.2584762777

TS-*Z,E*[1,1]^{MeOH} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,E*-diimine **1** complex in MeOH)
cydiimph2_ZE_b2cat2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.132178

Zero-point correction= 0.571485 (Hartree/Particle)
Thermal correction to Energy= 0.602250
Thermal correction to Enthalpy= 0.603194
Thermal correction to Gibbs Free Energy= 0.510825
Sum of electronic and ZPE= -1696.560693
Sum of electronic and thermal Energies= -1696.529928
Sum of electronic and thermal Enthalpies= -1696.528984
Sum of electronic and thermal Free Energies= -1696.621353

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.918	127.891	194.408

H,-1.5463130803,-4.0548413641,-0.2076268779
C,-1.1645260668,-3.5521752251,0.6866796203
C,-1.5208563312,-3.2160405012,3.1878303328
C,-0.7411816236,-1.3286680016,1.7888236697
C,-1.5871079458,-1.6926557148,3.0026931151
C,-1.3120806166,-2.0423144904,0.5423564391
C,-1.9575408582,-3.9781083452,1.9300916267
H,-0.4889793365,-3.4951279932,3.4369649492
H,0.2784237114,-1.6819855162,1.9680448074
H,-2.6271523704,-1.377013025,2.8565644537
H,-2.3766776483,-1.8079369064,0.499324107
H,-3.0244272512,-3.7925380915,1.747107879
H,-0.1067966786,-3.8149699386,0.7941478692
H,-2.1450864982,-3.5104260317,4.036756616
H,-1.2019165846,-1.1782772869,3.8883787364
H,-1.8432830958,-5.0546166064,2.0881778668
N,-0.6182217551,0.1112215056,1.4748993804
N,-0.6800429867,-1.4281730126,-0.6455890305
C,-1.7478384816,0.747941007,1.1850701649
H,-2.6637207819,0.161621833,1.1688676309
C,-1.3994708818,-0.707813371,-1.4836491612
H,-0.8169892146,-0.0851655449,-2.1606762343
B,0.6913353604,0.4224076685,0.81047563
B,0.7763837623,-1.1364746512,-0.5097664416
O,1.6313295808,-2.1560359472,0.0669550181
O,1.4622547972,-0.5765042373,-1.6522102679
O,1.933240446,0.2850957584,1.5453461169

O,0.791769583,1.5840230311,-0.0335280116
C,2.7572072523,-0.9937007519,-1.5221126098
C,5.2052900527,-2.0485458946,-0.836267311
C,3.8640466763,-0.5576305617,-2.2206199895
C,2.8579899026,-1.935390825,-0.490428241
C,4.072494286,-2.4808470845,-0.1267664527
C,5.1041614589,-1.1083667213,-1.8577184004
H,3.7722865556,0.1880540316,-3.0033801026
H,4.1420893548,-3.2027090341,0.6800054791
H,5.99870279,-0.786526464,-2.381345014
H,6.1776248512,-2.4536101962,-0.5747644585
C,2.1197382877,1.8977753253,-0.0391186927
C,4.8542003144,2.1090496233,0.2279162922
C,2.7792069242,2.8000484674,-0.8489991914
C,2.8050068871,1.1161010187,0.9005114384
C,4.1751300293,1.1948391921,1.0498383162
C,4.1721519572,2.8946977496,-0.6975130289
H,2.239121729,3.3945574471,-1.5781764644
H,4.696424973,0.5658841602,1.7638408856
H,4.7251480168,3.5896097156,-1.321385976
H,5.9325358221,2.1969480542,0.314659777
C,-1.9042246209,2.1785040702,1.0242539654
C,-2.3760180433,4.9278922158,0.7211124101
C,-0.9610174957,3.1198914973,1.4797545696
C,-3.1034175195,2.6443850545,0.451960095
C,-3.3307435772,4.0049813406,0.2922632002
C,-1.2000133,4.4792306906,1.3244736741
H,-0.0602102707,2.7837991422,1.9828233447
H,-3.8517659436,1.9236098578,0.132543443
H,-4.2562149908,4.3477116686,-0.1601016929
H,-0.4687254083,5.195580857,1.6861426281
H,-2.5551083333,5.9920344781,0.6030838755
C,-2.8422682658,-0.7025475262,-1.704109222
C,-5.5800181615,-0.5296883737,-2.292370901
C,-3.3866435515,0.4719489755,-2.2556575093
C,-3.6867936605,-1.8092161997,-1.5017113001
C,-5.0438407391,-1.7141540095,-1.7881195026
C,-4.7441027994,0.5606417728,-2.534908168
H,-2.7330275779,1.3194430153,-2.445115019
H,-3.2792554611,-2.7551863313,-1.1592706089
H,-5.6835446342,-2.5767420781,-1.6305025266
H,-5.1501087543,1.4800025097,-2.9451322994
H,-6.6404371657,-0.4634838801,-2.5140877159

TS-*Z,Z*[1,1]^{MeOH} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in MeOH)
cydiimph2_ZZ_b2cat2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1177778

Zero-point correction= 0.572004 (Hartree/Particle)
Thermal correction to Energy= 0.602692
Thermal correction to Enthalpy= 0.603636
Thermal correction to Gibbs Free Energy= 0.511405
Sum of electronic and ZPE= -1696.545773
Sum of electronic and thermal Energies= -1696.515086
Sum of electronic and thermal Enthalpies= -1696.514142
Sum of electronic and thermal Free Energies= -1696.606373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.195	127.869	194.117

H,-1.4386497862,-2.7290910754,-2.2346679996
C,-1.0302274446,-2.8312354984,-1.2237210343
C,-1.3151312349,-3.9711396735,1.0226578153
C,-0.5989331101,-1.6089863136,0.9498943462
C,-1.4659674374,-2.6081469834,1.7110042088
C,-1.1177453973,-1.4892719268,-0.5004209336
C,-1.791428342,-3.8986032407,-0.431409084
H,-0.2649050074,-4.2886664535,1.0534409413
H,0.4070294618,-2.0386958586,0.9303973788
H,-2.5194940785,-2.3275819489,1.6688468261
H,-2.1592673189,-1.1748021361,-0.415853843
H,-2.863664767,-3.6618585354,-0.4442511549
H,0.0226003585,-3.115866027,-1.3205011189
H,-1.8952360884,-4.719328198,1.5709613639
H,-1.1586593206,-2.6544453862,2.7603479648
H,-1.671879423,-4.8696652045,-0.9211200486
N,-0.3849158917,-0.2124924492,1.4413050071
N,-0.3743372594,-0.3987106721,-1.1734142685
C,-1.3196617531,0.7324374093,1.4839505252
H,-0.9221439543,1.7434460189,1.5187543817
C,-1.007444251,0.6978130252,-1.5751601151
H,-0.3446787339,1.5233120797,-1.826331655
B,0.9966161075,0.2177337749,1.101051784
B,1.0728348989,-0.3382222623,-0.8907040465
O,1.8437337786,-1.5638068596,-0.9421035054
O,1.8609390015,0.7148672749,-1.4893471051
O,2.1412498827,-0.496279537,1.6301421713

O,1.2853249218,1.6281279072,1.1456834062
C,3.1259311757,0.2004305024,-1.5660427511
C,5.4731971738,-1.2366344812,-1.50165474
C,4.2975163839,0.8685068481,-1.85605927
C,3.1141004014,-1.1608232588,-1.2358595641
C,4.2755504445,-1.905511549,-1.1990828371
C,5.484828225,0.1185619658,-1.8195697673
H,4.2935327881,1.9283762585,-2.0878056077
H,4.2567478401,-2.9573903195,-0.9345799988
H,6.4272796386,0.6106939005,-2.0376292336
H,6.4065575302,-1.7899890676,-1.4783734157
C,2.6351833226,1.7006394251,1.351469057
C,5.337310782,1.3366933956,1.7415390983
C,3.4538349887,2.8077872482,1.2624921251
C,3.1463983046,0.4283819498,1.6371611847
C,4.4966588786,0.2156601486,1.8310152536
C,4.8283413421,2.6030989178,1.4660610768
H,3.0473121177,3.7867467413,1.0318961081
H,4.8828478853,-0.7784908373,2.0298778786
H,5.503935509,3.4497873264,1.3988516282
H,6.4055241401,1.2076564472,1.8843372106
C,-2.7686543794,0.6294091153,1.6582191535
C,-5.5561703884,0.665680478,2.0136541779
C,-3.3895051985,-0.2670565813,2.5440294785
C,-3.564423064,1.6050020901,1.0321886555
C,-4.9449997128,1.6095491686,1.1887110403
C,-4.7704861459,-0.2530911112,2.7088413538
H,-2.7853430394,-0.9349032262,3.1460169576
H,-3.0854844815,2.3601383979,0.4188075769
H,-5.5415696989,2.3581700575,0.6760153525
H,-5.2322200504,-0.9503525074,3.4010800987
H,-6.6340344496,0.6681669307,2.1422325878
C,-2.4060971876,0.9097341142,-1.9088118334
C,-5.0543079331,1.6011012816,-2.5930392505
C,-2.7899858329,2.2559685919,-2.0883248892
C,-3.3754793623,-0.0859314952,-2.1458002102
C,-4.6824465306,0.2638704401,-2.4687327238
C,-4.0932456343,2.5978847084,-2.4170543406
H,-2.0469796765,3.0363796336,-1.9446294687
H,-3.112595193,-1.1371402619,-2.1272756122
H,-5.4116517968,-0.5211850014,-2.6429789106
H,-4.3608019811,3.6432076799,-2.5361355815
H,-6.0764769467,1.8632956851,-2.8468182562

TS-*E*,*E*[1,2]^{MeOH} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in MeOH)
cydiimph2_EE_b2cat2_1-2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1355814

Zero-point correction= 0.571644 (Hartree/Particle)
Thermal correction to Energy= 0.602116
Thermal correction to Enthalpy= 0.603060
Thermal correction to Gibbs Free Energy= 0.511992
Sum of electronic and ZPE= -1696.563937
Sum of electronic and thermal Energies= -1696.533465
Sum of electronic and thermal Enthalpies= -1696.532521
Sum of electronic and thermal Free Energies= -1696.623590

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.833	127.867	191.669

H,2.0265818374,2.5297136464,3.2792958968
C,2.2437074426,2.6546290891,2.2139503174
C,2.7600978885,4.3758613213,0.3958922719
C,1.3252604094,2.4360235336,-0.1245411396
C,1.5596601299,3.9064184992,-0.4426179071
C,1.0193918474,2.2875654103,1.3837582277
C,2.5697313408,4.1241067128,1.8986204194
H,3.6554579839,3.84100205,0.0536026244
H,2.2462625247,1.8963638642,-0.355061784
H,0.67384783,4.5042737229,-0.1966548014
H,0.2495774022,3.0208498826,1.6417252662
H,1.7515655253,4.7559031039,2.2683147548
H,3.0912800888,2.013689027,1.9596008504
H,2.9385630543,5.4408515482,0.2191788428
H,1.7638945945,4.0312582501,-1.5104155702
H,3.4722138089,4.4231063919,2.4403034844
N,0.2463729288,1.7334088049,-0.8432822068
N,0.3873106901,0.9592180326,1.588909673
C,-0.9869320695,2.2086854946,-0.6181952892
H,-1.0536197552,3.1280101431,-0.0440783365
C,-0.9344477461,1.0232030944,1.7649135826
H,-1.3658197261,1.997404234,1.9642612474
B,0.5166483438,0.2745525219,-0.9787904735
B,1.1012477325,-0.1870679108,0.974662937
O,2.5195230068,-0.0551760943,0.9769119642
O,1.6729818057,-0.1077062633,-1.7213465912
O,0.6886593984,-1.5331338219,1.135510004

O,-0.6611337532,-0.4967150241,-1.1176988105
C,2.7441091002,-0.8348267507,-1.2909565292
C,5.0393584868,-2.2396508472,-0.5326615208
C,3.4562595803,-1.5775575406,-2.2291138566
C,3.1841828654,-0.8030451163,0.0427486553
C,4.3260157914,-1.5054856891,0.4123007129
C,4.6003713667,-2.2777622236,-1.8538709646
H,3.0989317537,-1.5847507471,-3.2542512795
H,4.6407836088,-1.4588184757,1.4503941593
H,5.1457750265,-2.8501730779,-2.5972229304
H,5.9305021736,-2.7814020519,-0.2331616412
C,-0.7467211105,-1.8126908019,-0.7879777898
C,-1.1104161373,-4.472059772,-0.0359606881
C,-1.5667771669,-2.6468715511,-1.5415319087
C,-0.1065244949,-2.3079418185,0.3563468216
C,-0.2910552009,-3.639226815,0.7219401896
C,-1.7513655853,-3.9760210624,-1.1692451586
H,-2.0624541422,-2.2242203967,-2.4105769511
H,0.211439011,-3.9982312998,1.6150604186
H,-2.3946367139,-4.6174077436,-1.7627381639
H,-1.2471031061,-5.5060042011,0.2639981078
C,-2.1724470324,1.8962589224,-1.4100793317
C,-4.5163059428,1.472955333,-2.9000598909
C,-3.4176152362,2.3528185815,-0.9415509666
C,-2.1197966595,1.2561214238,-2.6592681188
C,-3.2841177358,1.0454822307,-3.3915497696
C,-4.5775500272,2.1358232797,-1.6728249898
H,-3.4643121311,2.8681953454,0.015130022
H,-1.1629904802,0.9511944073,-3.0694930316
H,-3.2258940887,0.5527703628,-4.3574073686
H,-5.5305810561,2.4865031227,-1.2889759285
H,-5.4214178477,1.304439954,-3.4750715622
C,-1.7442022355,-0.1746615797,2.0585118846
C,-3.2696637496,-2.4512149152,2.6303894008
C,-2.9268108443,-0.4281479468,1.3556993329
C,-1.3451404027,-1.061228359,3.0694486903
C,-2.1069320945,-2.188430976,3.3555111101
C,-3.6777397599,-1.5679591931,1.6331658519
H,-3.2371131831,0.2504639418,0.5664891123
H,-0.4350823404,-0.8595549158,3.6268329666
H,-1.788473547,-2.8681791401,4.1400599367
H,-4.5806014618,-1.7673220355,1.0640479884
H,-3.8557538147,-3.3396911264,2.8444985248

TS-*E,Z*[1,2]^{MeOH} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E,Z*-diimine **1** complex in MeOH)
cydiimph2_EZ_b2cat2_1-2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1278944

Zero-point correction= 0.571911 (Hartree/Particle)
Thermal correction to Energy= 0.602209
Thermal correction to Enthalpy= 0.603153
Thermal correction to Gibbs Free Energy= 0.512526
Sum of electronic and ZPE= -1696.555983
Sum of electronic and thermal Energies= -1696.525686
Sum of electronic and thermal Enthalpies= -1696.524742
Sum of electronic and thermal Free Energies= -1696.615368

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.892	127.569	190.740

H,1.4013067588,-1.7052218092,3.4968961119
C,1.4005802157,-2.2032966373,2.5223516037
C,2.721786324,-3.7465264173,0.988182785
C,1.4935539947,-1.8417926955,0.0202847859
C,2.7682034533,-2.6722317905,-0.1096610489
C,1.4833070824,-1.1578889404,1.4143700925
C,2.617505384,-3.1295272774,2.3880464267
H,1.8600444176,-4.4037712662,0.8139580174
H,0.665599456,-2.5524350281,-0.0185213684
H,3.6605439053,-2.0576203112,0.0310581972
H,2.4461066938,-0.6483538287,1.526902369
H,3.5307821528,-2.5567305025,2.595638933
H,0.4773619009,-2.7799092304,2.4357252503
H,3.6189369707,-4.3694645048,0.9218895915
H,2.820848546,-3.134423121,-1.099982944
H,2.5580484033,-3.919978164,3.1423297157
N,1.1151620637,-0.7798185153,-0.9481360451
N,0.4545229015,-0.0888746922,1.3970365663
C,1.8053506969,0.3580521043,-1.038466913
H,1.2689907811,1.1612740458,-1.5348605746
C,0.9913281947,1.1142673292,1.2095349364
H,2.0555225944,1.2043726605,1.3940677725
B,-0.3776024351,-0.6843307327,-1.0376194684
B,-0.8932132168,-0.493880761,0.8725952997
O,-1.2899326763,-1.7983206389,1.3230744777
O,-1.0279434601,-1.8942997147,-1.4705846061
O,-1.9901600304,0.4194439817,0.8920104718

O,-0.7765201342,0.515147005,-1.7071739382
C,-2.1020664396,-2.4515885299,-0.8436549013
C,-4.2455204597,-3.7495603613,0.3946638269
C,-3.0501373041,-3.1270636024,-1.6071436825
C,-2.2326163019,-2.4229247265,0.5552328629
C,-3.3033987736,-3.0685333019,1.1638751334
C,-4.1193581112,-3.7755832519,-0.9919095163
H,-2.924957084,-3.1402866174,-2.6856137381
H,-3.3763413863,-3.0305947933,2.2466213509
H,-4.8496655828,-4.3001016085,-1.5996706001
H,-5.0750034782,-4.2528101698,0.8807436089
C,-1.8742453988,1.2482262749,-1.3873360563
C,-4.0696306089,2.8777673093,-0.8029177845
C,-2.396891853,2.1058574182,-2.3534746356
C,-2.4517274878,1.2116933257,-0.1078158732
C,-3.5505941582,2.0246083898,0.1668909327
C,-3.4875763049,2.9221721545,-2.0676688906
H,-1.9204507353,2.1190648202,-3.3291867965
H,-3.9771350866,1.9766110304,1.164461914
H,-3.8790016838,3.5851992247,-2.832414004
H,-4.9225738286,3.5054381526,-0.5656543607
C,3.2792011473,0.4974906113,-1.0173746303
C,6.0479318123,0.9048259945,-1.228686397
C,3.8820458046,1.623999173,-0.4396621852
C,4.0795244945,-0.3932494188,-1.7472579652
C,5.4537103389,-0.1955083614,-1.8426283964
C,5.2560073687,1.8191503742,-0.5362954192
H,3.2734697271,2.356233971,0.0836729278
H,3.6163485923,-1.2300900824,-2.2603951114
H,6.0575772676,-0.897092391,-2.4096832314
H,5.7074857552,2.690481669,-0.0724549076
H,7.119867444,1.0585763278,-1.3034975186
C,0.1928463955,2.3570269342,1.1937041832
C,-1.2927826984,4.7284090432,1.217673461
C,-0.7265598151,2.6074364381,2.2220715814
C,0.378108338,3.3175879695,0.193502516
C,-0.3719535029,4.4916474144,0.1998293423
C,-1.4600997704,3.7881500532,2.2346595081
H,-0.8586754516,1.8712927737,3.00935858
H,1.0953866558,3.1381492031,-0.6023101681
H,-0.2358469726,5.2199552493,-0.5935798953
H,-2.1696649882,3.971967051,3.0357002983
H,-1.877364214,5.643279168,1.2207016203

TS-*Z,E*[1,2]^{MeOH} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z,E*-diimine **1** complex in MeOH)
cydiimph2_ZE_b2cat2_1-2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.135184

Zero-point correction= 0.572331 (Hartree/Particle)
Thermal correction to Energy= 0.602746
Thermal correction to Enthalpy= 0.603691
Thermal correction to Gibbs Free Energy= 0.512517
Sum of electronic and ZPE= -1696.562853
Sum of electronic and thermal Energies= -1696.532438
Sum of electronic and thermal Enthalpies= -1696.531493
Sum of electronic and thermal Free Energies= -1696.622667

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.229	127.481	191.892

H,0.8494244632,-4.0141819632,1.2067190575
C,0.4718048641,-3.6891208425,0.2317959578
C,0.6704365601,-4.0476626636,-2.2893501751
C,0.2916541191,-1.7776320947,-1.3937692939
C,0.9743504323,-2.5570567897,-2.5098678655
C,0.8686515211,-2.2430125918,-0.0333827302
C,1.0828036562,-4.53741465,-0.8941661657
H,-0.4076015705,-4.2068095326,-2.4206390058
H,-0.7740946853,-2.0111081897,-1.4245723109
H,2.0579540986,-2.3869821149,-2.495550839
H,1.9543702216,-2.215354864,-0.1296744996
H,2.1770054598,-4.499708201,-0.8072857393
H,-0.6179273773,-3.7880236645,0.2427671763
H,1.1759428886,-4.6434401782,-3.0553007873
H,0.5947720292,-2.2268235619,-3.4816674124
H,0.7893534421,-5.583838676,-0.7677999991
N,0.3861945513,-0.3029775976,-1.4326307807
N,0.5046289325,-1.2118017159,0.9637523994
C,1.6206425743,0.1937533104,-1.3341108134
H,2.4338176357,-0.5265049333,-1.2965264932
C,1.4649540764,-0.3857917912,1.3750145939
H,1.1034304937,0.5412745255,1.8134950393
B,-0.824339571,0.3363087974,-0.8445737512
B,-0.8895193931,-0.7194512328,0.9340331561
O,-1.8828293844,-1.7224249347,0.7032457242
O,-2.0641643475,0.0102708627,-1.48259427
O,-1.1999174023,0.2600863865,1.9314706115

O,-0.6610818319,1.6653111524,-0.3606520376
C,-3.1841457311,-0.3697808874,-0.798877125
C,-5.5066667306,-1.2176666741,0.4985179741
C,-4.4269438442,0.0921524126,-1.2185723856
C,-3.1030024071,-1.2569277773,0.2868610088
C,-4.2619419608,-1.6744535598,0.9300720875
C,-5.5875291812,-0.3318524951,-0.5726761356
H,-4.4635945114,0.7815833474,-2.0565640098
H,-4.1674436229,-2.3601031936,1.7666058321
H,-6.5521082664,0.0340279463,-0.9095054603
H,-6.406813434,-1.5505843451,1.0048517915
C,-1.6405534814,2.116984935,0.4830985092
C,-3.5809727202,3.0185403847,2.2595207307
C,-2.3340743414,3.2879064456,0.2099438187
C,-1.9158263773,1.387069613,1.6490487429
C,-2.887807047,1.8390904526,2.5334781403
C,-3.3045315677,3.7434128239,1.1032028452
H,-2.0970598053,3.830584466,-0.7002309109
H,-3.0878002106,1.2572916604,3.4279680865
H,-3.8440079162,4.6602497862,0.8892986039
H,-4.3388796461,3.3664564093,2.9539884669
C,2.0193006336,1.570147735,-1.5802369588
C,2.9709738792,4.1621112813,-2.0957506702
C,3.342478435,1.929982373,-1.2616763136
C,1.1982935145,2.5208601441,-2.2146976172
C,1.6738760098,3.803044652,-2.4625994707
C,3.8077595896,3.2159255184,-1.5030734189
H,4.0022561083,1.1859967226,-0.8237980839
H,0.2019591333,2.2445159064,-2.5401027701
H,1.0307055148,4.5247665182,-2.9569791302
H,4.8277966953,3.4779364387,-1.2392487693
H,3.3346193518,5.165993065,-2.2916342855
C,2.8851453733,-0.6580495413,1.5753726406
C,5.6312590009,-0.9656970533,2.0846320748
C,3.7176808831,0.463298965,1.7501441384
C,3.448064462,-1.9398697973,1.7168505599
C,4.8093376517,-2.0850471326,1.9603875268
C,5.0768931221,0.3109506404,1.9897987077
H,3.2832798869,1.4574801073,1.6857822183
H,2.8202772002,-2.8244127299,1.6782511387
H,5.2270112793,-3.0809064054,2.0706422428
H,5.7036043331,1.1892508177,2.1095651048
H,6.6925851985,-1.0874379972,2.2763629186

TS-*Z,Z*[1,2]^{MeOH} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in MeOH)
cydiimph2_ZZ_b2cat2_1-2_ts_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.1213537

Zero-point correction= 0.572175 (Hartree/Particle)
Thermal correction to Energy= 0.602712
Thermal correction to Enthalpy= 0.603656
Thermal correction to Gibbs Free Energy= 0.511220
Sum of electronic and ZPE= -1696.549179
Sum of electronic and thermal Energies= -1696.518642
Sum of electronic and thermal Enthalpies= -1696.517698
Sum of electronic and thermal Free Energies= -1696.610133

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.207	127.664	194.547

H,-1.1473812978,-1.7249105353,-3.1626179394
C,-0.769871386,-2.1819311148,-2.241740714
C,-1.0895788008,-4.0778228472,-0.5880489689
C,-0.4513855606,-1.8436546073,0.2475578874
C,-1.2997517534,-3.07510178,0.5556639867
C,-0.9520383846,-1.213957155,-1.0773076742
C,-1.5185413199,-3.4828370314,-1.9329815749
H,-0.0313531257,-4.3659287128,-0.6340360936
H,0.5632814454,-2.2141215986,0.0948091059
H,-2.3619463099,-2.8258477357,0.6018554372
H,-2.0167166152,-1.0304808617,-0.9239246274
H,-2.5975849217,-3.2798790116,-1.9064576218
H,0.2955813819,-2.3844572205,-2.3852802609
H,-1.6622832342,-4.9867376808,-0.3805011439
H,-1.0029695562,-3.5105506962,1.5147973262
H,-1.3482064066,-4.2034127689,-2.7385700203
N,-0.2819540964,-0.7058831398,1.204953277
N,-0.301026783,0.1067280563,-1.2272375593
C,-1.2690607343,0.1417938478,1.5135924882
H,-0.9307497719,1.1062486676,1.8800656805
C,-1.0587729722,1.1916014617,-1.0341450359
H,-0.4907076709,2.0959695513,-0.8325245601
B,1.0861933845,-0.1474281488,1.0716776612
B,1.1440701467,0.1841447769,-0.9597196181
O,1.9175570483,-0.908308282,-1.4653065344
O,2.1549278721,-1.0750384135,1.2962205808
O,1.7214029664,1.4893479129,-1.0926944496

O,1.2420984483,1.1644978688,1.610703754
C,3.2660135788,-1.1379805258,0.5042591261
C,5.5332336038,-1.3860977593,-1.1029288221
C,4.5155217352,-1.3176191072,1.0865846985
C,3.1513471596,-1.0742388347,-0.8927840926
C,4.2825161798,-1.196069431,-1.6899858638
C,5.6487104617,-1.4431393932,0.2835288289
H,4.5795599445,-1.359935211,2.1695961979
H,4.1626543269,-1.142271841,-2.7677424371
H,6.6199497314,-1.5843266449,0.7466736453
H,6.4128006687,-1.4831190425,-1.730944644
C,2.3540942126,1.8511844651,1.1986212556
C,4.5779398321,3.2796618981,0.3262961642
C,3.2242787207,2.4103502471,2.1249097641
C,2.5948320679,2.0017085135,-0.1767167378
C,3.7085633755,2.7139291474,-0.6063898941
C,4.3366092986,3.1308978286,1.6892849667
H,3.0128335711,2.274762366,3.1811245069
H,3.8777163573,2.8150316037,-1.674021643
H,5.0125110512,3.5680596825,2.4169240117
H,5.4444850225,3.8346428855,-0.0184428851
C,-2.6810450258,-0.1623117281,1.7659967753
C,-5.3931861485,-0.5631668127,2.3877807416
C,-3.6235107731,0.8627903428,1.5817294597
C,-3.1111737243,-1.3599495681,2.3606549261
C,-4.455584524,-1.5592569338,2.6570643444
C,-4.9679045562,0.6581334865,1.8663839832
H,-3.2891860991,1.8272825704,1.2194490487
H,-2.3847225099,-2.1146474133,2.6375274803
H,-4.7676155602,-2.4906899803,3.1193611053
H,-5.6808638601,1.4585273939,1.6926135539
H,-6.4421053614,-0.7252631239,2.6155721365
C,-2.4496900482,1.4224797035,-1.4094643951
C,-5.0952967266,2.1542748439,-2.0601534583
C,-2.9758416887,2.6766954292,-1.0393086091
C,-3.2690125749,0.56762437,-2.1718507084
C,-4.5769816911,0.9305102674,-2.4779316886
C,-4.2793081514,3.0356023464,-1.3503267306
H,-2.3446394097,3.3658569027,-0.4835213676
H,-2.8870335733,-0.3655266593,-2.5698077431
H,-5.1894315049,0.2531531937,-3.0649585981
H,-4.6583326455,4.0046997056,-1.0411500045
H,-6.1166127353,2.4280840152,-2.3048311864

TS-*E*,*E*[1,1]^{DMF} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
maxstep5_cydiimph2_EE_b2cat2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1277715

Zero-point correction= 0.572168 (Hartree/Particle)
Thermal correction to Energy= 0.603046
Thermal correction to Enthalpy= 0.603990
Thermal correction to Gibbs Free Energy= 0.509568
Sum of electronic and ZPE= -1696.555603
Sum of electronic and thermal Energies= -1696.524726
Sum of electronic and thermal Enthalpies= -1696.523781
Sum of electronic and thermal Free Energies= -1696.618204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.417	127.676	198.728

H,1.1996471346,4.4540917887,0.6578112196
C,1.2340651691,3.9325671381,-0.3035723216
C,0.8974645047,4.2155207142,-2.8233155797
C,0.2049877192,2.1252325355,-1.7126955535
C,-0.140749874,3.0814802182,-2.8463270105
C,0.1244939533,2.8904180166,-0.3703221779
C,0.9851540177,4.9160906737,-1.4595797069
H,1.878954627,3.7926034132,-3.0726889094
H,1.235375948,1.7894074483,-1.855878529
H,-1.1500938237,3.4893636972,-2.713616239
H,-0.8200873389,3.4414823582,-0.3622878304
H,0.0468666846,5.4535667048,-1.2708032268
H,2.213070577,3.4581475914,-0.4020304549
H,0.6591268442,4.9477096196,-3.6005189585
H,-0.1125246371,2.5534607419,-3.8041910293
H,1.7821585497,5.6652717354,-1.4814827369
N,-0.6028164071,0.8871802796,-1.5919003037
N,0.0182392087,1.8796844699,0.7204809576
C,-1.8875781138,1.0554994107,-1.3468172399
H,-2.2644072711,2.0761927973,-1.3291623243
C,-1.1824398651,1.8548959191,1.2640304
H,-1.7872316183,2.7383722988,1.0769179103
B,0.2979477215,-0.2111478283,-1.0271843888
B,1.0194884488,0.7560620301,0.5691101418
O,2.3593281649,1.2087766532,0.1949226653
O,1.1883214286,-0.2037883992,1.6434595835
O,1.4629755329,-0.5396593415,-1.8410897316

O,-0.2756074964,-1.4588521618,-0.5801214183
C,2.5162684459,-0.4914642595,1.6760431863
C,5.2509131109,-0.7207950512,1.4077882801
C,3.1615296061,-1.4593216171,2.4192705772
C,3.2159185759,0.3554750553,0.8039047657
C,4.5855595037,0.2597186652,0.6520158182
C,4.5556417372,-1.561092389,2.271238309
H,2.608398102,-2.1114517466,3.0868447876
H,5.1187222952,0.917423474,-0.0262289242
H,5.0941133954,-2.3126510572,2.8396548225
H,6.3270924291,-0.8229852834,1.3100206151
C,0.6026878988,-2.4305846947,-0.9456522679
C,2.6411860153,-4.0279918382,-1.8836012634
C,0.5519410963,-3.7791571166,-0.6562849431
C,1.6477883203,-1.8736295317,-1.6971638477
C,2.6838684179,-2.6539311398,-2.1737757445
C,1.5995223634,-4.5790676063,-1.1434219373
H,-0.2646334698,-4.1948376095,-0.0750916347
H,3.4937100875,-2.2161667354,-2.7476606269
H,1.5943224688,-5.6437765283,-0.933254933
H,3.4399561891,-4.6683753297,-2.2440752849
C,-2.8680986823,-0.0082110484,-1.1726809398
C,-4.8123819836,-1.9772182164,-0.743703369
C,-3.9928848434,0.2587798749,-0.3729331569
C,-2.7523706329,-1.2647881928,-1.7870922445
C,-3.7202603026,-2.239529638,-1.5702526902
C,-4.9510528969,-0.7213880005,-0.1503361732
H,-4.0913990942,1.2365848823,0.0922860779
H,-1.9169295459,-1.4632090919,-2.4497019267
H,-3.6240750458,-3.20717721,-2.0527715138
H,-5.8040861092,-0.5083490963,0.4861904921
H,-5.5605240938,-2.7449330284,-0.5723744823
C,-1.8290915152,0.8874833948,2.147757973
C,-3.423503934,-0.8058721452,3.7176228535
C,-1.6417883642,-0.5035355844,2.1049520056
C,-2.8518603987,1.4084010425,2.9628476491
C,-3.6297379825,0.5731867095,3.7533241561
C,-2.4373625966,-1.3351735298,2.8869660057
H,-0.9053576568,-0.9383441341,1.4439954198
H,-3.0298284775,2.4805700933,2.970211201
H,-4.4042267976,0.9954656086,4.3855158445
H,-2.2919624613,-2.4098811301,2.8354085588
H,-4.0387369632,-1.464774743,4.3224232977

TS-*E,Z*[1,1]^{DMF} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E,Z*-diimine **1** complex in DMF)
cydiimph2_EZ_b2cat2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1158672

Zero-point correction= 0.571928 (Hartree/Particle)
Thermal correction to Energy= 0.602738
Thermal correction to Enthalpy= 0.603682
Thermal correction to Gibbs Free Energy= 0.510675
Sum of electronic and ZPE= -1696.543939
Sum of electronic and thermal Energies= -1696.513129
Sum of electronic and thermal Enthalpies= -1696.512185
Sum of electronic and thermal Free Energies= -1696.605192

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.224	127.775	195.750

H,-1.3277713925,-1.8129586106,-3.4524179085
C,-1.134792785,-2.3106272828,-2.4970144106
C,-1.9105612217,-4.1624125829,-0.9350319551
C,-1.1598937893,-2.0144422952,0.0124271709
C,-2.1666577382,-3.147459152,0.1890024589
C,-1.3987914525,-1.3331649281,-1.3559392168
C,-2.0626394171,-3.520275452,-2.3188044499
H,-0.8976844062,-4.5720289448,-0.830537506
H,-0.1689321694,-2.477061165,-0.0030688023
H,-3.1921237404,-2.7804468029,0.1057162228
H,-2.4569162969,-1.0550661508,-1.3900932903
H,-3.1039049131,-3.1985954526,-2.4504125731
H,-0.0898725745,-2.6282364345,-2.4829373752
H,-2.6083073937,-4.998781376,-0.8325096939
H,-2.0450830268,-3.6125911987,1.1718861894
H,-1.8541092768,-4.2569226413,-3.1003328337
N,-1.0271849344,-0.9125112931,1.0100307149
N,-0.628195023,-0.0539547823,-1.3973349891
C,-1.9623140399,-0.0166880347,1.2487030904
H,-1.6014586264,0.8937416594,1.7253878609
C,-1.4083031175,1.0095232109,-1.3772709162
H,-2.4562393838,0.8136034596,-1.5839866307
B,0.4114653387,-0.4624606907,1.0266733854
B,0.7831753565,-0.2050335323,-0.8977180166
O,1.4756248172,-1.4079823074,-1.3628129569
O,1.7390926599,0.8843463318,-0.9911684758
O,1.428855568,-1.4245565358,1.4386804485

O,0.676778102,0.7748512582,1.7392913047
C,2.9536253812,0.2804454624,-1.0858396593
C,5.1581158263,-1.3617181126,-1.2887974222
C,4.2015647952,0.8519703828,-0.9437921023
C,2.792888474,-1.0953375115,-1.3096808159
C,3.8819530803,-1.9372728883,-1.420125562
C,5.3150177898,0.0002861546,-1.0530159156
H,4.3094569332,1.913358925,-0.746060266
H,3.7502226212,-3.0009260914,-1.5883512619
H,6.3117309193,0.4157260668,-0.9434097702
H,6.0343419847,-1.997773607,-1.3653188514
C,1.962634635,0.6537740131,2.1712132093
C,4.548428532,-0.0435119976,2.8268650312
C,2.7864491224,1.6333492006,2.6866955808
C,2.4105431103,-0.6641262369,1.9854546649
C,3.7035295768,-1.0350576123,2.2993480507
C,4.1007729959,1.2599150944,3.018084049
H,2.4306039416,2.6501340028,2.8177821004
H,4.0477515933,-2.0502865045,2.1321507584
H,4.7769003101,2.0067467666,3.4217684544
H,5.5714868772,-0.3021613021,3.0811468407
C,-3.4273370002,-0.1733167355,1.1683337135
C,-6.2248086625,-0.3224700352,1.2322651611
C,-4.0684189763,-1.24711909,1.801474375
C,-4.2086369358,0.8529297276,0.615979652
C,-5.5960607786,0.7711041079,0.6367532536
C,-5.4583091049,-1.3239300345,1.8234813179
H,-3.4745029962,-2.0068331384,2.2993562675
H,-3.7206565044,1.7132736899,0.1654100052
H,-6.187879394,1.5642933874,0.1912011455
H,-5.94072612,-2.1622443229,2.3158883129
H,-7.3083077139,-0.383981714,1.2500183461
C,-1.0708564649,2.4359313392,-1.3072491763
C,-0.7150050814,5.2180190725,-1.2348730825
C,-1.8867678083,3.2874971127,-2.0739159218
C,-0.1002840104,3.0044714224,-0.4677405639
C,0.0713232036,4.3846467997,-0.4404289856
C,-1.7006616332,4.664225453,-2.0504389662
H,-2.6633077041,2.8557469883,-2.6999643364
H,0.4978611226,2.3726085934,0.1753158139
H,0.8212021055,4.8133265957,0.2175354858
H,-2.3292332382,5.3037687298,-2.6618865169
H,-0.5709775573,6.2935608228,-1.2064961196

TS-*Z,E*[1,1]^{DMF} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,E*-diimine **1** complex in DMF)
freq_cydiimph2_ZE_b2cat2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1299319

Zero-point correction= 0.571399 (Hartree/Particle)
Thermal correction to Energy= 0.602269
Thermal correction to Enthalpy= 0.603213
Thermal correction to Gibbs Free Energy= 0.510272
Sum of electronic and ZPE= -1696.558533
Sum of electronic and thermal Energies= -1696.527663
Sum of electronic and thermal Enthalpies= -1696.526719
Sum of electronic and thermal Free Energies= -1696.619659

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.930	127.957	195.611

H,-1.559449,-4.044194,-0.215398
C,-1.170341,-3.545179,0.677843
C,-1.50287,-3.219551,3.182731
C,-0.736966,-1.325844,1.783706
C,-1.572691,-1.695865,3.002872
C,-1.316447,-2.034286,0.539181
C,-1.952104,-3.976324,1.926241
H,-0.46802,-3.498488,3.419304
H,0.285864,-1.676993,1.948827
H,-2.614527,-1.382599,2.864757
H,-2.380275,-1.793985,0.499824
H,-3.020407,-3.788521,1.754368
H,-0.110537,-3.803912,0.773246
H,-2.117616,-3.517871,4.037087
H,-1.182793,-1.182686,3.887194
H,-1.837569,-5.053553,2.078761
N,-0.619716,0.115163,1.474762
N,-0.681623,-1.42802,-0.649579
C,-1.750361,0.754865,1.209959
H,-2.667182,0.169078,1.193348
C,-1.392954,-0.74548,-1.518754
H,-0.80475,-0.14837,-2.2133
B,0.692773,0.424388,0.799249
B,0.778275,-1.122373,-0.50139
O,1.622366,-2.155374,0.070196
O,1.463887,-0.577151,-1.650566
O,1.931063,0.296184,1.542602

O,0.78572,1.596629,-0.030645
C,2.750894,-0.998634,-1.517614
C,5.194683,-2.073309,-0.834734
C,3.862264,-0.572088,-2.215634
C,2.845758,-1.941895,-0.482454
C,4.058285,-2.496364,-0.123765
C,5.099881,-1.132145,-1.855224
H,3.776548,0.17476,-2.997998
H,4.125494,-3.219336,0.682225
H,5.996116,-0.816568,-2.379816
H,6.163928,-2.486648,-0.574483
C,2.107953,1.910882,-0.037328
C,4.844527,2.133236,0.235224
C,2.767273,2.821599,-0.838571
C,2.796399,1.125502,0.901758
C,4.166899,1.211566,1.0512
C,4.160576,2.921646,-0.685829
H,2.227075,3.419891,-1.564582
H,4.691445,0.581898,1.762209
H,4.711132,3.622868,-1.304866
H,5.92246,2.224669,0.32392
C,-1.904185,2.184982,1.042801
C,-2.367605,4.93417,0.728055
C,-0.958077,3.124963,1.49355
C,-3.100807,2.651709,0.466411
C,-3.324404,4.012423,0.301083
C,-1.192838,4.48439,1.333364
H,-0.058341,2.78631,1.996125
H,-3.849201,1.931203,0.146195
H,-4.247812,4.356059,-0.154584
H,-0.459469,5.200136,1.6918
H,-2.543625,5.998298,0.606013
C,-2.838839,-0.72532,-1.728124
C,-5.579742,-0.528003,-2.291305
C,-3.374637,0.448276,-2.289112
C,-3.693921,-1.818823,-1.501799
C,-5.052604,-1.712003,-1.776606
C,-4.733993,0.54965,-2.555453
H,-2.713255,1.285621,-2.495512
H,-3.293571,-2.763636,-1.148048
H,-5.700808,-2.564509,-1.60066
H,-5.133671,1.468495,-2.972653
H,-6.64135,-0.452284,-2.503594

TS-*Z,Z*[1,1]^{DMF} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in DMF)
maxstep1_cfc_cydiimph2_ZZ_b2cat2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1165081

Zero-point correction= 0.572293 (Hartree/Particle)
Thermal correction to Energy= 0.602950
Thermal correction to Enthalpy= 0.603894
Thermal correction to Gibbs Free Energy= 0.512231
Sum of electronic and ZPE= -1696.544216
Sum of electronic and thermal Energies= -1696.513558
Sum of electronic and thermal Enthalpies= -1696.512614
Sum of electronic and thermal Free Energies= -1696.604277

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.357	127.753	192.922

H,-1.4570409996,-2.6934073669,-2.2538961766
C,-1.0425867849,-2.8090593701,-1.2467956186
C,-1.3162837939,-3.9696023064,0.9890523325
C,-0.5922618835,-1.6083543165,0.9374018783
C,-1.4573486704,-2.6134081815,1.6928229425
C,-1.1157616011,-1.4736055421,-0.5097537281
C,-1.8039301945,-3.8803000552,-0.4604004736
H,-0.2665877864,-4.2899346149,1.0072609866
H,0.416438945,-2.0311026587,0.9097222098
H,-2.5100769144,-2.3282755609,1.6613156915
H,-2.1532414793,-1.1464701949,-0.4189692276
H,-2.8748032476,-3.6373029808,-0.4619712197
H,0.0093068546,-3.0939678952,-1.3524298699
H,-1.8935308112,-4.7222548473,1.5340898604
H,-1.1438790223,-2.6719550505,2.7396970547
H,-1.6937726417,-4.8470480311,-0.9606338015
N,-0.3846057594,-0.2154531452,1.4377676208
N,-0.3595147057,-0.3922534236,-1.1807846506
C,-1.3260742714,0.7158919053,1.5143840748
H,-0.9382497494,1.7301491302,1.5591273267
C,-0.9736165561,0.6969144023,-1.6223152221
H,-0.2956357016,1.5022026173,-1.8961952783
B,0.993128121,0.2346329974,1.086562398
B,1.0890485299,-0.3478600861,-0.8855851384
O,1.833668202,-1.5895138223,-0.9204643505
O,1.8964555336,0.6792061675,-1.4975592818
O,2.1453419707,-0.4500818017,1.6328081013

O,1.2488552111,1.6503994147,1.123196731
C,3.14657866,0.1419847775,-1.562193682
C,5.4678102177,-1.3425433797,-1.47731017
C,4.3329042592,0.7791650193,-1.8642481314
C,3.1079935308,-1.2161833421,-1.2102031728
C,4.2561892292,-1.9814667201,-1.1634528966
C,5.505798604,0.006255826,-1.817677742
H,4.3519997406,1.834890514,-2.1135380914
H,4.2177823502,-3.0289993996,-0.8843003765
H,6.4573536629,0.4761947799,-2.0450304854
H,6.3897024648,-1.9144543981,-1.4463704418
C,2.5911075444,1.7514768343,1.3267270623
C,5.3007291618,1.4487263663,1.7407559351
C,3.3894886972,2.8736507132,1.2344160783
C,3.1277328834,0.4902575416,1.6293880514
C,4.481808989,0.3111191406,1.8347417362
C,4.7672001141,2.7009209487,1.4492998904
H,2.9653952148,3.8425785881,0.9934066773
H,4.8889342718,-0.6719355025,2.0467953204
H,5.4249380988,3.5613577878,1.3794303797
H,6.3702251418,1.343301787,1.8929949642
C,-2.775500584,0.5906239845,1.6867534814
C,-5.5598451714,0.5866223413,2.0632479599
C,-3.3742743791,-0.2998724667,2.5934486459
C,-3.5920798543,1.5354304894,1.0417165738
C,-4.9715701615,1.520694477,1.2111848384
C,-4.7539155927,-0.305986515,2.769397181
H,-2.7530990564,-0.950061451,3.1981179779
H,-3.1323574966,2.2807681516,0.4017217223
H,-5.585081464,2.2462014582,0.6856697298
H,-5.1987841602,-0.9980610053,3.4775474266
H,-6.6363429127,0.5748815655,2.2015925832
C,-2.3733162887,0.9354637935,-1.9336639291
C,-5.0200174365,1.6763319634,-2.5745729941
C,-2.7336649674,2.2885571296,-2.114125604
C,-3.3671511482,-0.0415669104,-2.1467074897
C,-4.672580048,0.3327907416,-2.4489848719
C,-4.0357817333,2.6546274435,-2.4202489057
H,-1.9728512422,3.0545091341,-1.9875303417
H,-3.1248265106,-1.0975880503,-2.123426544
H,-5.4205738209,-0.4383202685,-2.6045822025
H,-4.2848820512,3.7045032702,-2.5387961869
H,-6.0410295504,1.9578884587,-2.8111741277

TS-*E*,*E*[1,2]^{DMF} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in DMF)
cydiimph2_EE_b2cat2_1-2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1342279

Zero-point correction= 0.571696 (Hartree/Particle)
Thermal correction to Energy= 0.602301
Thermal correction to Enthalpy= 0.603245
Thermal correction to Gibbs Free Energy= 0.510859
Sum of electronic and ZPE= -1696.562532
Sum of electronic and thermal Energies= -1696.531927
Sum of electronic and thermal Enthalpies= -1696.530983
Sum of electronic and thermal Free Energies= -1696.623369

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.950	127.899	194.443

H,2.0064834789,2.522925618,3.2817186533
C,2.231745849,2.6447265758,2.2176428425
C,2.7641086736,4.3602938772,0.3991543495
C,1.3266875099,2.423379389,-0.1258486219
C,1.5664962458,3.8930593649,-0.4443075943
C,1.0130276736,2.2757465119,1.3801500209
C,2.5634750863,4.1124922709,1.9011736313
H,3.659220788,3.8208977403,0.0634474249
H,2.2464702904,1.879625915,-0.351511957
H,0.68101549,4.4927981583,-0.2018213194
H,0.2390238119,3.0073127305,1.6314479791
H,1.7441455442,4.7471391188,2.263221194
H,3.0763861574,1.9975042049,1.9697215995
H,2.9477758328,5.4240952335,0.2210252706
H,1.7746889886,4.0167937054,-1.5114579156
H,3.4629434244,4.4111406631,2.4479720704
N,0.2496949681,1.7226693287,-0.8492323738
N,0.3866401625,0.9441250226,1.5875336577
C,-0.9815559035,2.2082020451,-0.6477969501
H,-1.0540925982,3.1240708071,-0.0685873522
C,-0.931617177,1.0044516903,1.7831520792
H,-1.3691345021,1.9843638139,1.933555098
B,0.5182675282,0.2611693688,-0.9788670448
B,1.1106285802,-0.1984963984,0.9748928831
O,2.5253464829,-0.0509493402,0.9771945199
O,1.6723792977,-0.1276941891,-1.7165849865
O,0.7046230046,-1.5445272232,1.1257489471

O,-0.66056312,-0.5043521824,-1.1067031789
C,2.7514335653,-0.8331602493,-1.2872659835
C,5.0771032592,-2.1955752922,-0.5328290378
C,3.4749793896,-1.5680869681,-2.2241769433
C,3.1971709154,-0.7894188036,0.0460910286
C,4.3537130939,-1.4703884579,0.4116911356
C,4.6330039794,-2.2469759855,-1.8518271329
H,3.1149193567,-1.5857451907,-3.2480531697
H,4.6724204273,-1.4145886386,1.4479512815
H,5.1851671768,-2.8122158209,-2.5956479807
H,5.9790277282,-2.7198843118,-0.2346091744
C,-0.7358602187,-1.8204214969,-0.7903299441
C,-1.0412685005,-4.50003328,-0.07887687
C,-1.5466294649,-2.6594799527,-1.5497142143
C,-0.0767655923,-2.3218254905,0.3418090761
C,-0.2333481173,-3.6629079252,0.686769172
C,-1.7023993404,-3.9980359318,-1.1980809933
H,-2.0549152107,-2.2334369311,-2.4095771712
H,0.2824730918,-4.0266523473,1.5700321469
H,-2.3377299736,-4.6422608123,-1.7969847529
H,-1.1545195083,-5.5414125784,0.2045624221
C,-2.1663668913,1.8836479916,-1.4315391251
C,-4.5163738177,1.4472667751,-2.9108145481
C,-3.4080783736,2.3615399704,-0.9739191065
C,-2.1211255619,1.2139564653,-2.6661114904
C,-3.2875842963,0.9982603007,-3.3928545755
C,-4.5709145046,2.1380390611,-1.6988183005
H,-3.4487865359,2.9030083023,-0.0314672963
H,-1.1678994179,0.8900025883,-3.068764574
H,-3.2345516372,0.4837049288,-4.3475214913
H,-5.5202082132,2.5062777384,-1.3224114319
H,-5.4230004239,1.2738159088,-3.4817888155
C,-1.7576081406,-0.1715814061,2.0870996882
C,-3.3755742553,-2.3808439872,2.6781602001
C,-3.0209779113,-0.3054740568,1.4960346686
C,-1.3271337423,-1.1431391002,3.003235388
C,-2.1331346105,-2.2379369657,3.2955123585
C,-3.8181984326,-1.4094237978,1.7812403773
H,-3.3617500352,0.4458151068,0.7895397371
H,-0.3612723418,-1.0312214795,3.4852048819
H,-1.7893814797,-2.983368257,4.0062138296
H,-4.7859890654,-1.5122659441,1.3002155771
H,-3.9983599366,-3.2417494993,2.9003412275

TS-*E,Z*[1,2]^{DMF}(Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E,Z*-diimine **1** complex in DMF)
cydiimph2_EZ_b2cat2_1-2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1266158

Zero-point correction= 0.571924 (Hartree/Particle)
Thermal correction to Energy= 0.602336
Thermal correction to Enthalpy= 0.603280
Thermal correction to Gibbs Free Energy= 0.511802
Sum of electronic and ZPE= -1696.554692
Sum of electronic and thermal Energies= -1696.524280
Sum of electronic and thermal Enthalpies= -1696.523336
Sum of electronic and thermal Free Energies= -1696.614814

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	377.971	127.640	192.531

H,1.4114703804,-1.6645712809,3.4910831753
C,1.3976630099,-2.1728900116,2.5218551388
C,2.6901221415,-3.7444576921,0.9929694096
C,1.4800281181,-1.8330139955,0.0152442317
C,2.7447402674,-2.6788530139,-0.1127997708
C,1.4797123463,-1.1389616705,1.4031294258
C,2.6030785294,-3.1137404251,2.3878999048
H,1.8178578427,-4.3904873755,0.8294706929
H,0.6429109168,-2.5330886512,-0.0175375208
H,3.6442051501,-2.0735225872,0.0220321216
H,2.4439004489,-0.6289978833,1.5040740383
H,3.524380025,-2.5493162142,2.582525857
H,0.4652769214,-2.7359639259,2.4460359014
H,3.5778882641,-4.3805390017,0.926386534
H,2.7904240972,-3.147631408,-1.1003735852
H,2.5410149289,-3.896401259,3.1500023115
N,1.1107962997,-0.7718336647,-0.9576314658
N,0.4494960639,-0.0706073874,1.3863731452
C,1.8148489452,0.353506284,-1.0663967296
H,1.2817491129,1.1631399785,-1.5554682977
C,0.9804653239,1.1360694808,1.2172185452
H,2.0487174907,1.2259025132,1.3750192114
B,-0.3832874973,-0.6626126532,-1.0455657088
B,-0.9003227282,-0.4810588675,0.8672300602
O,-1.2819958959,-1.7872575875,1.3172912293
O,-1.0455807585,-1.8613164615,-1.4813752433
O,-1.9976792406,0.4280810564,0.8815665662

O,-0.7637213631,0.5494013594,-1.6994197612
C,-2.0949116891,-2.4430062065,-0.8468096426
C,-4.1961830403,-3.8032094275,0.4049795391
C,-3.0362546743,-3.1376544228,-1.6033210562
C,-2.2134968869,-2.4259813114,0.5554168813
C,-3.262575775,-3.1038287645,1.1683128717
C,-4.0836487309,-3.8163654251,-0.9829218716
H,-2.9219471346,-3.1418582773,-2.6829142652
H,-3.3252986516,-3.0754259952,2.2518318238
H,-4.8066027512,-4.3547100792,-1.5873927782
H,-5.0075681901,-4.3303670778,0.8962494723
C,-1.8683144022,1.2691744821,-1.389907361
C,-4.0876888114,2.8733932176,-0.8164318495
C,-2.3929672635,2.1269255043,-2.3555522974
C,-2.4577792522,1.2194623065,-0.1141502971
C,-3.5678257903,2.020547562,0.1535963864
C,-3.4950730776,2.9304250281,-2.0757593773
H,-1.9090016852,2.1505326795,-3.3271894228
H,-4.0022412599,1.9637601076,1.147044858
H,-3.886774782,3.5930476384,-2.8406968335
H,-4.9491514498,3.4909600487,-0.5834737449
C,3.288946025,0.4796413824,-1.0394357485
C,6.0629113141,0.8613006875,-1.2365735286
C,3.8983893001,1.6057034258,-0.4674107196
C,4.0865451203,-0.4243216335,-1.7562897414
C,5.4629896619,-0.2393646603,-1.844636613
C,5.274563848,1.7883398507,-0.5569475316
H,3.2917666904,2.3461144254,0.0462961167
H,3.6186899662,-1.2616440277,-2.2643865665
H,6.0643518891,-0.950901536,-2.4016967267
H,5.7307474813,2.6594607235,-0.0975299378
H,7.136480656,1.0051424568,-1.306002108
C,0.1812520261,2.3761930153,1.2133331361
C,-1.2990535999,4.7510709351,1.2531824151
C,-0.762856466,2.6064056684,2.2238733209
C,0.3927704701,3.3587370144,0.2391489434
C,-0.3534976822,4.5346720098,0.2531747664
C,-1.4936406828,3.7888327721,2.24428766
H,-0.9157709825,1.8530210322,2.9902767614
H,1.1284589405,3.1926741971,-0.5428185408
H,-0.196094869,5.2803562627,-0.5197723802
H,-2.2221338418,3.9574449281,3.0315020263
H,-1.8809765074,5.6674926777,1.2626980245

TS-*Z,E*[1,2]^{DMF} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z,E*-diimine **1** complex in DMF)
cydiimph2_ZE_b2cat2_1-2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1343495

Zero-point correction= 0.572316 (Hartree/Particle)
Thermal correction to Energy= 0.602816
Thermal correction to Enthalpy= 0.603760
Thermal correction to Gibbs Free Energy= 0.512027
Sum of electronic and ZPE= -1696.562033
Sum of electronic and thermal Energies= -1696.531533
Sum of electronic and thermal Enthalpies= -1696.530589
Sum of electronic and thermal Free Energies= -1696.622322

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.273	127.562	193.069

H,0.8478852486,-4.0045121781,1.2190259868
C,0.4678941827,-3.6824159471,0.2439770544
C,0.6591746361,-4.0498329889,-2.2764331047
C,0.287889867,-1.7765378236,-1.3867090304
C,0.9672402333,-2.5607487023,-2.5015732738
C,0.8658419332,-2.2377237361,-0.0267329442
C,1.0734358816,-4.5362481256,-0.8805417567
H,-0.4197446541,-4.2056720736,-2.4042139743
H,-0.778253274,-2.0076599363,-1.4135010127
H,2.0513440652,-2.3941938416,-2.4880235368
H,1.9516638551,-2.2079113426,-0.1230258344
H,2.1679230829,-4.5004164571,-0.796882204
H,-0.6224500072,-3.7727029183,0.2600475658
H,1.1607337922,-4.6497591696,-3.0416459192
H,0.58837301,-2.2317709034,-3.4740661226
H,0.7781328154,-5.58162996,-0.7503228231
N,0.3828173156,-0.3021428433,-1.4295439072
N,0.4974368146,-1.2088351368,0.9701526971
C,1.6158405379,0.196342739,-1.348359911
H,2.4299686069,-0.5226442221,-1.30134807
C,1.4533464876,-0.3988308236,1.4124717258
H,1.0884086184,0.5183662246,1.867586344
B,-0.8328301416,0.3364540663,-0.8452904209
B,-0.8994317313,-0.7136228068,0.9333625593
O,-1.884971937,-1.7220259316,0.7018336285
O,-2.0664158585,0.0006151704,-1.4873157183
O,-1.2065439883,0.2676965625,1.9270165439

O,-0.6707364122,1.6670081556,-0.3725339705
C,-3.18346403,-0.3862300042,-0.8142485047
C,-5.5112378058,-1.2625094064,0.4615612764
C,-4.4297664618,0.0557042581,-1.2477001851
C,-3.1026915685,-1.2701129522,0.2769027419
C,-4.2644670143,-1.7007204382,0.9073411962
C,-5.5921669951,-0.3813808048,-0.6133055442
H,-4.467978553,0.740622162,-2.0891047782
H,-4.1707577581,-2.3836396806,1.7460394067
H,-6.557728406,-0.0299122404,-0.9624659454
H,-6.412107611,-1.6064525214,0.9591548476
C,-1.6353587168,2.1257304079,0.4773554745
C,-3.5434677455,3.0572958374,2.2781464237
C,-2.315091483,3.3081190283,0.2156526758
C,-1.9088762499,1.3981814489,1.6479019163
C,-2.8644359665,1.8672319111,2.5424705518
C,-3.2689099054,3.7786461874,1.1194331955
H,-2.0796210448,3.8495822563,-0.6955488796
H,-3.0621719316,1.2896262676,3.44000173
H,-3.7958687606,4.7041965417,0.911949029
H,-4.2875382686,3.416159717,2.9819246709
C,2.0138826473,1.5731302596,-1.5848870368
C,2.972145625,4.1668168571,-2.0840820339
C,3.3407241766,1.9262086591,-1.2720685445
C,1.1908621991,2.5338246761,-2.2018716475
C,1.6701560012,3.8158422219,-2.4424655548
C,3.8095659144,3.2124257944,-1.505486763
H,3.999789885,1.1762008837,-0.8431771611
H,0.1891633441,2.2660053873,-2.5156976521
H,1.0257360829,4.5449985208,-2.9241215606
H,4.8322999331,3.4682612773,-1.2463250554
H,3.3381680071,5.1707757746,-2.2746338931
C,2.87784342,-0.6632089729,1.5903243737
C,5.6335170027,-0.9583327835,2.0565776456
C,3.7067162825,0.4618234601,1.7607564758
C,3.4507323737,-1.9427276032,1.7140254825
C,4.8163053558,-2.0816621002,1.9362604337
C,5.0702444097,0.3157036063,1.9789309866
H,3.2659550801,1.4538174763,1.7074459816
H,2.8267893487,-2.830014361,1.6772556131
H,5.241400894,-3.0757175441,2.0326887853
H,5.6937093419,1.1967907858,2.094407798
H,6.6981968816,-1.0750410711,2.231472597

TS-*Z,Z*[1,2]^{DMF}(Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in DMF)
cydiimph2_ZZ_b2cat2_1-2_ts_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.1213922

Zero-point correction= 0.572434 (Hartree/Particle)
Thermal correction to Energy= 0.602974
Thermal correction to Enthalpy= 0.603918
Thermal correction to Gibbs Free Energy= 0.511365
Sum of electronic and ZPE= -1696.548958
Sum of electronic and thermal Energies= -1696.518418
Sum of electronic and thermal Enthalpies= -1696.517474
Sum of electronic and thermal Free Energies= -1696.610027

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.372	127.603	194.794

H,-1.1494743682,-1.7123332388,-3.1595658557
C,-0.7679632636,-2.1723399513,-2.2417631899
C,-1.0794595254,-4.0749755634,-0.5938092985
C,-0.4419088354,-1.8429378806,0.246534591
C,-1.288443888,-3.0759779538,0.5533238211
C,-0.9459907392,-1.208462985,-1.0732925066
C,-1.5131834193,-3.4758081767,-1.9355390029
H,-0.0206322428,-4.3601550713,-0.6436952828
H,0.5730486759,-2.2100346619,0.08898868
H,-2.3506906734,-2.8273808542,0.6013548474
H,-2.009464762,-1.0213466374,-0.9149901922
H,-2.5924210449,-3.2746252773,-1.9043893944
H,0.2985284144,-2.3680500789,-2.3868708722
H,-1.6495063174,-4.9858899832,-0.388127348
H,-0.9907879447,-3.5134046351,1.511286893
H,-1.3445453583,-4.1934889757,-2.7439992936
N,-0.270663269,-0.7088073189,1.2064974455
N,-0.2899658338,0.1090080039,-1.2259769638
C,-1.255064511,0.131058068,1.534903544
H,-0.9132963404,1.0952346982,1.8984803542
C,-1.0419452937,1.2007778938,-1.065444769
H,-0.4690526421,2.1060880457,-0.885048096
B,1.1006749986,-0.1508290501,1.0750128282
B,1.1575981616,0.1834683982,-0.957842167
O,1.9213775687,-0.9130560555,-1.4637637939
O,2.1625263358,-1.0837567172,1.2953236534
O,1.7319338136,1.4873777134,-1.0892287065

O,1.2517371697,1.1571494086,1.6180858321
C,3.2661109235,-1.1626032286,0.5038531622
C,5.5262886792,-1.4611231742,-1.1099125725
C,4.5144027428,-1.3715356285,1.0811561938
C,3.1498719598,-1.0959500902,-0.8949745133
C,4.2780497358,-1.2431101989,-1.6932009345
C,5.6434489434,-1.5216980919,0.2761306765
H,4.5807151568,-1.4183931035,2.1636817133
H,4.1576549723,-1.18833942,-2.7707108027
H,6.6120394748,-1.6855998038,0.7373621779
H,6.4017394681,-1.5778428343,-1.7403188547
C,2.3455879375,1.8622589651,1.2050139432
C,4.5312602314,3.3558898592,0.334516363
C,3.1989585275,2.4502882795,2.1302579774
C,2.5860489304,2.0166790445,-0.1721955156
C,3.6804346389,2.7621185094,-0.598001561
C,4.2911113533,3.2027820029,1.69706487
H,2.9885864599,2.3131929978,3.1863555368
H,3.8483456149,2.8682364393,-1.6651640724
H,4.9513471715,3.6613560434,2.4258922785
H,5.3811537453,3.9362348076,-0.0098989239
C,-2.669718151,-0.167479646,1.7744894747
C,-5.3893553042,-0.5561489321,2.3729403378
C,-3.6056466479,0.8631804562,1.5855142683
C,-3.1116786609,-1.3658970381,2.3593535309
C,-4.4594461635,-1.5590824097,2.644195934
C,-4.9533010436,0.6648148955,1.8594528392
H,-3.2631894491,1.8258621969,1.225292638
H,-2.3911279147,-2.1260644113,2.6367729507
H,-4.7804755403,-2.4909970091,3.0991051308
H,-5.6607874925,1.4693128635,1.682800364
H,-6.4407456964,-0.7132065573,2.5921799585
C,-2.4381699584,1.4262429064,-1.4201951547
C,-5.0957942222,2.1498497747,-2.0366500766
C,-2.9618807149,2.6823689142,-1.0507231472
C,-3.2686383772,0.5649151389,-2.163942703
C,-4.5817761836,0.923698463,-2.4527386993
C,-4.2702526652,3.0371204938,-1.3449287078
H,-2.3239141474,3.3756586979,-0.5080874278
H,-2.8909158409,-0.3702785923,-2.5609308617
H,-5.2018763144,0.2410389474,-3.025307563
H,-4.6461959119,4.0075741611,-1.036464768
H,-6.1209111327,2.4205501483,-2.2680032164

TS-*E*,*E*[1,1]^{benzene} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E*,*E*-diimine **1** complex in benzene)
cydiimph2_EE_b2cat2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1219456

Zero-point correction= 0.572217 (Hartree/Particle)
Thermal correction to Energy= 0.603081
Thermal correction to Enthalpy= 0.604025
Thermal correction to Gibbs Free Energy= 0.510510
Sum of electronic and ZPE= -1696.549728
Sum of electronic and thermal Energies= -1696.518864
Sum of electronic and thermal Enthalpies= -1696.517920
Sum of electronic and thermal Free Energies= -1696.611436

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.439	127.668	196.820

H,1.2182741198,4.4347142995,0.6335524827
C,1.2556056111,3.9028106858,-0.3220247966
C,0.9321056236,4.1544126684,-2.8476209141
C,0.2352982473,2.074691325,-1.7131833505
C,-0.1012612281,3.0158433639,-2.8625206452
C,0.1506559235,2.8551193508,-0.3815990149
C,1.0122952209,4.8714894333,-1.4915369885
H,1.9157957531,3.7314188078,-3.0866442728
H,1.2651860587,1.7309216471,-1.8449995779
H,-1.1156434191,3.419119679,-2.7477115815
H,-0.7982912599,3.4016067681,-0.3844115946
H,0.0735317331,5.4139600773,-1.3160062348
H,2.23412049,3.4248731146,-0.405340993
H,0.6982405164,4.8763962783,-3.6355651203
H,-0.0653296629,2.4742172086,-3.8121862074
H,1.8075712064,5.6220118363,-1.518749725
N,-0.5772089967,0.8476074153,-1.580333441
N,0.0478487811,1.8602390502,0.7170434946
C,-1.8623881098,1.011233983,-1.3398451204
H,-2.2426094096,2.0312359661,-1.3043076026
C,-1.1417633919,1.8424947665,1.2802818453
H,-1.7540083594,2.7198942401,1.0821811405
B,0.3191605596,-0.2648872582,-1.0038641628
B,1.0556627193,0.725422831,0.581170402
O,2.3849826952,1.1833082121,0.1983996005
O,1.2135795511,-0.1833579019,1.6885714464
O,1.4522664718,-0.6159234409,-1.8391064499

O,-0.2946999642,-1.4861975515,-0.5591372938
C,2.5541804696,-0.3499282327,1.8510882728
C,5.308363389,-0.3614098459,1.8182192235
C,3.2083309835,-1.1780833929,2.7394845156
C,3.2548153696,0.4657862493,0.9542869724
C,4.6344814355,0.4767896382,0.9162720956
C,4.6116422406,-1.1698752294,2.7097695403
H,2.6518985433,-1.8063486351,3.4259455699
H,5.1666507934,1.1092354266,0.2143445431
H,5.1589717459,-1.8102537946,3.3937243103
H,6.3934164327,-0.3778079871,1.8148783253
C,0.4536359417,-2.4986188017,-1.0800649558
C,2.235503048,-4.1797584848,-2.3303965757
C,0.2701592837,-3.8576449046,-0.9314869217
C,1.5023473554,-1.9714422239,-1.8443112787
C,2.4121271234,-2.7954216418,-2.4772340798
C,1.1887665814,-4.7004403846,-1.5763439243
H,-0.5511647462,-4.2454838914,-0.3387348203
H,3.2258735683,-2.3800277951,-3.0609638838
H,1.0790785295,-5.7757427291,-1.48102292
H,2.9328957179,-4.8548293767,-2.8157598757
C,-2.8326591392,-0.0687241209,-1.2149897664
C,-4.7472560596,-2.0890641236,-0.9355637894
C,-3.9601288959,0.1242387325,-0.4020816271
C,-2.6898039218,-1.2820304209,-1.9052555864
C,-3.6420501665,-2.2827634457,-1.7630699242
C,-4.90703934,-0.8810237944,-0.2582089348
H,-4.0730394071,1.0604945825,0.1389562798
H,-1.8413563701,-1.4238530382,-2.5667383966
H,-3.5220066206,-3.2164096167,-2.3032814339
H,-5.7651822283,-0.7253776356,0.3874578518
H,-5.4866124563,-2.8759028185,-0.8240265968
C,-1.7600886789,0.8986570312,2.2088072232
C,-3.2585290477,-0.7452926795,3.9115808544
C,-1.5966258321,-0.4943615149,2.1689595106
C,-2.7129997465,1.4472543348,3.0864777853
C,-3.4431263073,0.6363468534,3.9429845038
C,-2.3457074675,-1.3009295959,3.0189764618
H,-0.9138237835,-0.9494602401,1.4645361103
H,-2.8675135321,2.5233050213,3.0979012191
H,-4.1603262555,1.0785331586,4.6268433656
H,-2.2189536251,-2.3776067875,2.97181918
H,-3.8350064051,-1.3863457004,4.5710882522

TS-*E*,*Z*[1,1]^{benzene} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
cydiimph2_EZ_b2cat2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1115261

Zero-point correction= 0.572532 (Hartree/Particle)
Thermal correction to Energy= 0.603424
Thermal correction to Enthalpy= 0.604368
Thermal correction to Gibbs Free Energy= 0.510205
Sum of electronic and ZPE= -1696.538994
Sum of electronic and thermal Energies= -1696.508102
Sum of electronic and thermal Enthalpies= -1696.507158
Sum of electronic and thermal Free Energies= -1696.601321

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.654	127.549	198.182

H,-1.2409440466,-1.9322430581,-3.4029266878
C,-1.0435809537,-2.3879834053,-2.4276876201
C,-1.7960393989,-4.1815569238,-0.7880789397
C,-1.0645097233,-1.9870087995,0.0699011616
C,-2.0583955392,-3.1239374453,0.2949153599
C,-1.31025633,-1.3665391649,-1.3258892254
C,-1.9598162132,-3.5974550838,-2.1964131137
H,-0.7787341201,-4.5759062258,-0.6716990846
H,-0.0683709157,-2.4392454865,0.0727767103
H,-3.089375749,-2.7738073167,0.2038979295
H,-2.3726346723,-1.1002116472,-1.3630229639
H,-3.0059417384,-3.2941667108,-2.3373720783
H,0.004846267,-2.6915811008,-2.4044974131
H,-2.4828771685,-5.0216927447,-0.6492082114
H,-1.9265480188,-3.5490699741,1.2947081448
H,-1.748952704,-4.3637757316,-2.9479820834
N,-0.9410838678,-0.8435970983,1.0149928036
N,-0.5504795413,-0.0887400879,-1.4134612428
C,-1.8741864041,0.0664182328,1.2030025209
H,-1.5069793839,0.9901764643,1.6484236231
C,-1.3358401902,0.9707468375,-1.4025705773
H,-2.3834305722,0.7624134514,-1.6005939594
B,0.5143856886,-0.393279359,1.0334359589
B,0.8799508534,-0.2112046802,-0.9135686132
O,1.5485274582,-1.4366698062,-1.3333233259
O,1.7978695195,0.878397997,-1.1411971643
O,1.4800684557,-1.3661307803,1.5114380562

O,0.7453164628,0.8476606008,1.741478886
C,2.9714681169,0.3088108058,-1.5271056792
C,5.1024639353,-1.26653076,-2.2788000409
C,4.1746776948,0.9303644495,-1.7896256668
C,2.8223597607,-1.0791921212,-1.6350729982
C,3.8747794427,-1.8907459779,-2.0077668879
C,5.2490629576,0.1122765247,-2.1728794014
H,4.2758776664,2.0060128939,-1.6984525463
H,3.7489734113,-2.9651392644,-2.0839373307
H,6.2108421679,0.5675248734,-2.3855027858
H,5.9511754156,-1.8749740077,-2.5739812528
C,1.8612839127,0.6389763935,2.4969327027
C,4.0936103277,-0.2392580158,3.8461417283
C,2.5248150056,1.5397585781,3.3032875806
C,2.2956492353,-0.6856551345,2.3556853916
C,3.4142044833,-1.1479587867,3.0205225451
C,3.6599546621,1.0747072813,3.9855067914
H,2.1756761326,2.5619782081,3.4001407383
H,3.7469536057,-2.1727385934,2.8998654599
H,4.2074434839,1.7557266425,4.6287844418
H,4.9763981478,-0.5717144845,4.3825993597
C,-3.3408241215,-0.083623602,1.1241955942
C,-6.1414041642,-0.2132016609,1.1783505762
C,-3.9941593041,-1.1381922305,1.7761232088
C,-4.1153228091,0.9382927077,0.5539210314
C,-5.5026044992,0.8663896307,0.569816038
C,-5.3841062836,-1.2070898015,1.7917129532
H,-3.4072390308,-1.8870590742,2.2975901866
H,-3.6187487629,1.7911468655,0.0980355479
H,-6.0871437383,1.6579816032,0.1122997618
H,-5.8742629217,-2.0312378882,2.2999016958
H,-7.2251749303,-0.2670574682,1.1923790781
C,-1.0191170246,2.4009386828,-1.3427712129
C,-0.7246125585,5.1885503712,-1.2574235316
C,-1.8846739225,3.2416429824,-2.0657987107
C,-0.0242309167,2.9831493261,-0.5421759179
C,0.1140705275,4.3660929616,-0.5080918698
C,-1.7304987707,4.6210854274,-2.0365587133
H,-2.6745835207,2.7989903627,-2.6675485431
H,0.6205406404,2.3632200824,0.0659281774
H,0.8839777067,4.8044686834,0.11884054
H,-2.3974336144,5.2515273475,-2.6156814994
H,-0.6031826309,6.2665954828,-1.2243222506

TS-*Z,E*[1,1]^{benzene} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,E*-diimine **1** complex in benzene)
cydiimph2_ZE_b2cat2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.125183

Zero-point correction= 0.571907 (Hartree/Particle)
Thermal correction to Energy= 0.602875
Thermal correction to Enthalpy= 0.603819
Thermal correction to Gibbs Free Energy= 0.509330
Sum of electronic and ZPE= -1696.553276
Sum of electronic and thermal Energies= -1696.522308
Sum of electronic and thermal Enthalpies= -1696.521364
Sum of electronic and thermal Free Energies= -1696.615854

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.310	127.791	198.870

H,-1.3985721388,-4.0816341597,0.4281810754
C,-0.9753757766,-3.4649108022,1.2281612946
C,-1.1678249521,-2.8366161568,3.6892429815
C,-0.5439571969,-1.1104193818,2.0224594611
C,-1.294790699,-1.3496601014,3.3272736699
C,-1.1647242787,-1.9857000415,0.9096346041
C,-1.669911367,-3.7533178856,2.5660589718
H,-0.1129910622,-3.0614186611,3.8914901194
H,0.499207944,-1.4052675129,2.1667469217
H,-2.3533760333,-1.0818269118,3.2215832725
H,-2.2347187681,-1.7676966958,0.8938849287
H,-2.752687274,-3.612050499,2.4431508002
H,0.094777018,-3.6878933471,1.2855173121
H,-1.7184536051,-3.041040392,4.6121467506
H,-0.8730680827,-0.7190790913,4.1155864477
H,-1.5179808918,-4.8005938114,2.8429561758
N,-0.5023665798,0.2799075499,1.5290466795
N,-0.6030728309,-1.5313736621,-0.3763231642
C,-1.6709328859,0.8481516057,1.2837478854
H,-2.5651161746,0.2423663666,1.4262359401
C,-1.3642044791,-0.990058594,-1.2980939936
H,-0.8128984294,-0.4930562383,-2.094119986
B,0.7376307434,0.5294299151,0.669287442
B,0.8645714517,-1.1743928689,-0.3287961289
O,1.729642797,-2.1136385964,0.3591538018
O,1.4894050295,-0.820977504,-1.5781889353
O,2.0283497294,0.6614378456,1.3052302505

O,0.6223014105,1.5400234055,-0.3471008268
C,2.751246682,-1.327599727,-1.5035806056
C,5.1557739905,-2.5403657109,-0.9258568677
C,3.7973425974,-1.1406670534,-2.3829116717
C,2.8951419291,-2.0991480774,-0.3425475523
C,4.0888537296,-2.7175090362,-0.0312344737
C,5.0138353718,-1.7686862638,-2.074136449
H,3.6755304671,-0.5248814711,-3.2669012549
H,4.1897558641,-3.3094310735,0.8717080293
H,5.8588905881,-1.6418273281,-2.7428532513
H,6.1094084326,-3.0115628125,-0.7109340506
C,1.8726977419,2.0589184321,-0.4726008781
C,4.5197435098,2.811933435,-0.3479464603
C,2.3281736384,2.9780698672,-1.3958412052
C,2.7169405186,1.5269341284,0.5134362945
C,4.0488657253,1.8815612001,0.5907005625
C,3.6789235123,3.3498844395,-1.3172942669
H,1.6623940385,3.3838358887,-2.1494381765
H,4.6958130204,1.4485920593,1.3453186961
H,4.073088811,4.0663523229,-2.0307322119
H,5.5621771361,3.111843351,-0.317013498
C,-1.8978305824,2.2316878252,0.9250974395
C,-2.4825391563,4.8793284687,0.223550683
C,-0.9457273936,3.2477280461,1.1239208883
C,-3.1586562152,2.5741699772,0.4045929782
C,-3.4443684375,3.8850669024,0.0481873216
C,-1.2401988996,4.5568986673,0.7709786204
H,0.009866658,3.0095846625,1.5789518269
H,-3.9060741357,1.7956891896,0.2727552724
H,-4.41794993,4.1337724445,-0.3621365604
H,-0.4981808284,5.3328440187,0.9292278525
H,-2.7048561222,5.905555464,-0.0511157146
C,-2.8216126273,-0.9933063571,-1.4202654965
C,-5.5954606248,-0.8739749278,-1.827284635
C,-3.4065801211,0.1101855072,-2.0662303052
C,-3.6488940114,-2.0595748776,-1.0257136587
C,-5.0230185299,-1.9915207349,-1.2221819181
C,-4.7806274731,0.1726613011,-2.2574296274
H,-2.7707253994,0.9285677595,-2.3930246396
H,-3.2124771903,-2.95812311,-0.6005164507
H,-5.6484147523,-2.8239588018,-0.9161209358
H,-5.216220968,1.0396383029,-2.7438155994
H,-6.6687219717,-0.8279955019,-1.9801420014

TS-*Z,Z*[1,1]^{benzene} (Reductive coupling transition state from dicoordinate 1,1-B_2cat_2-*Z,Z*-diimine **1** complex in benzene)
cydiimph2_ZZ_b2cat2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1123544

Zero-point correction= 0.572514 (Hartree/Particle)
Thermal correction to Energy= 0.603395
Thermal correction to Enthalpy= 0.604339
Thermal correction to Gibbs Free Energy= 0.510977
Sum of electronic and ZPE= -1696.539841
Sum of electronic and thermal Energies= -1696.508959
Sum of electronic and thermal Enthalpies= -1696.508015
Sum of electronic and thermal Free Energies= -1696.601377

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.636	127.733	196.497

H,-1.2109770647,-3.1753641051,1.6970470036
C,-0.8568364144,-2.2524079318,2.1688147651
C,-1.2236804236,-0.6127945746,4.0636669013
C,-0.5592887704,0.2454391005,1.8403240475
C,-1.4279675287,0.5324071542,3.0624978223
C,-1.0016133024,-1.0878039437,1.19175344
C,-1.6379847996,-1.9548151231,3.4522206166
H,-0.169385581,-0.6565051352,4.3653087445
H,0.4676186153,0.1414591205,2.2027115292
H,-2.4862219716,0.5736898359,2.7974438678
H,-2.0497678052,-0.9453246455,0.9161052009
H,-2.7130250819,-1.9280343542,3.2275794033
H,0.2065749566,-2.3876001483,2.391891688
H,-1.8080192446,-0.4142764034,4.966933607
H,-1.1471258276,1.4938513083,3.503508442
H,-1.4839858678,-2.7647814584,4.1712005122
N,-0.4548649602,1.2188412817,0.7154648823
N,-0.2302623825,-1.2805811421,-0.0549720169
C,-1.4669801759,1.5726999818,-0.0538442717
H,-1.1719920557,2.0026921216,-1.0077453169
C,-0.8272076062,-1.380457458,-1.2318003759
H,-0.1384526093,-1.3269908813,-2.0716670859
B,0.908540555,1.1235738934,0.0864008046
B,1.1974637456,-0.8682385985,0.0073533071
O,1.9594608761,-1.2701495687,1.1708421428
O,2.0173790669,-1.051794346,-1.1608276417
O,2.0703719241,1.5446078839,0.833950389

O,1.0089846419,1.639411524,-1.2520758913
C,3.2723289151,-1.2729375217,-0.6763952675
C,5.5948833753,-1.6878900469,0.7432996952
C,4.4556115167,-1.346723548,-1.3810105682
C,3.237290854,-1.3950569973,0.7195642232
C,4.3871553183,-1.6031913633,1.4534228059
C,5.6286304052,-1.5618401771,-0.641432026
H,4.4679990923,-1.2278931274,-2.458556859
H,4.3493927739,-1.6907291429,2.5335574576
H,6.5785343973,-1.6219510249,-1.1624263231
H,6.518513281,-1.8501151982,1.2894415986
C,2.3000836255,2.0616160913,-1.3622313258
C,4.9449588386,2.7855234769,-1.1038785695
C,2.9671167806,2.486894761,-2.4921856046
C,2.9345774235,2.0007684267,-0.1130757149
C,4.2609115196,2.3506044381,0.0409317406
C,4.3130752799,2.8544524706,-2.3414665729
H,2.4659087892,2.5247330637,-3.4529950094
H,4.7464235338,2.2744053467,1.007326039
H,4.8700542448,3.1909622605,-3.2098479722
H,5.9898151048,3.0660855086,-1.0197899502
C,-2.9005246568,1.6269417735,0.2812824927
C,-5.6428675163,1.9388311751,0.7777354656
C,-3.3480921963,2.331454734,1.4103866121
C,-3.8504386279,1.1324761353,-0.6234851598
C,-5.21056827,1.2735516369,-0.3662937663
C,-4.7072389558,2.4800234081,1.6582121923
H,-2.6210289959,2.7869176551,2.0750012638
H,-3.5217918517,0.6311682606,-1.5278782299
H,-5.9310335981,0.8661984165,-1.0682938909
H,-5.0362716345,3.032849582,2.5322818043
H,-6.7041450653,2.0550695498,0.97304409
C,-2.2140551399,-1.6432694981,-1.5777921066
C,-4.8438857918,-2.06815887,-2.5064418022
C,-2.584350084,-1.325744938,-2.9026749633
C,-3.1849969032,-2.2441077388,-0.7527153011
C,-4.4830763975,-2.4373439454,-1.2133696198
C,-3.8784954485,-1.5246415584,-3.3566184077
H,-1.8386698075,-0.8929883205,-3.5640022489
H,-2.9251151883,-2.6010386275,0.2371680874
H,-5.2148379314,-2.8966889439,-0.5563404808
H,-4.1374959396,-1.2558272774,-4.3757628725
H,-5.8586479469,-2.2240207034,-2.8575264721

TS-*E*,*E*[1,2]^{benzene} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E*,*E*-diimine **1** complex in benzene)
cydiimph2_EE_b2cat2_1-2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1302657

Zero-point correction= 0.572234 (Hartree/Particle)
Thermal correction to Energy= 0.602816
Thermal correction to Enthalpy= 0.603760
Thermal correction to Gibbs Free Energy= 0.511665
Sum of electronic and ZPE= -1696.558032
Sum of electronic and thermal Energies= -1696.527450
Sum of electronic and thermal Enthalpies= -1696.526506
Sum of electronic and thermal Free Energies= -1696.618600

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.273	127.884	193.830

H,1.9675566224,2.5204032284,3.2933576883
C,2.2083089844,2.6343512658,2.231802932
C,2.7841356585,4.3307110808,0.4091002418
C,1.3269038668,2.4070851761,-0.1234730294
C,1.5906808889,3.8726831971,-0.4451229889
C,1.000192137,2.2635797576,1.379430576
C,2.5606505021,4.0958912684,1.9100868994
H,3.6762165085,3.7775671208,0.088914784
H,2.2402819768,1.8505407996,-0.3414823081
H,0.7119510123,4.4893061271,-0.2183284242
H,0.2196577116,2.995041635,1.6181486255
H,1.7456089064,4.7451861974,2.2573227183
H,3.0475558944,1.9738710675,2.0020383138
H,2.9860816889,5.390132358,0.2252625082
H,1.8089771406,3.9882125344,-1.5108500256
H,3.4550124343,4.3896049088,2.4674177279
N,0.2488034513,1.7182334868,-0.8533266665
N,0.3799758652,0.9322927741,1.5917552848
C,-0.9719282347,2.2327661108,-0.6969630561
H,-1.0426881422,3.1495890848,-0.1172042156
C,-0.9275143633,0.9770192929,1.826779292
H,-1.3804365577,1.9574869288,1.9218500311
B,0.5031927073,0.243404992,-0.9662315123
B,1.1062448156,-0.2136405256,0.9669882436
O,2.518406553,-0.0529252235,0.9757845865
O,1.6458154156,-0.1528593268,-1.7139315196
O,0.6972721461,-1.5527935182,1.1256624381

O,-0.6884903579,-0.5001230618,-1.0809598467
C,2.7484506338,-0.8262714638,-1.2920976704
C,5.1139421409,-2.1256589635,-0.5566850111
C,3.4849275935,-1.5388290768,-2.2350185648
C,3.20210041,-0.7737683954,0.0370151234
C,4.3784678941,-1.4230170532,0.393590347
C,4.6623630507,-2.1859047245,-1.8720913032
H,3.1139293517,-1.5646009845,-3.2542765933
H,4.6982602622,-1.3609553021,1.4287601887
H,5.2239075739,-2.7356938665,-2.6202023853
H,6.0309098767,-2.6273467989,-0.2661343712
C,-0.7632722411,-1.8214962571,-0.7750540973
C,-1.0489228049,-4.5050232577,-0.083373681
C,-1.5799925528,-2.6550246726,-1.5313434989
C,-0.0898285993,-2.3299521579,0.3432100722
C,-0.235473716,-3.6728227111,0.6793969694
C,-1.7260095506,-3.9957657103,-1.1885620917
H,-2.0999259046,-2.2211373788,-2.379500197
H,0.296771108,-4.0393989423,1.5511180973
H,-2.3656820122,-4.6378452897,-1.7849426496
H,-1.1538055746,-5.5496940577,0.1905625445
C,-2.1564990432,1.9011262373,-1.4723228062
C,-4.506111976,1.4433565403,-2.941952444
C,-3.3952258313,2.4000052862,-1.0305191428
C,-2.1144163196,1.195537939,-2.6866217814
C,-3.2809064012,0.9709153682,-3.4081584369
C,-4.5581237802,2.166719013,-1.7501860752
H,-3.43544067,2.9676460729,-0.1032748057
H,-1.1627853176,0.8503790547,-3.0742368734
H,-3.2308518093,0.4287455243,-4.3473183284
H,-5.5051038579,2.5521855287,-1.3859256937
H,-5.4128035688,1.2618217555,-3.5099020691
C,-1.7551615774,-0.190853369,2.1350259209
C,-3.3977778994,-2.3775958766,2.7204161309
C,-3.0334211772,-0.2899882315,1.5693948761
C,-1.3184923871,-1.1888343445,3.0184973906
C,-2.1376755115,-2.2733558874,3.3064297319
C,-3.8439846015,-1.3821799801,1.8537244855
H,-3.3693747325,0.473725926,0.8734636356
H,-0.3366195663,-1.1066766255,3.4725080603
H,-1.7893204271,-3.0427012596,3.9883900727
H,-4.8216903543,-1.4611213375,1.3894055641
H,-4.0297373623,-3.2324810074,2.9387150621

TS-*E*,*Z*[1,2]^{benzene} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*E*,*Z*-diimine **1** complex in benzene)
cydiimph2_EZ_b2cat2_1-2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1222623

Zero-point correction= 0.572688 (Hartree/Particle)
Thermal correction to Energy= 0.603067
Thermal correction to Enthalpy= 0.604011
Thermal correction to Gibbs Free Energy= 0.512897
Sum of electronic and ZPE= -1696.549575
Sum of electronic and thermal Energies= -1696.519195
Sum of electronic and thermal Enthalpies= -1696.518251
Sum of electronic and thermal Free Energies= -1696.609365

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.430	127.575	191.765

H,1.4579277108,-1.6016226126,3.4842285387
C,1.4175724619,-2.1223347188,2.5223054833
C,2.6511366699,-3.7354602427,0.9893327139
C,1.4648838764,-1.8082220419,0.0076460688
C,2.710013425,-2.6818179414,-0.1277779316
C,1.4870157225,-1.103809345,1.3882300174
C,2.6027554435,-3.0867889275,2.3779503866
H,1.762521741,-4.3639224203,0.8488449492
H,0.6118684681,-2.4885376189,-0.0170639548
H,3.6258175504,-2.0965439137,-0.0150250282
H,2.4542922628,-0.5925616493,1.4640147643
H,3.5397220316,-2.5399810159,2.5491991854
H,0.4719861044,-2.6660000204,2.4736507683
H,3.5224041659,-4.3929785766,0.9144824659
H,2.7303624176,-3.1620806195,-1.1108431745
H,2.5415943183,-3.8586339785,3.1508144102
N,1.1119489229,-0.7433085413,-0.9666310446
N,0.4539999528,-0.0382048834,1.3851207234
C,1.8451207442,0.3507365711,-1.1156344287
H,1.3209124307,1.17432482,-1.5918291319
C,0.9658445011,1.1770580787,1.2609526426
H,2.0413784893,1.2661288645,1.3598809413
B,-0.3896604739,-0.6024286165,-1.0385741871
B,-0.9019900898,-0.454900739,0.8654040431
O,-1.2611442991,-1.7677630354,1.3096035805
O,-1.0665057841,-1.7794960577,-1.4981267607
O,-1.9920650579,0.4556800203,0.90128751

O,-0.7367923715,0.6377039525,-1.6502141931
C,-2.0881650417,-2.4033842895,-0.8564887135
C,-4.1313776821,-3.8438527251,0.3968006493
C,-3.0204463372,-3.1083239483,-1.6131005245
C,-2.1871236288,-2.4169994665,0.5458538702
C,-3.2072626485,-3.1346982078,1.1601005729
C,-4.0384619354,-3.8267626803,-0.99190655
H,-2.9209331776,-3.082608664,-2.6933574752
H,-3.254192669,-3.1237309262,2.244336719
H,-4.756590092,-4.3711738114,-1.5964124563
H,-4.9221135517,-4.4011141115,0.8881427823
C,-1.8901279067,1.2967385541,-1.3689321463
C,-4.194964971,2.7768884447,-0.8257545072
C,-2.4495294525,2.1162475374,-2.3454039571
C,-2.4897677885,1.2176276482,-0.1016557205
C,-3.6407026301,1.9598801891,0.1542942784
C,-3.5961461438,2.85828307,-2.079820545
H,-1.957905142,2.1567601564,-3.3121562582
H,-4.081200509,1.8792662342,1.142942426
H,-4.0190349912,3.4919013061,-2.8524722577
H,-5.0916450577,3.3470984915,-0.6060318889
C,3.3202572811,0.4486715611,-1.0705138592
C,6.1055337976,0.7669542584,-1.2251625519
C,3.9499167418,1.5518227173,-0.4768950171
C,4.1076142905,-0.4636700897,-1.7879070407
C,5.4882087549,-0.3105386572,-1.8556119546
C,5.3306441209,1.7032011796,-0.5448049111
H,3.3536710568,2.3001398393,0.0375371073
H,3.6244775029,-1.2817151451,-2.3125996106
H,6.0801392646,-1.0279618992,-2.4148479887
H,5.8006060484,2.5574363244,-0.0683380877
H,7.1827766065,0.8861623641,-1.2786828601
C,0.1730991126,2.4155962525,1.2610764757
C,-1.2758934929,4.8074637126,1.2726470356
C,-0.8299259905,2.6309703773,2.2156589886
C,0.4543827318,3.4206569032,0.3278417636
C,-0.2717380058,4.6066696325,0.3293788236
C,-1.5474577317,3.8207012445,2.2187293949
H,-1.0422329511,1.8578789194,2.9465024098
H,1.2240590105,3.2548882775,-0.4216114616
H,-0.0609030825,5.3682864016,-0.4141905389
H,-2.3267208528,3.9756469761,2.9582444387
H,-1.8480515916,5.7296321077,1.269365269

TS-*Z*,*E*[1,2]^{benzene} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z*,*E*-diimine **1** complex in benzene)
cydiimph2_ZE_b2cat2_1-2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1318243

Zero-point correction= 0.572967 (Hartree/Particle)
Thermal correction to Energy= 0.603430
Thermal correction to Enthalpy= 0.604375
Thermal correction to Gibbs Free Energy= 0.512733
Sum of electronic and ZPE= -1696.558857
Sum of electronic and thermal Energies= -1696.528394
Sum of electronic and thermal Enthalpies= -1696.527450
Sum of electronic and thermal Free Energies= -1696.619091

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.658	127.452	192.875

H,0.8380990415,-3.995844901,1.2389279153
C,0.459186757,-3.6761530979,0.2623884669
C,0.6424748352,-4.0532795337,-2.257127898
C,0.2755125644,-1.774106133,-1.3738300155
C,0.9505957174,-2.5649472323,-2.4872652555
C,0.8516490743,-2.2299894275,-0.0124457276
C,1.0604892886,-4.5350985682,-0.8605025479
H,-0.4365588706,-4.2095236805,-2.38130696
H,-0.7913653092,-2.0012454389,-1.3991687755
H,2.0356507119,-2.4007772265,-2.4811273219
H,1.9385110577,-2.1921261509,-0.105513703
H,2.1560593285,-4.5032627594,-0.7824616044
H,-0.6310590518,-3.7635130299,0.2860275819
H,1.1396577987,-4.6570378841,-3.0220909568
H,0.5714886576,-2.2371096896,-3.4596817925
H,0.7657847121,-5.579924132,-0.725706893
N,0.3724027893,-0.3020401366,-1.4223224972
N,0.474130727,-1.2079876447,0.9844526188
C,1.6015660026,0.1991863415,-1.3695440629
H,2.4180142666,-0.5174669534,-1.3130976655
C,1.4187636294,-0.4156830962,1.4687267379
H,1.0406425666,0.4838176255,1.947139216
B,-0.8474581714,0.3383736981,-0.825247754
B,-0.9300263061,-0.7106052425,0.933014436
O,-1.8967402813,-1.733493052,0.6943328249
O,-2.0725097215,0.0122813,-1.4829516645
O,-1.2401538741,0.2571367266,1.9332485088

O,-0.6630401596,1.6662960833,-0.3611219107
C,-3.1933203119,-0.4183693884,-0.8430128581
C,-5.5252814684,-1.3878502562,0.3509764927
C,-4.4399185999,-0.018158216,-1.3123465469
C,-3.1155248487,-1.3091424715,0.241021399
C,-4.2794892565,-1.785484923,0.8316716523
C,-5.6037723008,-0.5017418297,-0.7191475296
H,-4.4722849029,0.6729408601,-2.1482132953
H,-4.183855844,-2.4712763774,1.6672788358
H,-6.5699074536,-0.1815568399,-1.0952450612
H,-6.4285330834,-1.7664072724,0.8178372635
C,-1.5967709469,2.1524407413,0.5084902088
C,-3.4244809888,3.1537535697,2.3525274508
C,-2.2169490553,3.3725326678,0.2764601242
C,-1.8898451805,1.4234040379,1.6718652658
C,-2.8054322094,1.9274296004,2.5877898797
C,-3.1298256747,3.8776965415,1.2012259303
H,-1.9628743135,3.9137945672,-0.6293361276
H,-3.0174255004,1.3437946787,3.4774768939
H,-3.6102385106,4.8327786642,1.0165358119
H,-4.1384752947,3.5397247977,3.0726972252
C,1.9995567475,1.5749852933,-1.6009361233
C,2.9557447395,4.1670263012,-2.094224991
C,3.3281086618,1.9249061712,-1.2948732798
C,1.1715831272,2.5389011788,-2.204371495
C,1.6508098451,3.8201568293,-2.4422864049
C,3.7964922222,3.2106214464,-1.5261645749
H,3.9880216452,1.1733049925,-0.8695265472
H,0.1665414588,2.2719326315,-2.5068498611
H,1.0030813302,4.5530774397,-2.9130510515
H,4.8211621989,3.4649904997,-1.2738287917
H,3.3213697373,5.1711815795,-2.2835839564
C,2.8500876156,-0.6612117797,1.615697821
C,5.6183151182,-0.9282219987,2.0221536266
C,3.67147347,0.4718704443,1.7654551842
C,3.439956784,-1.9336046883,1.72893505
C,4.8107663002,-2.0593533504,1.9211176835
C,5.0401030434,0.3390908683,1.9546281042
H,3.2205842742,1.4591803443,1.7129089055
H,2.8208477845,-2.824958525,1.7110266298
H,5.2480029481,-3.048571286,2.0114923659
H,5.6566976726,1.2266980772,2.0548837754
H,6.6873021496,-1.0334781555,2.1753027558

TS-*Z,Z*[1,2]^{benzene} (Reductive coupling transition state from dicoordinate 1,2-B_2cat_2-*Z,Z*-diimine **1** complex in benzene)
cydiimph2_ZZ_b2cat2_1-2_ts_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.1195834

Zero-point correction= 0.573052 (Hartree/Particle)
Thermal correction to Energy= 0.603520
Thermal correction to Enthalpy= 0.604465
Thermal correction to Gibbs Free Energy= 0.512783
Sum of electronic and ZPE= -1696.546531
Sum of electronic and thermal Energies= -1696.516063
Sum of electronic and thermal Enthalpies= -1696.515119
Sum of electronic and thermal Free Energies= -1696.606800

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	378.715	127.525	192.960

H,-1.1908543106,-1.6593221126,-3.171204392
C,-0.8111565808,-2.126069503,-2.2557283942
C,-1.1429527619,-4.0187196919,-0.5997753247
C,-0.4516297409,-1.7971371563,0.2323173738
C,-1.3118198546,-3.0176458757,0.5528201638
C,-0.9492552511,-1.1558671797,-1.0871940491
C,-1.5824749774,-3.41148423,-1.9362867208
H,-0.0915670901,-4.3265240936,-0.666506338
H,0.5609307084,-2.1720243683,0.0786229227
H,-2.3686645508,-2.7541902574,0.6366587193
H,-2.0048774047,-0.9321118925,-0.917487668
H,-2.6572945891,-3.1883468517,-1.8903587105
H,0.2493580105,-2.3427835093,-2.4146871603
H,-1.727006072,-4.9189638941,-0.3867064852
H,-0.9944326842,-3.4632934617,1.5005119838
H,-1.4432922272,-4.1349332536,-2.7450493308
N,-0.2809546528,-0.6577873624,1.181952924
N,-0.2544740957,0.1389852498,-1.2579389296
C,-1.282204542,0.1506072807,1.5139342678
H,-0.9746244454,1.1276634585,1.8745372854
C,-0.9616848997,1.2631495274,-1.1499424098
H,-0.345549171,2.1466678308,-1.0098321214
B,1.0914848352,-0.0896002355,1.0442116467
B,1.1982033912,0.174736094,-0.983973671
O,1.9187242965,-0.9625871452,-1.4552162772
O,2.1473115688,-1.010648712,1.315712617
O,1.814159003,1.4513687004,-1.1481443355

O,1.202211103,1.2341674106,1.5489634586
C,3.2452998108,-1.1782225668,0.5296522512
C,5.4893197808,-1.6708583911,-1.0555251139
C,4.4792235098,-1.4224326807,1.1222483577
C,3.1364847017,-1.1751688655,-0.8699691406
C,4.2567633048,-1.4183101666,-1.6543842351
C,5.5995996193,-1.6689491667,0.331850891
H,4.5366938622,-1.4165887995,2.2057418509
H,4.1383896029,-1.4081211959,-2.7330442976
H,6.5577282063,-1.8578143106,0.8048135818
H,6.3596167994,-1.8616065516,-1.6746635077
C,2.3018889266,1.9441073737,1.1557490304
C,4.492757555,3.4469993407,0.3249484189
C,3.0925110132,2.5958315706,2.0928497196
C,2.6081312716,2.0391461742,-0.212125684
C,3.7053504094,2.7900280359,-0.6183683974
C,4.1866932419,3.3535363697,1.6791192049
H,2.8293203853,2.5004117781,3.1412578207
H,3.9235342872,2.8451265154,-1.6797386202
H,4.7991216499,3.8619188623,2.4163545876
H,5.3470653395,4.0298142043,-0.0035002993
C,-2.6773511052,-0.2503404858,1.7641565936
C,-5.3187212844,-0.9113921205,2.4488822718
C,-3.7436807212,0.5743095706,1.3808739417
C,-2.9547223602,-1.3822078063,2.5485956647
C,-4.2627580833,-1.7119659999,2.8814790438
C,-5.0531028341,0.2364200861,1.7069113159
H,-3.546954725,1.4809316466,0.8214616327
H,-2.130986648,-1.9844297313,2.9179562009
H,-4.4566993044,-2.5878925201,3.4924260959
H,-5.8654227106,0.8787222913,1.3817848625
H,-6.3403955192,-1.1703594501,2.707872088
C,-2.3554568777,1.5387101072,-1.4673504144
C,-5.0097350252,2.3487625859,-1.9825973573
C,-2.8129942471,2.8262633676,-1.1130724595
C,-3.2512101826,0.6931583671,-2.1489592667
C,-4.5620664733,1.0943929746,-2.3864856625
C,-4.1181623992,3.2223964436,-1.3572634952
H,-2.1254550259,3.5072974067,-0.6182381054
H,-2.9250295686,-0.2660185416,-2.5337260075
H,-5.234153599,0.4209470761,-2.9088801282
H,-4.4424048263,4.2151983061,-1.0618290446
H,-6.0333187715,2.6533201307,-2.1739972339

P-*E*,*E*[1,1]^{MeOH} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,1]^{MeOH}** and **TS-*Z*,*Z*[1,1]^{MeOH}** in MeOH)
cis-diph-tetrahydroquinoxaline_1-1-dieq_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2419426

Zero-point correction= 0.575765 (Hartree/Particle)
Thermal correction to Energy= 0.606691
Thermal correction to Enthalpy= 0.607635
Thermal correction to Gibbs Free Energy= 0.511105
Sum of electronic and ZPE= -1696.666178
Sum of electronic and thermal Energies= -1696.635252
Sum of electronic and thermal Enthalpies= -1696.634308
Sum of electronic and thermal Free Energies= -1696.730838

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.704	126.238	203.165

C,1.7938723875,-0.4175576646,-0.703202217
C,3.3293377535,-1.8500711783,-2.0867675304
C,0.9018312123,-2.4773835095,-1.8581902212
C,2.3295291213,-2.9992460853,-2.0155627109
C,0.762646908,-1.5576692576,-0.6427906861
C,3.2109479874,-0.9703315051,-0.8448360912
H,3.1336854087,-1.2484039147,-2.9841938795
H,0.6062041375,-1.9215662271,-2.7580362827
H,2.5778424382,-3.6406696072,-1.159675807
H,1.0014995335,-2.1389371245,0.2662824927
H,3.4632747805,-1.5608499828,0.0443655332
H,1.5789584385,0.1743431087,-1.6055373377
H,4.3515290317,-2.2320876429,-2.1722218601
H,0.2159376643,-3.3230558416,-1.7616527726
H,2.3905057234,-3.6246361833,-2.9118453574
H,3.9175926996,-0.1373138801,-0.894234602
N,-0.6147984047,-1.0269868151,-0.5029848855
N,1.6341844393,0.4559517589,0.4622268883
C,0.2858428326,1.0304777953,0.576694129
C,-0.7600058788,-0.1095242198,0.6346540635
H,-0.53380105,-0.6497994363,1.5687108537
H,0.2219013389,1.509565418,1.5561452595
C,-2.1409064747,0.507246348,0.7806771626
C,-4.6202680678,1.7653077941,1.1716192806
C,-2.5727401821,0.8512061683,2.0631973321
C,-2.9678963082,0.8041681207,-0.3079359313
C,-4.2003996309,1.4215466504,-0.1124253224

C,-3.8007477839,1.47964447,2.2604995625
H,-1.9408057204,0.6180329354,2.9171694794
H,-2.6582919171,0.5465948007,-1.3174928581
H,-4.8335034302,1.6363710598,-0.9679619095
H,-4.1189617143,1.7364860117,3.2663245917
H,-5.5810389986,2.2480786478,1.3213742226
C,0.0621641964,2.1299347668,-0.4543125842
C,-0.2159454115,4.2719871586,-2.2559760269
C,0.2821089696,3.4493680208,-0.0438875943
C,-0.3018369172,1.9001077592,-1.7878030879
C,-0.4401242574,2.963388116,-2.678229534
C,0.146144013,4.5131408602,-0.9327411476
H,0.565265071,3.6421190287,0.9883257674
H,-0.4914032218,0.8876561886,-2.1288104766
H,-0.7262391587,2.7655453537,-3.7069557157
H,0.3193915178,5.5287516241,-0.5897896125
H,-0.3254613541,5.0975262708,-2.9526242581
H,-5.2348747295,-3.341924901,0.7197243923
C,-4.873093155,-3.4531115879,-0.2963962929
C,-3.8882696973,-3.7289928835,-2.9669974184
C,-3.6702296826,-2.9067823188,-0.6946312465
C,-5.5917346699,-4.1555911309,-1.272865234
C,-5.111228109,-4.2902027281,-2.5757812445
C,-3.1922736298,-3.0381352888,-1.9963514842
H,-6.5432095643,-4.6040408112,-1.0065558077
H,-5.6959695498,-4.8404387094,-3.3056196649
H,-3.5052465076,-3.8249231248,-3.9768743415
O,-1.9887076532,-2.3838279515,-2.1036069261
O,-2.7667504435,-2.1842785557,0.0452821356
B,-1.7326301625,-1.8462419499,-0.8360507376
H,6.4584711391,0.3376000732,2.713463636
C,5.7032574088,0.9816485904,3.1502494888
C,3.6900445315,2.6675563579,4.2759887984
C,4.434742633,1.0647423446,2.6153343905
C,5.9582229664,1.7703301535,4.2813110676
C,4.9758147009,2.5928742075,4.8306106735
C,3.4527731141,1.8867460836,3.1639423102
H,6.9428071964,1.7367768962,4.7361241345
H,5.2075208663,3.1900844544,5.7064039508
H,2.9175118813,3.3036806227,4.6936963244
O,2.2993574187,1.768679838,2.4296939757
O,3.9234939165,0.4072303775,1.522738602
B,2.5931780492,0.8420857922,1.4075781694

P-*E,Z*[1,1]^{MeOH} (*N*,*N*-Diborylated product **2a** from reductive coupling transition state **TS-*E,Z*[1,1]^{MeOH}** in MeOH)
trans-dieq-diph-tetrahydroquinoxaline_1-1-dieq_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2425235

Zero-point correction= 0.575788 (Hartree/Particle)
Thermal correction to Energy= 0.606884
Thermal correction to Enthalpy= 0.607828
Thermal correction to Gibbs Free Energy= 0.510274
Sum of electronic and ZPE= -1696.666735
Sum of electronic and thermal Energies= -1696.635639
Sum of electronic and thermal Enthalpies= -1696.634695
Sum of electronic and thermal Free Energies= -1696.732249

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.826	126.470	205.319

C,0.5614074099,-1.3933375091,1.4997579273
C,0.7542964813,-3.013146387,3.410912091
C,-1.4685194248,-1.9472485432,2.8519597283
C,-0.5854663452,-2.5206386626,3.9658711643
C,-0.7017806797,-0.8287495593,2.1501375617
C,1.4762191078,-1.9255618303,2.6086094016
H,0.5751784324,-3.8759775961,2.7556410302
H,-1.7221948719,-2.7414609615,2.1441285434
H,-0.4034770022,-1.7430819813,4.7192350174
H,-0.3836539064,-0.1336955848,2.941580673
H,1.7465849681,-1.0862043071,3.2637800658
H,0.2413798342,-2.2428388557,0.8747088135
H,1.3967723833,-3.3620734101,4.2257325689
H,-2.4053374446,-1.5504623574,3.2575856854
H,-1.1091784001,-3.3388363514,4.4703931779
H,2.4028685492,-2.3207136097,2.1848288844
N,-1.4345483646,-0.0116060413,1.1814333335
N,1.2355623417,-0.4085985247,0.6271174722
C,0.6642418949,0.903330039,0.2334288139
C,-0.6632438403,1.2169612225,0.9588862544
H,-0.3956903445,1.5726943203,1.962077296
H,0.4594229856,0.8616822679,-0.8430106599
C,-1.4795647513,2.3431437564,0.3428721854
C,-3.1171714298,4.4077394158,-0.6252915802
C,-2.4333639495,2.9490605294,1.1677546334
C,-1.3570167819,2.7864158333,-0.9748720261
C,-2.1687062762,3.8143513822,-1.4535291146

C,-3.2495725314,3.9696717754,0.6915121629
H,-2.5341296071,2.6096237621,2.1961703579
H,-0.6453452219,2.3274046788,-1.6525088278
H,-2.0599441988,4.1464962542,-2.481544232
H,-3.9840482189,4.4258382381,1.3482602314
H,-3.7483952389,5.206793231,-1.0019095694
C,1.6592979941,2.02544675,0.4910827527
C,3.4500687171,4.1165008373,1.0140088445
C,2.193585517,2.1996796737,1.7714423704
C,2.0415381641,2.9010860557,-0.5256465915
C,2.9314065577,3.9427967788,-0.2666269697
C,3.0809449132,3.2390669364,2.0337212687
H,1.9176353262,1.5062728237,2.5634361671
H,1.6511327986,2.7579105554,-1.5300151199
H,3.2229585687,4.6143538938,-1.0685480016
H,3.4880776784,3.3631291055,3.0327146193
H,4.1441440028,4.9264535987,1.2165409274
H,-4.7826579389,-3.7962542255,-0.3912612934
C,-4.7577940936,-2.8769108833,-0.9658667004
C,-4.6691322734,-0.4414313042,-2.4582949638
C,-3.9079743293,-1.8433289442,-0.631075439
C,-5.5815050046,-2.6721198972,-2.0819987166
C,-5.5383641997,-1.4837781311,-2.8102507956
C,-3.8641361623,-0.6568204899,-1.3591722962
H,-6.2665187136,-3.4580885167,-2.3826558597
H,-6.1906112494,-1.359315109,-3.6684543097
H,-4.6254134191,0.4883858603,-3.0147645506
O,-2.9322803812,0.1850761668,-0.8038713065
O,-3.0042719163,-1.7763989247,0.4013270377
B,-2.4033524558,-0.5106725113,0.2943695242
H,4.4529555446,-4.2491386326,-1.0780512917
C,4.5035419502,-3.288619299,-1.5787393578
C,4.6122469651,-0.7445888402,-2.8755880302
C,3.7055189874,-2.2334716389,-1.1885152773
C,5.3757254715,-3.0502358226,-2.6501026166
C,5.4286832931,-1.8089051366,-3.2830056307
C,3.7585754763,-0.9923855632,-1.8208694223
H,6.0221620911,-3.8519638331,-2.9916511751
H,6.1162179458,-1.6595484709,-4.1090302905
H,4.6441437808,0.2255330089,-3.3590075192
O,2.8608400295,-0.1375729902,-1.2263899595
O,2.7722592752,-2.1929149388,-0.1796048866
B,2.2549905305,-0.8889745757,-0.2082062056

P-*Z*,*E*[1,1]^{MeOH} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z*,*E*[1,1]^{MeOH}** in MeOH)
trans-diax-diph-tetrahydroquinoxaline_1-1-dieq_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2551567

Zero-point correction= 0.576348 (Hartree/Particle)
Thermal correction to Energy= 0.607158
Thermal correction to Enthalpy= 0.608103
Thermal correction to Gibbs Free Energy= 0.512450
Sum of electronic and ZPE= -1696.678809
Sum of electronic and thermal Energies= -1696.647998
Sum of electronic and thermal Enthalpies= -1696.647054
Sum of electronic and thermal Free Energies= -1696.742706

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.998	126.239	201.317

C,0.5332653288,0.4104333842,-1.5855812913
C,0.5466186048,0.2736317247,-4.1026061842
C,-1.3636383844,-0.7159374226,-2.8129520514
C,-0.480153411,-0.8548606223,-4.0515859113
C,-0.517357922,-0.7159766004,-1.5424443887
C,1.4021413545,0.2900979656,-2.8362273353
H,0.0241367684,1.2341139969,-4.2034250841
H,-1.9267073437,0.2227893625,-2.8752318937
H,0.0404154924,-1.8212718025,-4.0259102316
H,0.0363788674,-1.6676715751,-1.5006017994
H,1.988991468,-0.6350987289,-2.7795459158
H,-0.0252510995,1.3585792934,-1.6441285358
H,1.1941580779,0.167898756,-4.9787890924
H,-2.0923235097,-1.5307101902,-2.7625570881
H,-1.1038647125,-0.8495476005,-4.9510840731
H,2.1101093483,1.1228244771,-2.868705766
N,-1.3149212568,-0.6170225612,-0.3133408052
N,1.3163964158,0.4268158694,-0.3390760099
C,0.4909881103,0.5253934777,0.8706589288
C,-0.4925105685,-0.6583916935,0.9003705232
H,-1.1552742491,-0.5294386134,1.7577408896
H,1.1501798789,0.4360320969,1.7372310184
C,0.1677738717,-2.0283209913,1.0820315488
C,1.2232144171,-4.6074916808,1.4797835035
C,1.4581525022,-2.2021251788,1.5892912598
C,-0.5865948375,-3.1695582731,0.7841487588
C,-0.0679016741,-4.4455712427,0.9792578389

C,1.9804870694,-3.481369719,1.7852585212
H,2.0788308423,-1.3488811126,1.8416661559
H,-1.5923935426,-3.0524564262,0.3896111318
H,-0.6732525761,-5.3146399098,0.7393071755
H,2.9877980247,-3.5910785547,2.1757760455
H,1.6329232219,-5.6016196631,1.6296656823
C,-0.1891312457,1.8942458335,0.9924139141
C,-1.3080256943,4.4621272524,1.2985825665
C,0.4033730518,3.0145539063,0.3993938873
C,-1.3481045701,2.0868466143,1.7524158028
C,-1.9030699196,3.3573396583,1.9009002097
C,-0.1481355457,4.2844511588,0.5482055538
H,1.305823755,2.8908264926,-0.1924567674
H,-1.836213838,1.2522680929,2.2438938685
H,-2.8056246036,3.4786278786,2.4924695043
H,0.3313014275,5.1358985032,0.0744802942
H,-1.7420627609,5.450527832,1.4133992206
H,-6.2536991178,0.1074682999,-2.1672144651
C,-6.1146844617,0.0169091551,-1.0955931254
C,-5.7138082059,-0.2243981414,1.7229897369
C,-4.8637723168,-0.1760935648,-0.547987481
C,-7.1873177816,0.0897210601,-0.1952314401
C,-6.9916863161,-0.0280323013,1.1800133325
C,-4.6680070834,-0.2945512924,0.8263954105
H,-8.1900733127,0.2410475072,-0.5811620609
H,-7.8444705653,0.0328642283,1.8481541961
H,-5.548378672,-0.3177307633,2.7906470285
O,-3.3327352556,-0.4809381984,1.080513954
O,-3.6547752447,-0.2805579547,-1.193257763
B,-2.7006535792,-0.4634052886,-0.1798817279
H,6.3338491735,0.182863751,-2.112834163
C,6.1701674826,0.3319718421,-1.0512863453
C,5.7032750454,0.7223461541,1.7405458005
C,4.8976019062,0.4093167083,-0.5254043377
C,7.2307632976,0.4550469623,-0.1423716477
C,7.0029168059,0.645464919,1.2198019022
C,4.6696385529,0.600115908,0.8355136296
H,8.2497871697,0.3999854944,-0.5109972248
H,7.847320879,0.7365348458,1.8951021006
H,5.5129185605,0.8704575138,2.7977780649
O,3.3173412427,0.6401306901,1.0675448036
O,3.694165101,0.3195099116,-1.1832075244
B,2.7103380623,0.4591220893,-0.1925262328

P-*E*,*E*[1,2]^{MeOH} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,2]^{MeOH}** in MeOH)
cydiimph2_EE_b2cat2_1-2_product_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2129144

Zero-point correction= 0.576205 (Hartree/Particle)
Thermal correction to Energy= 0.606215
Thermal correction to Enthalpy= 0.607159
Thermal correction to Gibbs Free Energy= 0.517199
Sum of electronic and ZPE= -1696.636710
Sum of electronic and thermal Energies= -1696.606699
Sum of electronic and thermal Enthalpies= -1696.605755
Sum of electronic and thermal Free Energies= -1696.695716

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.406	126.237	189.338

C,0.1346109869,2.7590343558,-0.4210047663
C,0.6231050158,5.1650624647,-0.1757456623
C,0.9404191518,3.5751341253,1.8131120873
C,0.6326253542,5.0118088532,1.3538792573
C,-0.0644836377,2.6662198335,1.1151999201
C,-0.2876585374,4.1473310003,-0.8857065166
H,1.6458657251,5.0288016369,-0.5513362318
H,1.9667754323,3.3032514521,1.5486652682
H,-0.3505543908,5.3000592823,1.7484639466
H,-1.04439811,3.1045677332,1.3496592182
H,-1.34014694,4.337912921,-0.6365825413
H,1.2043668256,2.6711291011,-0.6256130004
H,0.3237586317,6.1845248993,-0.4395288937
H,0.8383766769,3.4932690416,2.9005268399
H,1.3619174812,5.7049732827,1.7853908239
H,-0.1811639413,4.2364694237,-1.9718345922
N,-0.5138339512,1.5811289459,-1.0333077902
N,-0.1822519055,1.2486709192,1.5089177807
C,-1.557968663,0.8243405168,1.1492044384
H,-2.2225201075,1.4668419507,1.7397976974
C,-1.7946335468,1.3094814184,-0.3665488193
H,-2.2550387244,2.2954926554,-0.2415242296
B,0.9269006497,0.38093584,1.3131545979
B,0.3768209343,0.4999637108,-1.2985511529
O,1.670450693,0.7478367568,-1.7460083962
O,0.8497179217,-0.9938688379,1.5021645748
C,3.051618301,0.2850273667,0.1632042543

C,4.881207965,-1.0006631856,-1.4840527533
C,2.801186396,0.1761438972,-1.21286183
C,4.209558865,-0.2473672488,0.7099286729
C,5.1269126134,-0.8945102172,-0.1173190831
C,3.7183312849,-0.4637440654,-2.0351270367
H,4.3742655377,-0.1511062909,1.7784986911
H,6.0314692339,-1.3144615667,0.3097213933
H,3.5039037398,-0.53929859,-3.0964050312
H,5.5939793542,-1.5039742196,-2.1289968193
O,2.1363840036,0.9602990982,0.9358949978
C,1.1341455436,-1.9719120288,0.5903223225
C,1.6234213777,-4.025446142,-1.2347089876
C,0.674836826,-1.87311399,-0.7319645713
C,1.8378786694,-3.101633925,0.9893269207
C,2.0817038725,-4.126546894,0.0764182072
C,0.9136709342,-2.8954477212,-1.6385443052
H,2.1865075578,-3.1597276156,2.0155220391
H,2.6328630972,-5.0049920524,0.3957524493
H,0.5373319762,-2.7898801627,-2.6512680304
H,1.8121275416,-4.823759543,-1.9445836766
O,-0.0839234101,-0.7839217437,-1.079253702
C,-1.8925066001,-0.5858249784,1.6264925526
C,-2.4536279268,-3.0865268561,2.7960140242
C,-1.9817447145,-0.7336461323,3.0178653896
C,-2.1154656533,-1.7118907012,0.8303911701
C,-2.3917292245,-2.9496784489,1.4130887895
C,-2.2496526519,-1.9665661481,3.6013004964
H,-1.823157482,0.1365242352,3.6508427005
H,-2.0686162862,-1.6399744867,-0.2477058373
H,-2.5549756725,-3.8118281787,0.772926674
H,-2.3037339203,-2.0522921517,4.6824853425
H,-2.6646493273,-4.0531167161,3.2433815602
C,-2.8185564396,0.5455980588,-1.1812131193
C,-4.8369432634,-0.7795997231,-2.6189039019
C,-2.5949568842,0.1196300564,-2.490535334
C,-4.0808060274,0.3281021498,-0.6126397479
C,-5.0786831336,-0.3324541364,-1.3195230342
C,-3.5959670222,-0.5440440601,-3.2017074723
H,-1.6398839959,0.3068151478,-2.9698668931
H,-4.2800728074,0.6747626324,0.3989720685
H,-6.0472834716,-0.4968188343,-0.8569630377
H,-3.4000257881,-0.8734618874,-4.2177866562
H,-5.613419012,-1.2980462834,-3.1728697139

P-*E,Z*[1,2]^{MeOH} (*N*,*N*-Diborylated product **2a** from reductive coupling transition state **TS-*E,Z*[1,2]^{MeOH}** in MeOH)
cydiimph2_EZ_b2cat2_1-2_product_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2192208

Zero-point correction= 0.576570 (Hartree/Particle)
Thermal correction to Energy= 0.606480
Thermal correction to Enthalpy= 0.607424
Thermal correction to Gibbs Free Energy= 0.518173
Sum of electronic and ZPE= -1696.642651
Sum of electronic and thermal Energies= -1696.612741
Sum of electronic and thermal Enthalpies= -1696.611797
Sum of electronic and thermal Free Energies= -1696.701048

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.572	126.268	187.845

C,-0.0813756064,2.3484319466,0.1366000006
C,-0.2883670983,4.6666491007,0.921281779
C,0.3929170111,2.796470084,2.5494670701
C,-0.2741172288,4.1744578873,2.3788447093
C,-0.31180252,1.8554581265,1.5809073901
C,-0.8714700301,3.6390650953,-0.0673946983
H,0.7407598669,4.893566763,0.6130253285
H,1.4626351706,2.86002957,2.3297119918
H,-1.3080726937,4.1058837948,2.7415223712
H,-1.379201842,1.9758640893,1.804391752
H,-1.938861243,3.4830472677,0.1291228677
H,0.9699497997,2.6288990295,0.0525068853
H,-0.850124966,5.6043173656,0.859945196
H,0.2775028598,2.4436635769,3.5798536878
H,0.2325225316,4.9137218475,3.0075536206
H,-0.769399002,4.003183504,-1.0954384341
N,-0.2535745316,1.206549345,-0.7834360819
N,-0.0760092068,0.3945984134,1.6246065328
C,-1.28730581,-0.1817142744,1.01613451
H,-2.1186869167,0.2894153527,1.5499828361
C,-1.3795056668,0.308271876,-0.4938941133
H,-1.2501994706,-0.5649314542,-1.1403173121
B,1.2077503888,-0.0493191727,1.1672688783
B,0.9104505481,0.6969501108,-1.4067314306
O,2.0558187714,1.4945065945,-1.4653058326
O,1.5652195276,-1.2905814862,0.6729495453
C,3.3563217487,0.6879341332,0.3988710438

C,5.5713846291,0.4686820725,-1.2761513075
C,3.2423069424,1.0069679057,-0.9654141997
C,4.5726863986,0.2569668467,0.9107839034
C,5.6826266618,0.1496219073,0.0745749989
C,4.3506958852,0.8955548444,-1.7955216838
H,4.633039031,0.0158303669,1.9674523539
H,6.631013281,-0.1845785617,0.4820919632
H,4.2390365003,1.1533346155,-2.8439603042
H,6.432793648,0.3866582338,-1.930808194
O,2.2693407641,0.8502218329,1.2321474333
C,1.0633125484,-2.1877927365,-0.2248313071
C,0.1504264054,-4.087048709,-2.0514052858
C,0.764428202,-1.8074463235,-1.540328373
C,0.9691185794,-3.5258852738,0.1444396325
C,0.5099216887,-4.4751528259,-0.761578555
C,0.2880464165,-2.7583733448,-2.4397488523
H,1.24521767,-3.7960280454,1.1582691917
H,0.4249993185,-5.5125648533,-0.4549069674
H,0.052945284,-2.4342764815,-3.4486394939
H,-0.2196968578,-4.8178566321,-2.7628178385
O,1.0180339333,-0.5478378036,-2.0058813595
C,-1.4989637783,-1.6650645761,1.2518561358
C,-2.1051702975,-4.3394257836,1.8543087236
C,-2.2727691844,-2.4336116136,0.37720565
C,-1.0411495338,-2.2495674905,2.4373161138
C,-1.3377791215,-3.5769313727,2.73373807
C,-2.5727137544,-3.7616293613,0.6767515755
H,-2.6563749545,-2.0046758825,-0.5448529033
H,-0.4492462546,-1.657723228,3.1288149229
H,-0.9698077055,-4.0160151078,3.6564692806
H,-3.1717292937,-4.344315301,-0.0168459801
H,-2.3375664138,-5.3743636669,2.0859265107
C,-2.724294207,0.9189204867,-0.874130222
C,-5.1907381381,1.9870868704,-1.70211908
C,-2.8014126656,1.7741122234,-1.9797843324
C,-3.9064297205,0.5907649897,-0.2038384858
C,-5.1295586043,1.1226841877,-0.6140546333
C,-4.0194327856,2.3074654658,-2.3879879913
H,-1.8920894432,2.0291321617,-2.5156350727
H,-3.8951928116,-0.093498805,0.6397408874
H,-6.0345912065,0.8574218158,-0.0759848875
H,-4.0539156145,2.9752323049,-3.2436527107
H,-6.1420578329,2.4041851611,-2.0177094198

P-*Z*,*E*[1,2]^{MeOH} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z*,*E*[1,2]^{MeOH}** in MeOH)
cydiimph2_ZE_b2cat2_1-2_product_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2252124

Zero-point correction= 0.576487 (Hartree/Particle)
Thermal correction to Energy= 0.606418
Thermal correction to Enthalpy= 0.607362
Thermal correction to Gibbs Free Energy= 0.517712
Sum of electronic and ZPE= -1696.648725
Sum of electronic and thermal Energies= -1696.618794
Sum of electronic and thermal Enthalpies= -1696.617850
Sum of electronic and thermal Free Energies= -1696.707500

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.533	126.200	188.685

C,-0.4222676963,1.8371399012,1.407870485
C,-0.4486997316,4.0998179761,2.3706318769
C,-0.4151572329,3.7725129256,-0.1796113921
C,-0.0501844363,4.685936846,1.0053545101
C,0.1998721705,2.4124182343,0.1160554081
C,0.0587089658,2.6628707022,2.5949165988
H,-1.5439703772,4.0897709523,2.4460013366
H,-1.5021387347,3.6961598796,-0.2867975605
H,1.0351650036,4.8509071392,0.9915216924
H,1.2597260775,2.6203220606,0.3134720569
H,1.1544697183,2.6501942164,2.6642287944
H,-1.5016718055,1.9780912371,1.3478974459
H,-0.0838499549,4.7545592111,3.1684892671
H,-0.0099803355,4.1799523915,-1.1122503422
H,-0.5201340334,5.6666302135,0.879741552
H,-0.3413398438,2.2625354189,3.5323374284
N,-0.186917392,0.3779703685,1.4141930023
N,0.204062063,1.3492388511,-0.9064884858
C,1.3224231238,0.4546814898,-0.5622002518
H,1.2262779204,-0.4578180562,-1.1540553865
C,1.1851677005,0.079768224,0.9726987851
H,1.8233584453,0.7793062017,1.5282028449
B,-1.0363169879,0.7202934229,-1.219454495
B,-1.3201186307,-0.4477684588,1.1903537984
O,-2.5834881358,0.0908458491,1.4607061181
O,-1.2085864128,-0.5401088514,-1.7666554494
C,-3.3839539928,0.7012893185,-0.7310576207

C,-5.7729780431,-0.6287131078,-0.2001098029
C,-3.5608956334,0.0338225936,0.4936498217
C,-4.3989398904,0.6945892655,-1.6780946775
C,-5.5959631444,0.031580428,-1.4130201643
C,-4.7544285346,-0.6289847049,0.7511100984
H,-4.2360794275,1.2185703326,-2.6147368482
H,-6.386293048,0.033256943,-2.1564306788
H,-4.8691378046,-1.1339524151,1.7050328564
H,-6.7028333382,-1.1468145711,0.0104412883
O,-2.2205597162,1.4051976457,-0.9658303122
C,-0.6178509555,-1.7551142498,-1.5477003933
C,0.3627471462,-4.3375288168,-1.1831795409
C,-0.7113769251,-2.371148529,-0.2918097546
C,-0.0124619549,-2.4257121526,-2.6057743383
C,0.4859897091,-3.7128284974,-2.4228922707
C,-0.238378126,-3.6678059323,-0.122400923
H,0.0483034102,-1.9231367196,-3.5659141409
H,0.9579736221,-4.2275406065,-3.2531301309
H,-0.3367197412,-4.1257972707,0.8570097808
H,0.7402188676,-5.3442630476,-1.036255918
O,-1.3483494405,-1.7608777303,0.7495404271
C,2.6621832953,1.0836098989,-0.937964277
C,5.098075258,2.2219285096,-1.7615091342
C,2.7635943341,1.754646631,-2.162787605
C,3.8016890637,0.9909828993,-0.133843393
C,5.0100651293,1.5563500805,-0.5433223876
C,3.9675924686,2.3175816086,-2.5725805887
H,1.8829753364,1.8388196602,-2.7923942857
H,3.7692629595,0.4700164197,0.8184705366
H,5.8820941199,1.4748419366,0.0984153455
H,4.0232742348,2.8342475941,-3.5260788559
H,6.0382872763,2.6627852985,-2.0781025957
C,1.6685248393,-1.3114223789,1.3459703145
C,2.6426294285,-3.8251091938,2.1402268781
C,1.2621787065,-1.8860611956,2.5559671333
C,2.575646076,-2.011465463,0.5450139067
C,3.0622322207,-3.2564030726,0.9415969487
C,1.7390500034,-3.1336216993,2.9468550295
H,0.5640077803,-1.3519871728,3.1936470219
H,2.909296835,-1.5992210847,-0.4028265214
H,3.7627015495,-3.7846756654,0.3016955233
H,1.4061738513,-3.5650289685,3.8861925174
H,3.0156767476,-4.7978041642,2.445842093

P-*Z*,*Z*[1,2]^{MeOH} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*Z*,*Z*[1,2]^{MeOH}** in MeOH)
cydiimph2_ZZ_b2cat2_1-2_product_meoh
M062X/6-31G(d,p)
E(RM062X) = -1697.2147945

Zero-point correction= 0.576648 (Hartree/Particle)
Thermal correction to Energy= 0.606671
Thermal correction to Enthalpy= 0.607615
Thermal correction to Gibbs Free Energy= 0.517183
Sum of electronic and ZPE= -1696.638147
Sum of electronic and thermal Energies= -1696.608124
Sum of electronic and thermal Enthalpies= -1696.607180
Sum of electronic and thermal Free Energies= -1696.697611

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.692	126.174	190.330

C,-0.0046409808,-1.9269374638,0.2984611047
C,-0.5783853573,-4.2875960995,-0.0901142964
C,-0.209272533,-2.7038900721,-2.0725051516
C,-0.9344220638,-3.9553308477,-1.5478346138
C,-0.5160344386,-1.5658986641,-1.1091194881
C,-0.8036648823,-3.1003555502,0.8620871053
H,0.4783571159,-4.5820911813,-0.0396578773
H,0.8694381618,-2.883352112,-2.12674736
H,-2.0172899779,-3.7859302346,-1.6201317211
H,-1.6093315312,-1.5064177306,-1.0701698799
H,-1.8714119431,-2.8685880206,0.9252271376
H,1.013913327,-2.3001332638,0.1844075824
H,-1.1641233047,-5.1504776303,0.2428546698
H,-0.5599185697,-2.4544680978,-3.0802449823
H,-0.7050417471,-4.813348947,-2.1878511954
H,-0.4538946311,-3.346268293,1.8707706538
N,0.1095129889,-0.6722946236,1.0691434315
N,-0.0601508207,-0.1955049355,-1.4282285043
C,-0.9446014835,0.7262983696,-0.7041680026
H,-0.4711714346,1.7064420953,-0.6959623844
C,-0.9905108997,0.2847330079,0.8390199993
H,-0.7367250938,1.183303055,1.4070183505
B,1.3384839775,0.0745321707,-1.2936435664
B,1.4151873162,-0.2297935543,1.3917436775
O,2.4570006928,-1.1604208438,1.3783106009
O,1.9363007177,1.2982539266,-1.0284589923
C,3.4803489342,-0.865731624,-0.7902654634

C,5.9767759229,-0.7496746944,0.4411562426
C,3.5785864264,-0.946274169,0.6102920502
C,4.6277276793,-0.7241647503,-1.5587060458
C,5.8778665493,-0.669275747,-0.9450923889
C,4.82726265,-0.8871774537,1.2168126427
H,4.5221887852,-0.6634479434,-2.637357768
H,6.7699981207,-0.56220022,-1.5531881609
H,4.8781517051,-0.9574377332,2.2987445736
H,6.9471848695,-0.7062473214,0.9245730511
O,2.2485639288,-0.9706269906,-1.4050139961
C,1.5711968455,2.3739957984,-0.2657995445
C,0.9372610607,4.5900842545,1.2976866952
C,1.4778542774,2.2450645876,1.1281938313
C,1.3651989991,3.6117722216,-0.8653223738
C,1.0450484213,4.7197095938,-0.08539597
C,1.1577651786,3.3556785053,1.9024417807
H,1.4532564586,3.681722076,-1.9448312226
H,0.8806571846,5.6806811168,-0.5611660428
H,1.0918926825,3.2297936532,2.9785590238
H,0.6866915141,5.4493849688,1.9107276512
O,1.7724773081,1.0635452243,1.7493872834
C,-2.274769785,0.9811195293,-1.3868855812
C,-4.7429380324,1.5563378548,-2.5875376156
C,-2.6353188775,0.3709950802,-2.5881668757
C,-3.1487845205,1.9105251861,-0.8107528859
C,-4.3745435872,2.1940246713,-1.4019942647
C,-3.8674788519,0.6516451004,-3.1806815491
H,-1.9508310587,-0.3248704158,-3.0645258674
H,-2.8657449935,2.4088001322,0.1143964516
H,-5.0433324871,2.9138106757,-0.9397286018
H,-4.1384150406,0.162239177,-4.1115195498
H,-5.7012368717,1.7731337452,-3.0493759443
C,-2.2806327778,-0.2241113691,1.4886501235
C,-4.4798113151,-1.188540507,2.964167197
C,-2.3064411747,-0.1509982822,2.8875496276
C,-3.3859156141,-0.7860682748,0.841605182
C,-4.4730838657,-1.2632921254,1.5747342532
C,-3.3868925003,-0.6275452635,3.6221722528
H,-1.4549320023,0.2844512751,3.4063350185
H,-3.4223082224,-0.8677152999,-0.2383537013
H,-5.3180756454,-1.6973618372,1.0488042615
H,-3.3762465526,-0.5576625014,4.7056594894
H,-5.3288503302,-1.5608953643,3.5291264331

P-*E*,*E*[1,1]^{DMF} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,1]^{DMF}** and **TS-*Z*,*Z*[1,1]^{DMF}** in DMF)
cis-diph-tetrahydroquinoxaline_1-1-dieq_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2425953

Zero-point correction= 0.576011 (Hartree/Particle)
Thermal correction to Energy= 0.606943
Thermal correction to Enthalpy= 0.607887
Thermal correction to Gibbs Free Energy= 0.511207
Sum of electronic and ZPE= -1696.666584
Sum of electronic and thermal Energies= -1696.635653
Sum of electronic and thermal Enthalpies= -1696.634708
Sum of electronic and thermal Free Energies= -1696.731388

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.862	126.155	203.480

C,1.7973607242,-0.4003782701,-0.7156921395
C,3.3306401264,-1.8357814297,-2.0974837824
C,0.9022230748,-2.4583445053,-1.8691800114
C,2.3286649431,-2.9835132758,-2.0266090656
C,0.7657192242,-1.5401647697,-0.6526965595
C,3.2136984184,-0.9552461601,-0.8558174328
H,3.1355698808,-1.2341511543,-2.9950174545
H,0.6073405539,-1.8994731606,-2.7669592296
H,2.5757390319,-3.6250585091,-1.1705230828
H,1.0080390687,-2.120808228,0.2562013045
H,3.465078017,-1.5438772467,0.0344747051
H,1.5819746411,0.1893487742,-1.6192811199
H,4.3520534884,-2.2196363288,-2.1831669592
H,0.2118064651,-3.3006689323,-1.7765803602
H,2.3890396879,-3.6088605949,-2.9228782949
H,3.9222630714,-0.12409805,-0.9025337783
N,-0.611023181,-1.010069674,-0.5119356975
N,1.6371903448,0.4743886909,0.4480788489
C,0.2889637384,1.0485869103,0.5610118695
C,-0.7555010186,-0.0926853327,0.6249889479
H,-0.5250183555,-0.62921544,1.5603919742
H,0.2275519852,1.5341199677,1.5374074752
C,-2.1372496949,0.5215566938,0.7723418533
C,-4.6174591281,1.779122243,1.162330472
C,-2.5627771465,0.8799618497,2.0531563892
C,-2.969925449,0.8063363697,-0.3147309108
C,-4.2029253802,1.423343509,-0.1200029208

C,-3.7912372695,1.5073444486,2.2500203544
H,-1.9252983364,0.6581197791,2.9059899758
H,-2.6621305833,0.5453602172,-1.3238371606
H,-4.8399326156,1.6289602866,-0.9747812712
H,-4.1046383943,1.7748759564,3.2544835372
H,-5.5784122043,2.2613469605,1.3119277844
C,0.0632908106,2.1411475297,-0.4774452637
C,-0.2212422465,4.2707878908,-2.2934786073
C,0.285396423,3.4634879302,-0.0777407851
C,-0.3062685221,1.9022373262,-1.8079410706
C,-0.4477756567,2.9592624636,-2.7053579971
C,0.1464830055,4.5211081267,-0.9734835393
H,0.5721652745,3.6640547887,0.9518218547
H,-0.4972270093,0.8871594242,-2.1401506746
H,-0.7382167996,2.7542048689,-3.7313529601
H,0.3215766547,5.5388979694,-0.6383688854
H,-0.3333036533,5.0913389637,-2.9954181548
H,-5.176102108,-3.399431589,0.7721861797
C,-4.8327322573,-3.4907980802,-0.2522685629
C,-3.9007421204,-3.7176272201,-2.945693444
C,-3.6439417585,-2.9238482828,-0.666094242
C,-5.5636203605,-4.1878882111,-1.2233519802
C,-5.108769375,-4.2986658245,-2.5377665256
C,-3.1914648734,-3.0313331008,-1.980529677
H,-6.5041487866,-4.6510220563,-0.9438417832
H,-5.7020986467,-4.8454969966,-3.2631237714
H,-3.5390175617,-3.7958527388,-3.964895385
O,-2.001610378,-2.3624281259,-2.1034879317
O,-2.7352936893,-2.2049105049,0.0635259429
B,-1.7268830065,-1.8403163787,-0.8343188384
H,6.451023298,0.3295539264,2.7184239171
C,5.6896459565,0.9604692756,3.1634032843
C,3.6642044545,2.6131287107,4.3144140475
C,4.4230785302,1.0478061209,2.6232137368
C,5.9362865064,1.7264795371,4.3117560889
C,4.9477119664,2.5330575072,4.8734784419
C,3.4339071618,1.8546131345,3.1849489005
H,6.9189566278,1.6877934037,4.7701226579
H,5.1726233291,3.1128894212,5.7625305479
H,2.8879143907,3.2374225817,4.7427366301
O,2.2869541182,1.7462356197,2.4458766444
O,3.9212435347,0.4123647059,1.5175502735
B,2.5906090486,0.8433762883,1.4070226411

P-*E,Z*[1,1]^{DMF} (*N*,*N*-Diborylated product **2a** from reductive coupling transition state **TS-*E,Z*[1,1]^{DMF}** in DMF)
trans-dieq-diph-tetrahydroquinoxaline_1-1-dieq_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2417054

Zero-point correction= 0.575872 (Hartree/Particle)
Thermal correction to Energy= 0.607022
Thermal correction to Enthalpy= 0.607966
Thermal correction to Gibbs Free Energy= 0.509688
Sum of electronic and ZPE= -1696.665833
Sum of electronic and thermal Energies= -1696.634683
Sum of electronic and thermal Enthalpies= -1696.633739
Sum of electronic and thermal Free Energies= -1696.732017

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.912	126.449	206.844

C,1.565783031,-1.2013841343,-0.2471728258
C,3.0195440762,-3.245317688,-0.4767251366
C,0.5529293514,-3.3661957752,-0.9927509749
C,1.7724578427,-4.1325281172,-0.4709420432
C,0.3483794051,-2.1157995081,-0.1394920903
C,2.7885728836,-1.9468265796,0.3007825093
H,3.2793308846,-2.9983419271,-1.5147346571
H,0.7146147108,-3.0925660237,-2.0386283412
H,1.5755101517,-4.4765811558,0.552855702
H,0.3010927167,-2.4637991556,0.9050889836
H,2.6061466891,-2.1709235183,1.3607449574
H,1.7278193607,-1.0049701228,-1.3190019525
H,3.8735982899,-3.7848703498,-0.0550891586
H,-0.3479984596,-3.9875867181,-0.9500604845
H,1.9379691428,-5.0249396745,-1.0828051726
H,3.6733579322,-1.3076163618,0.2474243121
N,-0.8875439558,-1.354806974,-0.3516817688
N,1.3427582131,0.0856437556,0.4362078784
C,0.0457667618,0.5176288876,0.9941246691
C,-1.1021168678,-0.5262391585,0.8386959013
H,-1.0295363275,-1.2085214377,1.6953294083
H,-0.2618145918,1.4158524514,0.4481973551
C,-2.4483510332,0.1643037614,0.9574483968
C,-4.919768354,1.4417894672,1.3144253133
C,-3.3619309561,-0.3030649694,1.9028946701
C,-2.7869207265,1.2857509622,0.1918923768
C,-4.0130006236,1.9179010499,0.3665028481

C,-4.5925459225,0.3284051625,2.0820354561
H,-3.1041107837,-1.1663862714,2.5109887545
H,-2.0978415587,1.6597046949,-0.5602828118
H,-4.2628102017,2.7846764449,-0.2376646858
H,-5.2888414872,-0.0473760456,2.8253483475
H,-5.8744494541,1.9397604534,1.4533435227
C,0.1572085409,0.8890621835,2.4644115579
C,0.2608460168,1.5080829177,5.1946216397
C,0.870799251,0.0758630971,3.348281349
C,-0.5041013803,2.0137324095,2.9605337692
C,-0.4532310778,2.323111981,4.3186498882
C,0.9233507421,0.3825565072,4.7055992397
H,1.3940813903,-0.796267291,2.9627894756
H,-1.0585803084,2.6515559655,2.2760739832
H,-0.9670608748,3.2042682847,4.6908579248
H,1.4834614458,-0.2556476022,5.3824316998
H,0.3044944097,1.749932681,6.2520878796
H,-1.5006051155,-2.7310273329,-5.4187005936
C,-2.3164910455,-2.1999365557,-4.9410509742
C,-4.4495705456,-0.7972039407,-3.6584400395
C,-2.2396587094,-1.7988650324,-3.622895569
C,-3.4993053691,-1.8835571654,-5.6247012533
C,-4.5402979267,-1.1988458238,-4.9988083254
C,-3.2810371175,-1.1153874432,-2.9968253052
H,-3.602731432,-2.179010801,-6.663571447
H,-5.4417308486,-0.9704719596,-5.5578773754
H,-5.2517563541,-0.2637294149,-3.1604956669
O,-2.9346168288,-0.8490289366,-1.6999815111
O,-1.2122035568,-1.9679405596,-2.7345838992
B,-1.6461091523,-1.3774179846,-1.5337515725
H,5.8928223061,1.94108548,-1.5301910195
C,5.2558589458,2.6302863724,-0.9869832968
C,3.5575544806,4.4233448103,0.4487095028
C,4.0592034406,2.2198933639,-0.4359623063
C,5.5998059538,3.9775279973,-0.807843954
C,4.7708047922,4.8527357376,-0.1071467322
C,3.2291938574,3.0956433543,0.2653487825
H,6.5320694589,4.3435336385,-1.2250901205
H,5.0681156293,5.8892729487,0.0125903833
H,2.9052441915,5.0948155254,0.995835064
O,2.1161527162,2.4226587552,0.6978375652
O,3.4880103444,0.9733460694,-0.4627236054
B,2.2839595201,1.1072523486,0.2436656435

P-*Z,E*[1,1]^{DMF} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z,E*[1,1]^{DMF}** in DMF)
trans-diax-diph-tetrahydroquinoxaline_1-1-dieq_dmf
M062x/6-31G(d,p)
E(RM062X) = -1697.2564229

Zero-point correction= 0.576818 (Hartree/Particle)
Thermal correction to Energy= 0.607577
Thermal correction to Enthalpy= 0.608522
Thermal correction to Gibbs Free Energy= 0.512565
Sum of electronic and ZPE= -1696.679605
Sum of electronic and thermal Energies= -1696.648846
Sum of electronic and thermal Enthalpies= -1696.647901
Sum of electronic and thermal Free Energies= -1696.743858

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.261	126.073	201.957

C,1.3961095473,-0.2563436677,-0.7428258224
C,3.0290277451,-1.7230751051,-1.9762185028
C,0.6357536574,-2.4441087335,-1.7445898664
C,2.0878316867,-2.9145104388,-1.8146432374
C,0.4412154196,-1.4568952176,-0.5964030187
C,2.8458285699,-0.7283904043,-0.83051442
H,2.8206286708,-1.2239779714,-2.931757517
H,0.3653432414,-1.9596058858,-2.689919622
H,2.3431781264,-3.4577938114,-0.8953024024
H,0.7123177757,-1.9652889263,0.342619088
H,3.1283820298,-1.2050666717,0.1156733122
H,1.1368158844,0.2369073723,-1.6933083072
H,4.0712479478,-2.0558252719,-2.0088390486
H,-0.0416600525,-3.2928008191,-1.6122972972
H,2.2073842337,-3.6160732335,-2.646225527
H,3.502458443,0.1357294259,-0.9642090746
N,-0.9451340094,-0.9896604723,-0.4614190197
N,1.1682075959,0.7132501631,0.339933081
C,-0.2239503349,1.1660467947,0.4321024845
C,-1.1284873507,-0.0604381053,0.6579878169
H,-2.1673648168,0.2739356011,0.646877518
H,-0.3080512477,1.8166793249,1.3049528703
C,-0.9218811386,-0.7544750824,2.008379814
C,-0.7145646855,-2.0819070548,4.4834871778
C,-0.4008641211,-0.1019991236,3.1296158031
C,-1.3402075766,-2.0827652392,2.1514678249
C,-1.239150616,-2.7412788347,3.3732317714

C,-0.2971875618,-0.7609207344,4.3550914536
H,-0.0666132568,0.928114158,3.0698734181
H,-1.7427452802,-2.6090658515,1.2903641297
H,-1.570376473,-3.7719806655,3.4568769417
H,0.1150238907,-0.2335094423,5.2100161949
H,-0.6313356146,-2.5936390062,5.4371893635
C,-0.6308547261,2.0187653884,-0.77527366
C,-1.325440785,3.717190692,-2.9132327769
C,0.3432899107,2.7606633897,-1.4527679262
C,-1.9624303599,2.151353495,-1.1833188965
C,-2.305211032,2.9901733995,-2.2433242756
C,0.0029059944,3.6000998528,-2.5101076225
H,1.3837916039,2.6734320664,-1.1529054254
H,-2.7544998852,1.6048310723,-0.6831888988
H,-3.3456481268,3.0713831568,-2.5432528533
H,0.7796069768,4.161882694,-3.0201977245
H,-1.5934134471,4.3679528901,-3.7396522357
H,-3.3453177734,-3.2199402328,-4.6576135848
C,-3.9493956879,-2.6486864258,-3.9615099928
C,-5.5153301905,-1.1366086702,-2.1117243126
C,-3.3916122599,-2.0467688138,-2.8524905088
C,-5.330442732,-2.4815297988,-4.1379984738
C,-6.0945992208,-1.7433848204,-3.2353636294
C,-4.1561006865,-1.3091724613,-1.9489715244
H,-5.8111784555,-2.9377812153,-4.9970203022
H,-7.1611175261,-1.6342686611,-3.4023142826
H,-6.099885187,-0.5604867833,-1.4030475265
O,-3.3462017483,-0.8347838623,-0.952227944
O,-2.0816381452,-2.0487361737,-2.4482849416
B,-2.0508704897,-1.2908689419,-1.2690115459
H,5.99385661,1.1470891115,2.548823303
C,5.2007444325,1.7910750859,2.9122265854
C,3.0909149807,3.4733705995,3.8502354033
C,3.928449831,1.7328556547,2.381903776
C,5.4095359985,2.7216513307,3.9400920691
C,4.3798288541,3.5424026122,4.3980736712
C,2.8986893246,2.5543010912,2.8392595297
H,6.3950672275,2.8013423039,4.3868004581
H,4.5762729024,4.2512447675,5.1956686855
H,2.282841864,4.107078626,4.1983973446
O,1.7562792313,2.2825654811,2.1342821681
O,3.4568922959,0.9216895832,1.3824340202
B,2.1050401072,1.2593554563,1.2293364605

P-*E*,*E*[1,2]^{DMF} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,2]^{DMF}** in DMF)
cydiimph2_EE_b2cat2_1-2_product_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2123665

Zero-point correction= 0.576632 (Hartree/Particle)
Thermal correction to Energy= 0.606583
Thermal correction to Enthalpy= 0.607527
Thermal correction to Gibbs Free Energy= 0.517737
Sum of electronic and ZPE= -1696.635735
Sum of electronic and thermal Energies= -1696.605783
Sum of electronic and thermal Enthalpies= -1696.604839
Sum of electronic and thermal Free Energies= -1696.694630

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.637	126.072	188.981

C,-1.9854072064,-0.4020072762,1.6739169886
C,-3.3071570498,-0.8009171038,3.7180908283
C,-0.7429808763,-0.8640075463,3.8054885906
C,-2.0617858881,-1.3713274432,4.416422752
C,-0.801424667,-1.1749081942,2.3147153407
C,-3.2917249457,-0.9920050021,2.1907299018
H,-3.3678612982,0.2752946591,3.9269846039
H,-0.631072824,0.2109896214,3.9745336844
H,-2.0808380625,-2.466524686,4.3421415029
H,-1.0372706905,-2.246886211,2.2616863458
H,-3.3635176268,-2.0585208938,1.9388449302
H,-1.9415549161,0.6297257538,2.03066041
H,-4.2066113123,-1.256225256,4.1446976739
H,0.1106743136,-1.3707602168,4.2681917026
H,-2.0974515933,-1.1261536176,5.4827309389
H,-4.1482769445,-0.4838141281,1.7358118436
N,-1.7583866363,-0.3565077449,0.2155144648
N,0.3999855271,-1.0098929947,1.4744449922
C,0.2320565747,-1.920498986,0.3157696731
H,0.1702455653,-2.9276236716,0.7462705531
C,-1.2487320809,-1.6512003228,-0.2543446959
H,-1.8551206098,-2.3949018157,0.2740941034
B,0.9543272541,0.2899525313,1.3098990705
B,-1.1431805897,0.8464234443,-0.2403075332
O,-1.4743056339,2.0668036178,0.3361706286
O,1.9741406738,0.5622872374,0.4096116469
C,0.4243169704,2.6140446289,1.6982221895

C,0.250070941,5.2566894004,0.8561102248
C,-0.5661921502,2.9934363686,0.7780014716
C,1.3199005359,3.5522672354,2.1901797797
C,1.2337496311,4.8780408742,1.7661126223
C,-0.6526047527,4.3156024062,0.3622100375
H,2.0774278522,3.2305464442,2.897785835
H,1.9363824266,5.6106764972,2.1486471531
H,-1.4235370254,4.5889984809,-0.3509578875
H,0.1807635145,6.287508575,0.5247685473
O,0.4513225614,1.3069843487,2.1173194766
C,1.9664525477,1.4722615454,-0.6049984003
C,2.0049210204,3.2607496353,-2.7499181282
C,0.8554872144,1.5882968731,-1.4563674199
C,3.090475904,2.2564934591,-0.8374160312
C,3.1083220141,3.1493241853,-1.907882325
C,0.8764217157,2.4735256754,-2.5244518331
H,3.9397928036,2.1558097087,-0.1694680719
H,3.9898844526,3.7580997021,-2.079770427
H,0.0041675262,2.5331167797,-3.1676815183
H,2.0187772588,3.9543131932,-3.5838357963
O,-0.2108538703,0.7497549312,-1.2554453597
C,1.4624292873,-1.9824548492,-0.5842139411
C,3.878109859,-2.2250485257,-2.0111892238
C,2.5831908123,-2.6013146034,-0.0138935467
C,1.5681820301,-1.5061853244,-1.8929103294
C,2.7670613729,-1.6268556132,-2.5971378605
C,3.7808409217,-2.7172084394,-0.7099651669
H,2.5112208275,-2.9866205894,1.0007594567
H,0.7215979501,-1.032961401,-2.3719657973
H,2.826678304,-1.2448490737,-3.6121177596
H,4.6351490934,-3.1954221088,-0.2402908589
H,4.8088953166,-2.3138262989,-2.5630902903
C,-1.4963368158,-1.9708698148,-1.7144205954
C,-1.9851083578,-2.7216341991,-4.377886537
C,-2.1809833061,-1.1167761896,-2.5787268477
C,-1.0884894987,-3.2227947648,-2.1940292263
C,-1.323619213,-3.5939128894,-3.5128051159
C,-2.4181007448,-1.4876280175,-3.90314996
H,-2.5407211518,-0.1571557007,-2.2234000324
H,-0.5740387703,-3.9106100274,-1.5267410301
H,-0.992510069,-4.5659123479,-3.8657007492
H,-2.9474909883,-0.8059164046,-4.5620589946
H,-2.1681743979,-3.0073775092,-5.4090006645

P-*E,Z*[1,2]^{DMF} (*N*,*N*-Diborylated product **2a** from reductive coupling transition state **TS-*E,Z*[1,2]^{DMF}** in DMF)
cydiimph2_EZ_b2cat2_1-2_product_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2198291

Zero-point correction= 0.576900 (Hartree/Particle)
Thermal correction to Energy= 0.606741
Thermal correction to Enthalpy= 0.607685
Thermal correction to Gibbs Free Energy= 0.518748
Sum of electronic and ZPE= -1696.642929
Sum of electronic and thermal Energies= -1696.613089
Sum of electronic and thermal Enthalpies= -1696.612144
Sum of electronic and thermal Free Energies= -1696.701081

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.735	126.128	187.182

C,-0.6019671582,-1.5190744098,-1.476452346
C,-1.5208828401,-2.5399719434,-3.5118405515
C,-0.2471487893,-0.308790056,-3.633794838
C,-1.3208638583,-1.2141316321,-4.266565585
C,-0.634738575,-0.1405989273,-2.1705372326
C,-1.7663789478,-2.3552303044,-2.0020956204
H,-0.6236474692,-3.1597751359,-3.6394951001
H,0.7434840122,-0.7630776666,-3.7247662793
H,-2.2718810232,-0.6658355782,-4.2794472794
H,-1.6800909047,0.1923674506,-2.1948217479
H,-2.7240543707,-1.8499298391,-1.8296628473
H,0.3031197832,-2.0283245171,-1.8111015229
H,-2.3526684064,-3.0919938914,-3.9610761484
H,-0.2241251613,0.6629567746,-4.1385007074
H,-1.0637450903,-1.424754927,-5.309577728
H,-1.8069105852,-3.3296131609,-1.503271675
N,-0.415388547,-1.3126535549,-0.0263432946
N,0.0595635787,0.8378645104,-1.3040260959
C,-0.9134192697,1.1244357715,-0.2370179122
H,-1.8428323444,1.3667511432,-0.7623742479
C,-1.1859036955,-0.2161771096,0.5742497522
H,-0.7941284745,-0.080866147,1.5866464363
B,1.4073023237,0.5047482319,-0.9410557652
B,0.8395786604,-1.676330217,0.5228958551
O,1.6620525307,-2.5483758774,-0.1897589869
O,2.1317393835,0.9220343259,0.1586439207
C,3.1846444106,-1.0590428648,-1.3153074216

C,5.3184269643,-2.6180145749,-0.4291481274
C,2.9473765702,-2.1771826717,-0.4949908079
C,4.4838333157,-0.7307715004,-1.6797924063
C,5.5521602265,-1.5102800715,-1.2396133118
C,4.0168667075,-2.9494469214,-0.0573460947
H,4.6400471792,0.1363924663,-2.3136195007
H,6.5638049961,-1.2482681231,-1.5311935888
H,3.8097168627,-3.810642915,0.569728826
H,6.1462791447,-3.2284433333,-0.083805732
O,2.1227922018,-0.3272065669,-1.7964801545
C,1.9244978941,1.0661967267,1.4969840096
C,1.6394512618,1.3693001004,4.2552633895
C,1.4935193869,-0.0150985171,2.2798851123
C,2.2741718785,2.2652810155,2.1101899301
C,2.129379266,2.4222241323,3.4842127368
C,1.3323740662,0.1530339128,3.6535803414
H,2.6414653801,3.0711942003,1.4838441136
H,2.3901241311,3.3685880894,3.9466185257
H,0.9855371466,-0.6949219942,4.2353648309
H,1.5119732588,1.4847048224,5.3264761254
O,1.31687965,-1.2598016121,1.7542511505
C,-0.6309364983,2.3641408692,0.5901711726
C,-0.3273211385,4.776069442,1.9943914884
C,-1.1336039937,2.4999312642,1.8875128771
C,0.0157850637,3.4550357718,0.0001751694
C,0.1710570186,4.6492602768,0.6984031042
C,-0.9824771684,3.697974637,2.5842770029
H,-1.6538805437,1.6750029107,2.3672196471
H,0.3975314066,3.3621903817,-1.011998459
H,0.6806158347,5.4845067937,0.2270766377
H,-1.3757514752,3.7838408216,3.5928229981
H,-0.2074033197,5.7077648087,2.5385390359
C,-2.6623608681,-0.5616492352,0.7364394932
C,-5.3556190893,-1.2470907496,1.1673517888
C,-3.0324978646,-1.8853145877,1.0022642758
C,-3.6615955449,0.4157614127,0.7099250143
C,-4.997943136,0.0746927057,0.9221342859
C,-4.364526507,-2.2273482284,1.2109608166
H,-2.2644569093,-2.6523168463,1.0333565674
H,-3.4128335528,1.4587163835,0.5358793784
H,-5.7579218138,0.8495240054,0.8932939587
H,-4.6293319691,-3.2618353537,1.407945744
H,-6.3959145824,-1.5123046162,1.3279036042

P-*Z*,*E*[1,2]^{DMF} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z*,*E*[1,2]^{DMF}** in DMF)
cydiimph2_ZE_b2cat2_1-2_product_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2256751

Zero-point correction= 0.576772 (Hartree/Particle)
Thermal correction to Energy= 0.606697
Thermal correction to Enthalpy= 0.607641
Thermal correction to Gibbs Free Energy= 0.517932
Sum of electronic and ZPE= -1696.648903
Sum of electronic and thermal Energies= -1696.618978
Sum of electronic and thermal Enthalpies= -1696.618034
Sum of electronic and thermal Free Energies= -1696.707743

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.708	126.103	188.809

C,-0.2811765011,-1.8604341554,1.1525750673
C,-0.0381090978,-4.2335166607,1.7483046895
C,2.0144526932,-2.8513320104,1.0473119341
C,1.3672046645,-4.2467586108,1.1222764648
C,1.0217297032,-1.9512065568,0.3269670451
C,-0.989428054,-3.2087320909,1.1020642768
H,0.0515970433,-3.9890204822,2.8148379894
H,2.2288678195,-2.4678125998,2.0498244444
H,1.2987902001,-4.649733702,0.1033221813
H,0.7934806014,-2.4753615663,-0.6105540609
H,-1.2143916097,-3.4955507714,0.0663241636
H,-0.0028457308,-1.692631425,2.1929557204
H,-0.472025774,-5.2367834137,1.6900837945
H,2.9579979467,-2.8994379927,0.4927915172
H,2.0105572132,-4.9277059499,1.6885623423
H,-1.9352792408,-3.1702224455,1.6524453425
N,-1.0142242273,-0.6554001162,0.7131962017
N,1.4029662625,-0.5861172708,-0.0809558019
C,0.5156276569,-0.2313804256,-1.2012813641
H,0.6050681525,0.8407632742,-1.387001796
C,-0.9735952929,-0.5429968113,-0.7531019189
H,-1.2115217143,-1.548170975,-1.1252309283
B,1.5593993795,0.3945886514,0.943387113
B,-1.0381051833,0.4377123912,1.6230548427
O,-0.8313491482,0.1563624538,2.9762656339
O,1.4614808195,1.7663496647,0.7903518026
C,1.4789346363,0.7522373238,3.3118200845

C,0.742375783,2.2228557133,5.5615142747
C,0.1233828361,0.8468522621,3.6780416015
C,2.4486742491,1.394301066,4.0705171232
C,2.0828064118,2.1290899024,5.1970315603
C,-0.2348849977,1.5833447962,4.8010925224
H,3.4870151161,1.3032262265,3.767642512
H,2.8471578457,2.6251084649,5.7860160255
H,-1.2853303928,1.6386413949,5.0681868276
H,0.4517155051,2.7932112061,6.43760749
O,1.8435928893,-0.0267268009,2.2364522396
C,0.615286978,2.5795303943,0.0922554245
C,-1.0675669733,4.4155516198,-1.1588922698
C,-0.7560386831,2.5914053851,0.3892228589
C,1.1298251542,3.4715175192,-0.8437997352
C,0.2889961203,4.3837510653,-1.4762843632
C,-1.5856829708,3.5236035494,-0.2250441429
H,2.1938140781,3.4399563339,-1.055560903
H,0.6991539995,5.0737995528,-2.2059770196
H,-2.6406031169,3.5188532336,0.0307912645
H,-1.7273044527,5.1293678856,-1.641258123
O,-1.2736964453,1.7722113197,1.3444701917
C,0.949197932,-0.9373935142,-2.4840278065
C,1.8592087471,-2.1559594879,-4.8490519708
C,2.317201871,-1.0093226872,-2.7742946
C,0.0451271754,-1.4853595476,-3.3982954467
C,0.4977266033,-2.0900783913,-4.571800311
C,2.7696104999,-1.6104261224,-3.9441140754
H,3.0276852706,-0.5946546139,-2.065440739
H,-1.0243841409,-1.4420307221,-3.2154076843
H,-0.2217118438,-2.5119693215,-5.2668584597
H,3.8349632113,-1.6558016172,-4.1489395807
H,2.2100331538,-2.628150106,-5.76136908
C,-2.0335924435,0.377306877,-1.3335748293
C,-4.0694112524,1.9610255473,-2.4491531166
C,-3.2967036205,0.4442902593,-0.7342436701
C,-1.8089848938,1.1091142055,-2.5031263911
C,-2.8206079135,1.8912422155,-3.0590526883
C,-4.3034961866,1.2331402944,-1.2825067452
H,-3.4884168231,-0.1245639593,0.1707071932
H,-0.839383987,1.0852997452,-2.9919232996
H,-2.6228971221,2.4550765447,-3.9656952715
H,-5.2747318113,1.276677163,-0.7988653074
H,-4.8552245973,2.5753774018,-2.8775882411

P-*Z,Z*[1,2]^{DMF} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*Z,Z*[1,2]^{DMF}** in DMF)
cydiimph2_ZZ_b2cat2_1-2_product_dmf
M062X/6-31G(d,p)
E(RM062X) = -1697.2155782

Zero-point correction= 0.576799 (Hartree/Particle)
Thermal correction to Energy= 0.606829
Thermal correction to Enthalpy= 0.607773
Thermal correction to Gibbs Free Energy= 0.517138
Sum of electronic and ZPE= -1696.638779
Sum of electronic and thermal Energies= -1696.608749
Sum of electronic and thermal Enthalpies= -1696.607805
Sum of electronic and thermal Free Energies= -1696.698440

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	380.791	126.125	190.757

C,0.2728592879,1.3555299084,1.1702988592
C,-0.1577823059,3.6576330865,1.9223647098
C,-2.104763582,2.133445558,1.2430703205
C,-1.5779320209,3.5757416029,1.3400266837
C,-1.0860625172,1.332478528,0.444687998
C,0.8465957373,2.7711755891,1.1656256146
H,-0.1847645273,3.338536148,2.9727666881
H,-2.2307101783,1.7027629624,2.2415735904
H,-1.5747137732,4.0133896871,0.3326233082
H,-0.9758886696,1.8659812736,-0.5062651324
H,0.9846724946,3.1476241116,0.1472798916
H,0.0800310057,1.1250744405,2.2186761841
H,0.1818232468,4.6982857138,1.9156140763
H,-3.0793024998,2.1160287642,0.7423512389
H,-2.2597479739,4.1810359611,1.9458698024
H,1.822398625,2.7857146064,1.6634695304
N,1.0760032306,0.2299800034,0.6528584523
N,-1.3864264618,-0.0680972858,0.0775228012
C,-0.5773475789,-0.3809188441,-1.1065056007
H,-0.5599970448,-1.4627742013,-1.2247971529
C,0.948674061,0.0144067236,-0.8010492408
H,1.5332690469,-0.8801524805,-1.0309969014
B,-1.3345035666,-1.0422807212,1.1254377033
B,1.3228305865,-0.8473411909,1.5405134022
O,1.2102638913,-0.6158286035,2.9111228499
O,-1.0690760185,-2.397129433,0.995615358
C,-1.0091555181,-1.3815130192,3.4693968784

C,0.0591038246,-2.796423757,5.6202780734
C,0.3805028217,-1.3785531582,3.6929796948
C,-1.8460367654,-2.091834659,4.3197078532
C,-1.3150202421,-2.7979379523,5.3976222087
C,0.9036736388,-2.0874327381,4.7682072733
H,-2.9136440638,-2.0767906437,4.1246337233
H,-1.9773470529,-3.3471880868,6.0584351342
H,1.9771856639,-2.065747907,4.925758536
H,0.4792430316,-3.3444795507,6.4571271201
O,-1.5443119061,-0.6408009215,2.4379646487
C,-0.2541531627,-3.1176879406,0.1700539743
C,1.4131023465,-4.6682849662,-1.436466376
C,1.1396811447,-2.9665472074,0.2543779273
C,-0.8003102509,-4.0545837259,-0.7011524346
C,0.0310046203,-4.8280129852,-1.5070955551
C,1.9644136211,-3.7427434108,-0.5544810825
H,-1.8801381014,-4.1565510323,-0.7378559429
H,-0.4043284966,-5.5522710598,-2.1872477686
H,3.0382252272,-3.608287288,-0.4723370165
H,2.0667552168,-5.2663356856,-2.0625129904
O,1.7038396883,-2.128782418,1.1691388491
C,-1.1709334833,0.1094011317,-2.4133076522
C,-2.2086510315,0.9325633994,-4.8847990534
C,-2.3739219286,0.8124314426,-2.4754024257
C,-0.5101681094,-0.2090576681,-3.6056219351
C,-1.0208087152,0.2016225079,-4.8316835152
C,-2.8853362324,1.2292149778,-3.7053721501
H,-2.9141257415,1.0331034175,-1.5593169042
H,0.4171655196,-0.7770929732,-3.5676520928
H,-0.4938863261,-0.0490670254,-5.7473017252
H,-3.8184176165,1.7836983861,-3.7378597451
H,-2.6074704793,1.2576675738,-5.8406457294
C,1.6551662699,1.1401511154,-1.5623315278
C,3.2226685196,3.1480339479,-2.7683559886
C,3.0543786874,1.1096639995,-1.4944062765
C,1.0555869589,2.1972746112,-2.2541143173
C,1.8343821183,3.1904586155,-2.849911757
C,3.8339218614,2.0983072954,-2.0848107553
H,3.5357325147,0.2941903064,-0.9587029098
H,-0.0219608524,2.2728822729,-2.3382339866
H,1.3447118436,4.0022727534,-3.3790587026
H,4.9160807189,2.0475329343,-2.0133241671
H,3.8231977432,3.9232351832,-3.2340744463

P-*E*,*E*[1,1]^{benzene} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,1]^{benzene}** and **TS-*Z*,*Z*[1,1]^{benzene}** in benzene)
cis-diph-tetrahydroquinoxaline_1-1-dieq_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2433188

Zero-point correction= 0.576784 (Hartree/Particle)
Thermal correction to Energy= 0.607675
Thermal correction to Enthalpy= 0.608619
Thermal correction to Gibbs Free Energy= 0.512070
Sum of electronic and ZPE= -1696.666535
Sum of electronic and thermal Energies= -1696.635644
Sum of electronic and thermal Enthalpies= -1696.634700
Sum of electronic and thermal Free Energies= -1696.731249

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.322	125.970	203.204

C,1.800991967,-0.4061348256,-0.6839109151
C,3.3493335498,-1.8529978563,-2.0388636307
C,0.9171804891,-2.4731711593,-1.8331158347
C,2.3452776567,-2.9996390957,-1.972254706
C,0.7689236783,-1.5471688365,-0.623515747
C,3.2193467097,-0.9609727503,-0.8064776438
H,3.167023438,-1.2589776534,-2.9441186076
H,0.6289928534,-1.9215443979,-2.7372789805
H,2.5832225508,-3.6371165213,-1.1104486787
H,1.0079902184,-2.1223043225,0.2908216246
H,3.465078489,-1.5383757535,0.0929294336
H,1.5924707593,0.1781319167,-1.592941009
H,4.3711444965,-2.238257627,-2.1104438655
H,0.2244959208,-3.3143114119,-1.7457671782
H,2.4154684245,-3.6312736758,-2.8632107562
H,3.9280156586,-0.1303631418,-0.8529168871
N,-0.6079014274,-1.0204687138,-0.4917928184
N,1.6281644566,0.4746135344,0.4713987499
C,0.2773336413,1.0469774259,0.5665179626
C,-0.7588062252,-0.1005850299,0.6422281852
H,-0.5146686883,-0.6342750738,1.5765186647
H,0.2108392615,1.5477094228,1.5349489359
C,-2.1478120658,0.4927011488,0.8008233211
C,-4.6472729055,1.6991218732,1.2129000647
C,-2.5890327471,0.7995968886,2.0886921473
C,-2.9756504313,0.8025240186,-0.2818853408
C,-4.2182475407,1.3933711559,-0.0763673933

C,-3.8266054575,1.4025227666,2.2968023832
H,-1.9570960613,0.5554497655,2.9394682411
H,-2.6545643581,0.5802577183,-1.295714808
H,-4.8512236638,1.6189775301,-0.9287361683
H,-4.1517766715,1.6307483718,3.3070384804
H,-5.616031073,2.1623632584,1.3707655156
C,0.0579681901,2.1236229086,-0.4897239852
C,-0.1984137849,4.2256757665,-2.3389117814
C,0.2967194592,3.4485613309,-0.1115547293
C,-0.3111342903,1.867877792,-1.8163162774
C,-0.4394059071,2.9116186729,-2.7300432243
C,0.171550742,4.4921937797,-1.0236411264
H,0.5888473323,3.6598086207,0.9141982102
H,-0.5096255642,0.8488257884,-2.131702673
H,-0.7301934867,2.6935799161,-3.7531526126
H,0.359653461,5.5128166688,-0.7051931045
H,-0.2996263084,5.0361899144,-3.0538395006
H,-5.201449693,-3.4046782958,0.6808062608
C,-4.8402900432,-3.4898395637,-0.3375200889
C,-3.8585801334,-3.6901505665,-3.0133162624
C,-3.6433719543,-2.9208227437,-0.7219996061
C,-5.5529161136,-4.1756994455,-1.3285338717
C,-5.0736862982,-4.2739410575,-2.6345296824
C,-3.1666971034,-3.0150620382,-2.0285766466
H,-6.4992466604,-4.6400078834,-1.0722600093
H,-5.6541109641,-4.8125894811,-3.3760008917
H,-3.4764539489,-3.7567867684,-4.0254571097
O,-1.973806578,-2.3464044944,-2.1215887093
O,-2.7475811463,-2.2123184931,0.0320322797
B,-1.724585907,-1.8393320831,-0.8417402567
H,6.4416139677,0.4206594361,2.7364088005
C,5.6752207232,1.0500088035,3.1739975076
C,3.6338457563,2.6963396071,4.3002176107
C,4.4082923139,1.1148051898,2.6330314273
C,5.9140146,1.8355005271,4.3096453006
C,4.9174928844,2.6390758704,4.8594212261
C,3.410840475,1.9190328195,3.1828710985
H,6.8969849906,1.8151903158,4.7680416725
H,5.1369078736,3.2347018582,5.7391193333
H,2.8499280317,3.3175340082,4.7180664563
O,2.2648431311,1.786955155,2.4461753507
O,3.9128292988,0.4570746267,1.5377649472
B,2.579017762,0.8728545889,1.4217118968

P-*E,Z*[1,1]^{benzene} (*N,N*-Diborylated product **2a** from reductive coupling transition state **TS-*E,Z*[1,1]^{benzene}** in benzene)
trans-dieq-diph-tetrahydroquinoxaline_1-1-dieq_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2419779

Zero-point correction= 0.576572 (Hartree/Particle)
Thermal correction to Energy= 0.607645
Thermal correction to Enthalpy= 0.608590
Thermal correction to Gibbs Free Energy= 0.510900
Sum of electronic and ZPE= -1696.665406
Sum of electronic and thermal Energies= -1696.634332
Sum of electronic and thermal Enthalpies= -1696.633388
Sum of electronic and thermal Free Energies= -1696.731078

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.303	126.236	205.604

C,1.5852473834,-1.1708561515,-0.2567507058
C,3.0252837009,-3.2263406401,-0.4976839769
C,0.5582899163,-3.3269598111,-1.0124013299
C,1.77182647,-4.1038489439,-0.4934707796
C,0.3579615285,-2.0732136836,-0.1618212325
C,2.8022282804,-1.9309615443,0.2862450008
H,3.2862380548,-2.9764985921,-1.5345049882
H,0.7186392236,-3.0534879851,-2.0585989872
H,1.5742195002,-4.4510274627,0.5293442478
H,0.2975890152,-2.4183829639,0.884844052
H,2.6182373121,-2.1619060554,1.3446692366
H,1.751572804,-0.9652269526,-1.3262435572
H,3.8767656808,-3.7731010341,-0.0805666014
H,-0.3463639578,-3.9426092907,-0.9737999061
H,1.9284263623,-4.9963824684,-1.1072028375
H,3.6904435068,-1.2969259936,0.2399422086
N,-0.8680826447,-1.3033496849,-0.3904869229
N,1.3710512415,0.1071300548,0.4413856853
C,0.0744550135,0.54703716,0.9894733811
C,-1.09761559,-0.4678862262,0.7915262376
H,-1.0797992855,-1.1458756144,1.655842794
H,-0.2080555612,1.4635613874,0.4603001669
C,-2.4191440489,0.2743588716,0.84811728
C,-4.8369457828,1.6723648179,1.0732278325
C,-3.3655235159,-0.0921031477,1.8030419559
C,-2.6967730171,1.356019159,0.0056805026
C,-3.8971166085,2.0468658707,0.1129733109

C,-4.5693170542,0.6011241416,1.9178186229
H,-3.1533141523,-0.9219472579,2.4717344695
H,-1.9783024976,1.6485683465,-0.7556290333
H,-4.1009102946,2.8797840643,-0.5525679463
H,-5.2922258095,0.3053125497,2.6714346532
H,-5.771867295,2.216884893,1.1613431195
C,0.1658742098,0.8884829645,2.46973375
C,0.2181760853,1.4463546539,5.2137704078
C,0.9411892949,0.1151184372,3.3351260994
C,-0.58166718,1.9454041556,2.9919204034
C,-0.5565396145,2.2230801056,4.3560544239
C,0.968275272,0.3913157198,4.6992152678
H,1.5384345739,-0.6969581337,2.9285102649
H,-1.1867670367,2.5529421004,2.3235417116
H,-1.1391679,3.0510901939,4.7477996542
H,1.5797057512,-0.2149910005,5.3605955346
H,0.2421758471,1.6653719804,6.2766695316
H,-1.6452949006,-2.909176149,-5.3660570133
C,-2.4579730398,-2.3838266581,-4.877607957
C,-4.5775121071,-0.9929382487,-3.5634310132
C,-2.3398650363,-1.9288535446,-3.5807572848
C,-3.675448656,-2.1285515069,-5.5227864078
C,-4.7099748153,-1.4497507863,-4.8814000525
C,-3.374974564,-1.2513269792,-2.9391523596
H,-3.8123564132,-2.4673804833,-6.5442063521
H,-5.6392112061,-1.2699904133,-5.411591518
H,-5.3723856304,-0.4636212805,-3.050530471
O,-2.9847983321,-0.92428722,-1.6693953983
O,-1.2731445234,-2.0327153245,-2.7288418301
B,-1.6774081468,-1.4068142316,-1.5371374038
H,5.9808013824,1.9333431966,-1.4012507131
C,5.3407931361,2.6247917025,-0.8653066465
C,3.6307801192,4.4186304711,0.5516024287
C,4.127663409,2.2216045218,-0.3477441561
C,5.6958023399,3.9646879546,-0.6615415579
C,4.8609417073,4.8400764299,0.0303941727
C,3.2910640186,3.0978714738,0.344271715
H,6.641665571,4.3252664465,-1.051537533
H,5.1679140165,5.8710005932,0.1709105447
H,2.9730872028,5.0886641672,1.0931214386
O,2.1611849519,2.4323490061,0.7416405403
O,3.5438369272,0.9816751018,-0.4018338606
B,2.3280053375,1.1219407816,0.2800157264

P-*Z*,*E*[1,1]^{benzene} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z*,*E*[1,1]^{benzene}** in benzene)
trans-diax-diph-tetrahydroquinoxaline_1-1-dieq_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.258502

Zero-point correction= 0.577660 (Hartree/Particle)
Thermal correction to Energy= 0.608371
Thermal correction to Enthalpy= 0.609316
Thermal correction to Gibbs Free Energy= 0.513639
Sum of electronic and ZPE= -1696.680842
Sum of electronic and thermal Energies= -1696.650131
Sum of electronic and thermal Enthalpies= -1696.649186
Sum of electronic and thermal Free Energies= -1696.744863

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.759	125.862	201.367

C,1.3948256093,-0.2194853079,-0.773320968
C,3.0187772076,-1.6815630394,-2.0228320649
C,0.6267593032,-2.4079308352,-1.7703259483
C,2.0795181981,-2.8742242258,-1.8566274504
C,0.4385149644,-1.418818945,-0.6217027055
C,2.8436967411,-0.6932501275,-0.8704560431
H,2.8023710515,-1.1793276727,-2.9749436503
H,0.3407581104,-1.9274605136,-2.7131827011
H,2.3458084427,-3.4210390493,-0.9424768846
H,0.7126157078,-1.9234905323,0.3188607226
H,3.1314925886,-1.1752973772,0.0710492909
H,1.128578424,0.2781688372,-1.7198608734
H,4.0606927265,-2.0135462834,-2.0669019411
H,-0.0454781769,-3.2594660849,-1.6323781331
H,2.1918445998,-3.5736392011,-2.6908603248
H,3.5022200129,0.1705358671,-0.9979910331
N,-0.9471365524,-0.9499704006,-0.4837673806
N,1.1741233713,0.7470502225,0.3111059375
C,-0.2152667624,1.2101647309,0.3956819903
C,-1.1287756258,-0.0092786028,0.6271506674
H,-2.1665059144,0.3302174559,0.606229097
H,-0.2922930177,1.8667714861,1.2648866896
C,-0.9316632517,-0.6931047555,1.9851819617
C,-0.7383176114,-2.0004262791,4.4709019146
C,-0.432828385,-0.0271638873,3.1079327565
C,-1.3363139812,-2.0241446236,2.1335657313
C,-1.242130611,-2.6727114548,3.3601852574

C,-0.3356644561,-0.676334761,4.3380358869
H,-0.1065939021,1.0049403143,3.0446567851
H,-1.723297635,-2.5599545208,1.2717371646
H,-1.562704841,-3.7063526022,3.4469017843
H,0.061879534,-0.1385232487,5.1932044951
H,-0.659795786,-2.504585564,5.428810364
C,-0.6018824956,2.0632935262,-0.8181658153
C,-1.2411352013,3.7689885556,-2.9646166849
C,0.3679322636,2.8891921969,-1.3967630214
C,-1.9004324451,2.1120435317,-1.332246667
C,-2.2153448274,2.9557480811,-2.3966749267
C,0.0552689275,3.7329486404,-2.4571516392
H,1.3838680161,2.8629205469,-1.0136433311
H,-2.6875691284,1.4918821781,-0.9181357205
H,-3.230198408,2.9696135124,-2.7820005713
H,0.8276570503,4.3627637319,-2.8877919969
H,-1.4878445969,4.4234049927,-3.7945590076
H,-3.3832622139,-3.3340382223,-4.5689321537
C,-3.9855531301,-2.7517437809,-3.8810947633
C,-5.5409020587,-1.2085572379,-2.0513565602
C,-3.4174651658,-2.1085783281,-2.8016208922
C,-5.3708925265,-2.6106271755,-4.0378818846
C,-6.1300756025,-1.8574501403,-3.1447473247
C,-4.1770726759,-1.3550674867,-1.9078955629
H,-5.8596895285,-3.09948678,-4.8738408368
H,-7.2007000923,-1.7697168717,-3.2960349727
H,-6.1202677881,-0.6207754887,-1.3485828571
O,-3.3566236198,-0.8382917434,-0.9408194427
O,-2.101261702,-2.0802199358,-2.4202274237
B,-2.0611625097,-1.2858992553,-1.2670598612
H,5.9681495553,1.0246330002,2.6018078279
C,5.185767562,1.6795933209,2.9676587347
C,3.101446738,3.3885773451,3.9075839766
C,3.9210759861,1.6587731865,2.4183216165
C,5.4000406284,2.5849610823,4.0155409413
C,4.3827005879,3.4191689141,4.474279209
C,2.9031741687,2.4935277244,2.8772194931
H,6.3802655788,2.6347886184,4.4775039776
H,4.5836061786,4.1086342729,5.2873574558
H,2.301737895,4.0330450492,4.2542393455
O,1.7653655261,2.260215972,2.1516928376
O,3.4466077429,0.8781914055,1.3964464
B,2.1049612381,1.2467840533,1.2337416977

P-*E*,*E*[1,2]^{benzene} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*E*,*E*[1,2]^{benzene}** in benzene)
cydiimph2_EE_b2cat2_1-2_product_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2112523

Zero-point correction= 0.577409 (Hartree/Particle)
Thermal correction to Energy= 0.607315
Thermal correction to Enthalpy= 0.608259
Thermal correction to Gibbs Free Energy= 0.518636
Sum of electronic and ZPE= -1696.633843
Sum of electronic and thermal Energies= -1696.603937
Sum of electronic and thermal Enthalpies= -1696.602993
Sum of electronic and thermal Free Energies= -1696.692616

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.096	125.886	188.627

C,0.1337742327,2.7421994974,-0.4212639531
C,0.6325526741,5.1477845343,-0.1905560274
C,0.9470723289,3.5657307667,1.8075177418
C,0.6463167565,5.0016068561,1.3403960821
C,-0.062575352,2.6565027664,1.1168658671
C,-0.2834963406,4.1296953086,-0.8935898731
H,1.6536341824,5.0060898142,-0.5680804042
H,1.9690611564,3.2809709687,1.5420511239
H,-0.3336766507,5.2997767211,1.7362760824
H,-1.041999422,3.0994081637,1.3504869092
H,-1.3349924789,4.3283030267,-0.6450796722
H,1.203111526,2.6484079123,-0.6244976778
H,0.3382302714,6.1675055423,-0.4583455909
H,0.8478250084,3.4887480486,2.8953354188
H,1.3793297701,5.694133632,1.7660824944
H,-0.1816384039,4.2099506937,-1.9802600813
N,-0.5157188314,1.5643559355,-1.0242390231
N,-0.1831772747,1.2433852336,1.5144853909
C,-1.5570255596,0.8163831843,1.1580814522
H,-2.2206623566,1.4609181354,1.7501686026
C,-1.7967887644,1.2976615755,-0.3597259547
H,-2.252900367,2.287105023,-0.2387450114
B,0.9261356972,0.3728251664,1.3125494498
B,0.3725007983,0.4814207741,-1.294412049
O,1.6654173967,0.7302626257,-1.7359311237
O,0.8458510965,-0.9980153966,1.4861686832
C,3.0548065865,0.2992582371,0.1724878217

C,4.9107218533,-0.9446248121,-1.4780175427
C,2.8018596025,0.1811586866,-1.2031925449
C,4.2280870386,-0.2035624569,0.7140457319
C,5.1586431111,-0.8291996602,-0.1135979464
C,3.7336322561,-0.4378500889,-2.0249273241
H,4.3939396623,-0.0982323119,1.7811230843
H,6.07489131,-1.2249280454,0.311067592
H,3.5171227956,-0.5192011028,-3.0847801815
H,5.6332675836,-1.4313762523,-2.1243855024
O,2.133918048,0.9607791148,0.9461368711
C,1.1194829695,-1.9799333014,0.5823161975
C,1.5818913929,-4.0555447937,-1.2267414771
C,0.6558331237,-1.8896305886,-0.7394627824
C,1.8121011303,-3.1144948728,0.9863449715
C,2.0438884934,-4.1485915903,0.0826511597
C,0.8813104006,-2.9230599262,-1.6362711577
H,2.1590252524,-3.166909382,2.0127194168
H,2.58717404,-5.0295094819,0.4079963239
H,0.4975956619,-2.8235418249,-2.6463610914
H,1.7597315971,-4.8619845853,-1.9299125082
O,-0.0985043057,-0.8006059549,-1.0958283831
C,-1.8883759478,-0.5924161551,1.6408601408
C,-2.4548498738,-3.0845549925,2.8144830916
C,-1.9679793775,-0.7366791474,3.0321604547
C,-2.1178750371,-1.7165030017,0.8460483328
C,-2.3976973249,-2.9509377278,1.4321744303
C,-2.2399862593,-1.966118347,3.6178574268
H,-1.7915002281,0.1332655832,3.660685739
H,-2.0732560675,-1.6429916849,-0.2321523952
H,-2.5645401526,-3.8132163557,0.7938869493
H,-2.2867671572,-2.0515055004,4.6992070858
H,-2.6687602442,-4.0493051498,3.2639653883
C,-2.8218397941,0.5400144186,-1.179992637
C,-4.8362174366,-0.7517395168,-2.6494046691
C,-2.6035090592,0.1624236825,-2.5040699322
C,-4.0761170056,0.288411775,-0.61079452
C,-5.0724358454,-0.3552627687,-1.3340159519
C,-3.6019478729,-0.4845856034,-3.2312145298
H,-1.6532568144,0.3814835705,-2.9781060262
H,-4.2696196186,0.5870098453,0.4167225211
H,-6.034305466,-0.5487812725,-0.8695896096
H,-3.4103022602,-0.7760076154,-4.2593811326
H,-5.6114588544,-1.2575365518,-3.2160857423

P-*E*,*Z*[1,2]^{benzene} (*N*,*N*-Diborylated product **2a** from reductive coupling transition state **TS-*E*,*Z*[1,2]^{benzene}** in benzene)
cydiimph2_EZ_b2cat2_1-2_product_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2200978

Zero-point correction= 0.577755 (Hartree/Particle)
Thermal correction to Energy= 0.607503
Thermal correction to Enthalpy= 0.608448
Thermal correction to Gibbs Free Energy= 0.519845
Sum of electronic and ZPE= -1696.642342
Sum of electronic and thermal Energies= -1696.612594
Sum of electronic and thermal Enthalpies= -1696.611650
Sum of electronic and thermal Free Energies= -1696.700253

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.214	125.898	186.480

C,-0.0757172914,2.3424739433,0.1338774397
C,-0.2565818206,4.6636815116,0.916549806
C,0.4071540373,2.7864480376,2.546058649
C,-0.2430259149,4.1725482554,2.3749915849
C,-0.308775754,1.8520956504,1.5793410679
C,-0.8516941369,3.6415273461,-0.0710700657
H,0.7739357593,4.8799432311,0.6060152642
H,1.4769346549,2.8289646683,2.3240645728
H,-1.2768188243,4.1191161532,2.7411554627
H,-1.3757810212,1.9819164392,1.8040902275
H,-1.9217724846,3.4987180247,0.1204497922
H,0.9784352306,2.6113874009,0.0515656146
H,-0.807555891,5.6075895145,0.8557074278
H,0.2891596909,2.4340361865,3.5760528545
H,0.273087738,4.9071409523,3.001190585
H,-0.7441706519,4.0036353354,-1.0990330973
N,-0.2539566091,1.2027752605,-0.7873907411
N,-0.0818021763,0.3924924016,1.6228452834
C,-1.2921200257,-0.1798239779,1.0148165328
H,-2.1255033991,0.2969709247,1.5420064762
C,-1.3794096344,0.3054720412,-0.4977277423
H,-1.2451902667,-0.5722386048,-1.1365600609
B,1.2011025011,-0.0553838616,1.1568102509
B,0.9143816778,0.6899143141,-1.4111517877
O,2.0560790544,1.4857653695,-1.4565111319
O,1.5430018399,-1.2905389185,0.646775922
C,3.3534786739,0.6866458071,0.406764763

C,5.5780212767,0.4959566675,-1.2579854038
C,3.2416870208,1.007629473,-0.9574719028
C,4.5731096137,0.271371676,0.9226858374
C,5.687380134,0.1776165371,0.0922406157
C,4.3555447318,0.9096758941,-1.7813525179
H,4.6301623314,0.0300416781,1.9789681221
H,6.637698525,-0.1460428219,0.5032087011
H,4.2432146053,1.1665536108,-2.8292780931
H,6.4428019947,0.4231578661,-1.9089372809
O,2.2635299377,0.8373191662,1.2346874913
C,1.0344374181,-2.1848868073,-0.2454500695
C,0.1146154379,-4.0773586424,-2.0757662898
C,0.7481154535,-1.8033161394,-1.5642970589
C,0.9154562029,-3.5195952082,0.1262704431
C,0.4526073266,-4.4645683525,-0.7812372638
C,0.2709272792,-2.7518634805,-2.4654382926
H,1.1719957105,-3.7886183407,1.1447806858
H,0.3470263257,-5.4985171875,-0.4703525522
H,0.0516702424,-2.4262396253,-3.4769073331
H,-0.2548836467,-4.806218991,-2.7892388114
O,1.0043879178,-0.5468514215,-2.023188299
C,-1.5029059573,-1.6618041876,1.2617797233
C,-2.0789523966,-4.3355986037,1.883391677
C,-2.2595692702,-2.4469754317,0.3887597525
C,-1.0493407274,-2.2279606355,2.4574397418
C,-1.3315436838,-3.5552713263,2.7634971736
C,-2.5437619877,-3.7754266131,0.6976248897
H,-2.6357105817,-2.0308568736,-0.54199562
H,-0.4721042463,-1.6169477268,3.1443630855
H,-0.9683021793,-3.9808429215,3.6941943384
H,-3.1247311405,-4.3733183948,0.0022537194
H,-2.2987871645,-5.37151097,2.1218689784
C,-2.7264789558,0.9092156769,-0.8798343003
C,-5.199240333,1.9600202459,-1.7053820297
C,-2.8048773344,1.7937548593,-1.9609467022
C,-3.9103450876,0.5448869248,-0.2319692756
C,-5.1365963247,1.0675637009,-0.6411212382
C,-4.0264493752,2.3187233177,-2.3673185285
H,-1.891590492,2.077372816,-2.4747960892
H,-3.8934903542,-0.1633585732,0.5916196576
H,-6.0431369952,0.773114953,-0.1216210829
H,-4.0626202963,3.0100233032,-3.2036704908
H,-6.153377911,2.3702465029,-2.020435058

P-*Z*,*E*[1,2]^{benzene} (*N*,*N*-Diborylated product **2c** from reductive coupling transition state **TS-*Z*,*E*[1,2]^{benzene}** in benzene)
cydiimph2_ZE_b2cat2_1-2_product_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2262009

Zero-point correction= 0.577557 (Hartree/Particle)
Thermal correction to Energy= 0.607421
Thermal correction to Enthalpy= 0.608365
Thermal correction to Gibbs Free Energy= 0.518879
Sum of electronic and ZPE= -1696.648644
Sum of electronic and thermal Energies= -1696.618780
Sum of electronic and thermal Enthalpies= -1696.617836
Sum of electronic and thermal Free Energies= -1696.707322

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.162	125.894	188.340

C,-0.4226802431,1.8240805523,1.4084276446
C,-0.4605363138,4.093131693,2.3579520197
C,-0.4247412745,3.7502278179,-0.1917822888
C,-0.0667052058,4.673170372,0.9880428837
C,0.1965545611,2.3951298219,0.1124135765
C,0.054537351,2.6599208435,2.5902103772
H,-1.5554533593,4.0772898913,2.4345641727
H,-1.5096903526,3.6613662779,-0.3038019463
H,1.0173219785,4.8471944925,0.9736938963
H,1.2567206299,2.6074583179,0.306876891
H,1.1507487489,2.6554608985,2.6597853498
H,-1.5027475773,1.9580636585,1.3472192452
H,-0.1002727871,4.7553862992,3.151519036
H,-0.019885523,4.1524917712,-1.126505309
H,-0.5424940768,5.6502283862,0.8574580574
H,-0.3402248516,2.2612809427,3.5301614845
N,-0.1815618458,0.3682602377,1.4243035786
N,0.2020688664,1.3277632283,-0.903294579
C,1.3210981884,0.4371398216,-0.5569962991
H,1.2239732883,-0.4823267652,-1.1377943861
C,1.188177036,0.072221148,0.982133968
H,1.8285647213,0.7794377,1.5268395828
B,-1.0428597304,0.708896262,-1.2276759705
B,-1.3129433054,-0.4613776372,1.1739353902
O,-2.572854781,0.0739369203,1.4414613517
O,-1.2144023239,-0.5435570737,-1.7865536786
C,-3.3859492994,0.7082202267,-0.7336752182

C,-5.7847685797,-0.5961304412,-0.1876540062
C,-3.5565230323,0.0308519059,0.4868406997
C,-4.4126694628,0.7242336064,-1.667106709
C,-5.6141202042,0.0740256847,-1.3951771662
C,-4.7560941869,-0.6177054905,0.7509106914
H,-4.2530106697,1.2555901689,-2.5995317722
H,-6.4128513714,0.0924461652,-2.1289827771
H,-4.8637875697,-1.1300682595,1.7010123609
H,-6.7183005225,-1.1048810942,0.0283443502
O,-2.2189089528,1.400666477,-0.9716544839
C,-0.617698075,-1.7528869964,-1.579722356
C,0.4233752979,-4.3116129247,-1.2216060522
C,-0.6822365843,-2.3672264076,-0.320022033
C,-0.0221339236,-2.4189335502,-2.6460929985
C,0.5043042341,-3.6949615423,-2.4676130718
C,-0.1725594129,-3.6497226166,-0.1536114118
H,0.0086752217,-1.9198526689,-3.608983836
H,0.9678442298,-4.2057493115,-3.3047777991
H,-0.2328099173,-4.0978124238,0.8328433569
H,0.8298726086,-5.3066284876,-1.0742973143
O,-1.3166552146,-1.7666013273,0.7221584892
C,2.6585730522,1.0679303729,-0.9383371347
C,5.0886443191,2.2139327582,-1.7627548681
C,2.7428924798,1.7865432146,-2.1364757569
C,3.8112801951,0.9354169153,-0.1596561766
C,5.0170177803,1.5037946222,-0.569830683
C,3.9443386865,2.3530775198,-2.5462981871
H,1.8468668704,1.9069623821,-2.737435753
H,3.7872783104,0.3777471913,0.7717878486
H,5.900030289,1.3896581166,0.0511497206
H,3.9871297921,2.9078728474,-3.4785374777
H,6.0269523623,2.6576477269,-2.0801232016
C,1.6719575866,-1.3149356921,1.3718483684
C,2.6348729779,-3.8200054129,2.2007946112
C,1.2663419523,-1.8691977249,2.5911517841
C,2.5700340109,-2.0326255348,0.5783800391
C,3.051239127,-3.2733720427,0.9920730266
C,1.7379913481,-3.1119406276,2.9996034775
H,0.5715729364,-1.3191373132,3.2184118858
H,2.8975565081,-1.6371989403,-0.3785680715
H,3.7432909819,-3.8161577614,0.3557939375
H,1.406474448,-3.5270141649,3.9464685799
H,3.0046115543,-4.7892080233,2.5204490396

P-*Z*,*Z*[1,2]^{benzene} (*N*,*N*-Diborylated product **2b** from reductive coupling transition state **TS-*Z*,*Z*[1,2]^{benzene}** in benzene)
cydiimph2_ZZ_b2cat2_1-2_product_benzene
M062X/6-31G(d,p)
E(RM062X) = -1697.2160513

Zero-point correction= 0.577649 (Hartree/Particle)
Thermal correction to Energy= 0.607606
Thermal correction to Enthalpy= 0.608550
Thermal correction to Gibbs Free Energy= 0.518402
Sum of electronic and ZPE= -1696.638403
Sum of electronic and thermal Energies= -1696.608446
Sum of electronic and thermal Enthalpies= -1696.607501
Sum of electronic and thermal Free Energies= -1696.697649

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	381.278	125.922	189.732

C,-0.0130981234,-1.9070549766,0.3354515653
C,-0.5728816583,-4.2742890873,-0.0292771124
C,-0.2209047343,-2.7046534706,-2.027219737
C,-0.9352937244,-3.9569436647,-1.4893445139
C,-0.5328898703,-1.5596753059,-1.0735309034
C,-0.8018060846,-3.0803932592,0.9141608101
H,0.4854070796,-4.5629654817,0.0196066126
H,0.8596619788,-2.8697789983,-2.0809567825
H,-2.0199582088,-3.797600249,-1.5592269451
H,-1.6273527175,-1.500615185,-1.0309541444
H,-1.8704162373,-2.8550914273,0.9850159734
H,1.0077742938,-2.2725409166,0.2176234442
H,-1.1514358846,-5.1384731063,0.3122813521
H,-0.5731169213,-2.4672110037,-3.0372584415
H,-0.7030297206,-4.8191090006,-2.1225467199
H,-0.4449122021,-3.3128343069,1.9229657969
N,0.0987628876,-0.6459374588,1.0927295278
N,-0.0781904284,-0.1931008522,-1.4043927754
C,-0.9550170111,0.7367604894,-0.6846007681
H,-0.4660597329,1.7088313667,-0.6683593596
C,-1.0132105123,0.2925628664,0.8576344327
H,-0.7797974709,1.19373217,1.4321693278
B,1.3235096066,0.074528218,-1.2836244538
B,1.4057699658,-0.1882242213,1.3982876152
O,2.4493093634,-1.1089997015,1.3793048696
O,1.9200439307,1.2987550827,-1.0260226354
C,3.4623414175,-0.870116295,-0.7960732631

C,5.9658833271,-0.7630448362,0.4200659923
C,3.5658918553,-0.9200441688,0.6058518857
C,4.6081740277,-0.7659224273,-1.5717723564
C,5.8616115921,-0.7154172891,-0.9664604621
C,4.8189042388,-0.8654891429,1.2032422773
H,4.4966102714,-0.729323284,-2.650399928
H,6.7521715523,-0.6366052108,-1.5807860656
H,4.8719633775,-0.9113963397,2.2857661707
H,6.9391600391,-0.7223477122,0.8975006886
O,2.2278392922,-0.970646013,-1.4012903445
C,1.5674534493,2.3863072505,-0.2827076419
C,0.9526377045,4.6377938746,1.2399941905
C,1.4644867845,2.2806418026,1.1145518666
C,1.379637416,3.6177463699,-0.9012277197
C,1.0691267032,4.7430554192,-0.14330484
C,1.1535677223,3.4106525601,1.8650151459
H,1.4758915466,3.6678752378,-1.9807079285
H,0.9200513736,5.69750218,-0.6362397971
H,1.0837772222,3.3032799681,2.9424756028
H,0.7111274921,5.5101522444,1.8376556652
O,1.7305309462,1.1122128474,1.7588614244
C,-2.272769076,1.0142945181,-1.3829472399
C,-4.7085608403,1.6207334908,-2.6292523203
C,-2.6065694326,0.4291118603,-2.6034250485
C,-3.1564397821,1.935596037,-0.810036196
C,-4.3662191394,2.2344355577,-1.4244433651
C,-3.8230925844,0.7245560475,-3.2186769446
H,-1.9056713191,-0.2535400468,-3.0740359011
H,-2.8971198873,2.4111594256,0.1333699403
H,-5.0439311109,2.9462741715,-0.9636916743
H,-4.0736067465,0.255063713,-4.1650453004
H,-5.6548735575,1.8498102527,-3.1088324268
C,-2.2955259427,-0.256553393,1.4925552465
C,-4.4619319541,-1.3304579955,2.9377379662
C,-2.2839667592,-0.3044420044,2.8926151951
C,-3.4206311036,-0.7542072041,0.8298126988
C,-4.4919863059,-1.2855238177,1.5488681837
C,-3.3476774502,-0.8347980674,3.6115959322
H,-1.4104658558,0.069443109,3.4219234739
H,-3.4849107252,-0.7418647802,-0.2510170281
H,-5.3537305135,-1.6668779703,1.0100234501
H,-3.3069908877,-0.8612020905,4.6960355521
H,-5.2980622409,-1.7458973683,3.4912592076

2a^{MeOH} (Diamine product **2a** in MeOH)
trans-dieq-diph-tetrahydroquinoxaline_meoh

M062X/6-31G(d,p)
E(RM062X) = -885.7669331

Zero-point correction= 0.406107 (Hartree/Particle)
Thermal correction to Energy= 0.423922
Thermal correction to Enthalpy= 0.424866
Thermal correction to Gibbs Free Energy= 0.360073
Sum of electronic and ZPE= -885.360826
Sum of electronic and thermal Energies= -885.343011
Sum of electronic and thermal Enthalpies= -885.342067
Sum of electronic and thermal Free Energies= -885.406860

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.015	73.669	136.368

H,1.5186467414,-3.4442180063,-1.9267503953
C,1.8453808493,-3.1097018078,-0.9348171296
C,3.833239866,-2.7635381677,0.5830397315
C,1.8970361792,-1.1570472596,0.6409724935
C,3.4064983574,-1.3093134832,0.7943714661
C,1.4428830564,-1.6532142848,-0.7302885557
C,3.356960533,-3.2864116235,-0.7753199477
H,3.4027318005,-3.3854381629,1.3792633482
H,1.3953173589,-1.7968229414,1.3929912494
H,3.8996050486,-0.6634286388,0.0557461278
H,1.9639010537,-1.0296772397,-1.4828234098
H,3.8711300008,-2.7349056723,-1.5737808362
H,1.3164587109,-3.7254509611,-0.1952340152
H,4.9216125052,-2.8513191444,0.6641808954
H,3.7112969581,-0.9563403975,1.7868913307
H,3.6264222301,-4.3411342079,-0.8927722945
N,-0.0071522975,-1.4955699062,-0.8255840644
H,-0.3198565911,-1.8374401283,-1.7333615496
N,1.4975542142,0.2415218603,0.7857277633
H,1.8093532067,0.5841538173,1.693529458
C,0.0463918027,0.4062515004,0.7007186617
H,-0.4826103621,-0.2174812169,1.4437720338
C,-0.4141263961,-0.0968337221,-0.6908847076
H,0.0867207485,0.5505890802,-1.4331851586
C,-0.3420561693,1.8511729511,0.9161800294
C,-1.1391475613,4.5227146646,1.218843144
C,0.4000764616,2.883598338,0.3348426211
C,-1.4858096549,2.1728912632,1.6513095799
C,-1.8843503528,3.4991706697,1.8018569768
C,0.004352,4.2111139419,0.4853159535

H,1.2931278187,2.639060991,-0.2324072924
H,-2.0717131216,1.3744957741,2.1010639095
H,-2.7754106577,3.7334041055,2.3767251882
H,0.5904764741,5.0035602293,0.0291907954
H,-1.4470333695,5.5572938404,1.336629745
C,-1.9101445238,0.0438647899,-0.8559517146
C,-4.6866122747,0.3791729824,-1.0630507707
C,-2.4449941449,1.1345500205,-1.5461920891
C,-2.782224798,-0.8792205684,-0.2711392486
C,-4.1618205415,-0.7129533137,-0.374136998
C,-3.8238548423,1.3038046193,-1.6492082478
H,-1.7726481958,1.8602114201,-1.9982580621
H,-2.3713831828,-1.7317996547,0.261241981
H,-4.8280702487,-1.4379809465,0.0841308678
H,-4.2244475332,2.1563887046,-2.1895350965
H,-5.7617075374,0.5082562329,-1.1438537152

2b^{MeOH} (Diamine product **2b** in MeOH)
cis-diph-tetrahydroquinoxaline_meoh
M062X/6-31G(d,p)
E(RM062X) = -885.7574577

Zero-point correction= 0.406964 (Hartree/Particle)
Thermal correction to Energy= 0.424653
Thermal correction to Enthalpy= 0.425597
Thermal correction to Gibbs Free Energy= 0.360397
Sum of electronic and ZPE= -885.350494
Sum of electronic and thermal Energies= -885.332805
Sum of electronic and thermal Enthalpies= -885.331861
Sum of electronic and thermal Free Energies= -885.397060

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.474	73.565	137.224

H,2.3030813076,-2.9870584036,1.516714549
C,2.6314738075,-1.9896349436,1.2055124398
C,4.5733303959,-0.6141818157,0.3482491764
C,2.2390090923,-0.1439786962,-0.4556706081
C,3.7163818765,-0.1527627185,-0.8325500499
C,1.7907172416,-1.5265876031,0.0208711515
C,4.1213676993,-1.9871871228,0.8538155422
H,4.4878485572,0.1166703346,1.1635374521
H,2.0994032127,0.5524727251,0.3954028702
H,3.855461464,-0.8332240172,-1.6836409475
H,1.942134511,-2.2215304408,-0.820166369

H,4.3053058207,-2.7357821022,0.0715609916
H,2.4525397973,-1.3108906477,2.0522312789
H,5.6288248296,-0.6451479421,0.0584602258
H,4.0193726482,0.8475049715,-1.1655109608
H,4.7138495494,-2.285379362,1.7250580541
N,0.3647109184,-1.5569769938,0.3543405391
H,0.2277649815,-0.9890176953,1.1908596056
N,1.4127353417,0.2286931835,-1.6026460808
H,1.7380658283,1.1224332264,-1.9674567331
C,-0.0151590548,0.3487024168,-1.2573994484
H,-0.533571761,0.5266013399,-2.206556263
C,-0.4669611358,-1.0349507857,-0.7350272215
H,-0.2894193645,-1.7100785281,-1.5851094795
C,-0.3086546205,1.5581068494,-0.3643544055
C,-0.7205619923,3.9060111483,1.1428498648
C,-0.8092052059,1.4967634057,0.939919581
C,-0.0318902666,2.8241464834,-0.8996573753
C,-0.2333109577,3.9853701968,-0.1614145803
C,-1.0103164086,2.6590111464,1.6866945716
H,-1.0764785938,0.5456199302,1.3878859918
H,0.3396296951,2.9006025148,-1.9199490094
H,-0.0150163424,4.952333131,-0.6048753763
H,-1.3989592117,2.5826645271,2.6978675043
H,-0.8796330748,4.8086428166,1.724794766
C,-1.9488013881,-1.1236642562,-0.3961080079
C,-4.6929682666,-1.3410748587,0.1949608164
C,-2.3969816916,-1.9548545524,0.6352509949
C,-2.9010080441,-0.4057689143,-1.1304050843
C,-4.2582510157,-0.5140168841,-0.8391294586
C,-3.7554766997,-2.0614042774,0.929718598
H,-1.6727212526,-2.5215237682,1.2098719947
H,-2.5899692507,0.2481440032,-1.9395777884
H,-4.9778510979,0.0540438847,-1.4213073703
H,-4.0789683163,-2.7111871453,1.7376856858
H,-5.751056602,-1.4218747806,0.424393362

2c^{MeOH} (Diamine product **2c** in MeOH)
trans-diax-diph-tetrahydroquinoxaline_meoh
M062X/6-31G(d,p)
E(RM062X) = -885.7582061

Zero-point correction= 0.406868 (Hartree/Particle)
Thermal correction to Energy= 0.424571
Thermal correction to Enthalpy= 0.425515
Thermal correction to Gibbs Free Energy= 0.360597
Sum of electronic and ZPE= -885.351338

Sum of electronic and thermal Energies= -885.333636
Sum of electronic and thermal Enthalpies= -885.332691
Sum of electronic and thermal Free Energies= -885.397609

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.422	73.419	136.631

H,2.0997341173,1.2553246072,-2.5725217141
C,2.1855996254,1.2965804375,-1.4799622129
C,2.6772389105,2.7743355838,0.5053129099
C,0.940379598,0.9588969723,0.673492395
C,1.3471134523,2.3550169558,1.1346520149
C,0.8553102376,0.8972221572,-0.8490147189
C,2.6120460127,2.6929465343,-1.0223217888
H,3.4739082451,2.1108257879,0.8674779392
H,1.7256110546,0.2423434138,0.9826229662
H,0.5575495481,3.0612931517,0.844590862
H,0.0838880022,1.6280496504,-1.1594950925
H,1.887976087,3.4314988844,-1.3915831535
H,2.9451659507,0.5592971718,-1.1869689029
H,2.9397273175,3.7891056166,0.8220180126
H,1.4120781335,2.374668596,2.229254498
H,3.5819505058,2.9520423952,-1.4594889358
N,0.5013750032,-0.4683441213,-1.2323942816
H,0.4535971084,-0.5247660892,-2.2491178757
N,-0.3688122471,0.6053679337,1.2194367436
H,-0.3274996959,0.6551069836,2.2367923021
C,-0.8129535427,-0.7496635811,0.8438717628
H,-1.8609642081,-0.8282231038,1.1574149334
C,-0.7946858006,-0.9120767039,-0.6867307046
H,-0.8630045722,-1.9874137963,-0.8911566237
C,-0.0546063039,-1.8400217746,1.5966321132
C,1.2963793584,-3.7641469121,3.1401310693
C,1.0313382537,-2.5449278798,1.0666893614
C,-0.4514180378,-2.1177732319,2.9105469819
C,0.2149275703,-3.0681741259,3.6787481359
C,1.6993964529,-3.4998399306,1.8336051247
H,1.3560388093,-2.3353725613,0.0525600617
H,-1.3006411562,-1.5828307054,3.3316075252
H,-0.1141282952,-3.2713313192,4.6936294834
H,2.5400337337,-4.0384603582,1.4057372933
H,1.8179412316,-4.5087986533,3.7338172177
C,-1.9787169363,-0.2617276972,-1.3978819606
C,-4.0888610639,0.8776914616,-2.8671758636
C,-2.6708998689,0.8501910614,-0.9064280141

C,-2.3637569623,-0.7921391973,-2.635373587
C,-3.4065501916,-0.2308542949,-3.3667783183
C,-3.7181244053,1.4131769132,-1.6362816098
H,-2.3792019354,1.277777528,0.0474505149
H,-1.8393047916,-1.6627819972,-3.0246889196
H,-3.6917901913,-0.6626655043,-4.3216144191
H,-4.2452729016,2.275835779,-1.2390561976
H,-4.9051112345,1.3177379335,-3.432057274

2a^{DMF} (Diamine product **2a** in DMF)
trans-dieq-diph-tetrahydroquinoxaline_dmf
M062X/6-31G(d,p)
E(RM062X) = -885.7655681

Zero-point correction= 0.406098 (Hartree/Particle)
Thermal correction to Energy= 0.423871
Thermal correction to Enthalpy= 0.424815
Thermal correction to Gibbs Free Energy= 0.360391
Sum of electronic and ZPE= -885.359470
Sum of electronic and thermal Energies= -885.341697
Sum of electronic and thermal Enthalpies= -885.340753
Sum of electronic and thermal Free Energies= -885.405177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	265.983	73.671	135.592

H,1.5155424088,-3.4395319702,-1.9287322822
C,1.8416126041,-3.1057032845,-0.9364716267
C,3.8291843844,-2.7603092737,0.5833262278
C,1.8923984706,-1.155869276,0.642213671
C,3.4019697236,-1.3063308796,0.7962478382
C,1.4408934021,-1.6488158991,-0.7313525043
C,3.3530801548,-3.2829631579,-0.7753942233
H,3.3983835089,-3.3825238262,1.3790084027
H,1.3891090551,-1.7980771501,1.3912772408
H,3.8932219016,-0.6584978866,0.0581309786
H,1.9641315166,-1.0233931799,-1.4809495419
H,3.867526447,-2.7311291989,-1.5733132426
H,1.3104397263,-3.7199463612,-0.1972872084
H,4.9174350642,-2.8481982131,0.6643355094
H,3.7062146517,-0.9541380644,1.7890921446
H,3.6226315164,-4.3375506062,-0.8927138242
N,-0.0080743015,-1.4896967118,-0.8263556493
H,-0.3254291275,-1.838137508,-1.7299032026
N,1.4916368859,0.2414033898,0.7866822455

H,1.8089817567,0.5898525624,1.690230065
C,0.0416140832,0.4099502575,0.7016124492
H,-0.491086984,-0.2121152044,1.4436244951
C,-0.4186116635,-0.0927384535,-0.6915307844
H,0.0799954562,0.5580142018,-1.4326310905
C,-0.3390171511,1.857407601,0.914898569
C,-1.1140914608,4.5353911437,1.2130379655
C,0.4235125845,2.8839065749,0.3496663841
C,-1.491743837,2.1877734493,1.6319179591
C,-1.8792750156,3.5175567791,1.7802667577
C,0.0384071468,4.2148793198,0.4975878576
H,1.324016165,2.6296871038,-0.2014741323
H,-2.0926087906,1.3934878692,2.0689540224
H,-2.7771511139,3.7591212989,2.3411043343
H,0.6399086008,5.0029535957,0.0543184401
H,-1.4135058594,5.5725093075,1.3293177899
C,-1.9157265892,0.0397699005,-0.854602248
C,-4.6946435218,0.3521715189,-1.0577008706
C,-2.4600557643,1.1373340381,-1.5262389988
C,-2.7789969035,-0.9019643367,-0.2866760603
C,-4.1601072174,-0.746814856,-0.3873654219
C,-3.8404215907,1.2950875674,-1.6273107256
H,-1.7939101006,1.8766913831,-1.9650207978
H,-2.3578534817,-1.7597998242,0.2291209942
H,-4.8198319725,-1.4858991138,0.0574610021
H,-4.2489572019,2.1527587868,-2.1532122622
H,-5.770747944,0.4724369247,-1.1371965939

2b^{DMF} (Diamine product **2b** in DMF)
cis-diph-tetrahydroquinoxaline_dmf
M062X/6-31G(d,p)
E(RM062X) = -885.755629

Zero-point correction= 0.406775 (Hartree/Particle)
Thermal correction to Energy= 0.424478
Thermal correction to Enthalpy= 0.425422
Thermal correction to Gibbs Free Energy= 0.360055
Sum of electronic and ZPE= -885.348854
Sum of electronic and thermal Energies= -885.331151
Sum of electronic and thermal Enthalpies= -885.330207
Sum of electronic and thermal Free Energies= -885.395574

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.364	73.632	137.576

H,2.2925097271,-2.9746117906,1.5336736437
C,2.6271002161,-1.9812760243,1.2162008701
C,4.5740957277,-0.6215137363,0.3446535788
C,2.2400692789,-0.1403664724,-0.4528147622
C,3.7160785304,-0.1598038206,-0.8354536162
C,1.7869384926,-1.5198860898,0.0306791168
C,4.1158169968,-1.989353524,0.8592251247
H,4.4954911685,0.1137576136,1.1565301087
H,2.1060915535,0.5601534707,0.3960705229
H,3.8458235161,-0.8451572147,-1.6840613481
H,1.9347214158,-2.2178131043,-0.8087375964
H,4.2920588401,-2.7428283631,0.0800135365
H,2.4543842746,-1.29621486,2.0589850341
H,5.6283141912,-0.6604135768,0.0516549006
H,4.0242661212,0.8367652137,-1.1743104733
H,4.7100584686,-2.2862593792,1.729555067
N,0.3617302308,-1.5422720862,0.3642238572
H,0.2240827976,-0.9722977514,1.1990162871
N,1.4120419716,0.2281756799,-1.5988878396
H,1.7411536573,1.1131759716,-1.9806693403
C,-0.0157305994,0.3529567549,-1.2580402819
H,-0.5321569963,0.5280105599,-2.2091271
C,-0.4682941263,-1.0287219717,-0.7298323002
H,-0.2844125689,-1.7075357447,-1.5757858044
C,-0.3080570054,1.5660304553,-0.3686389234
C,-0.716546331,3.9183258926,1.1323200732
C,-0.8129960624,1.508975985,0.9341194992
C,-0.0245077086,2.8298220266,-0.9056408014
C,-0.224482423,3.9933007991,-0.1704803423
C,-1.0124034133,2.6734797148,1.6779351115
H,-1.0846748538,0.5594572958,1.3828572665
H,0.3516646798,2.9022066129,-1.9244194454
H,-0.0010779081,4.9584985858,-0.6149835272
H,-1.4043698923,2.6006225185,2.6879635728
H,-0.8743284656,4.8226273475,1.71181627
C,-1.9500808598,-1.1235954039,-0.3928858925
C,-4.6922441427,-1.3644394989,0.1948300251
C,-2.3948069861,-1.9881790875,0.6124876576
C,-2.903842505,-0.3832657231,-1.1020471368
C,-4.2606415441,-0.5033067254,-0.8124116714
C,-3.7525555781,-2.1064594333,0.9052945212
H,-1.6663720808,-2.56996228,1.1666820347
H,-2.5939926862,0.2983678867,-1.8883775156
H,-4.9821031472,0.0822642944,-1.3743806807
H,-4.0742189044,-2.7822007524,1.6922860978
H,-5.7497781077,-1.4544412844,0.4229076115

2c^{DMF} (Diamine product **2c** in DMF)
trans-diax-diph-tetrahydroquinoxaline_dmf
M062X/6-31G(d,p)
E(RM062X) = -885.7571777

Zero-point correction= 0.406770 (Hartree/Particle)
Thermal correction to Energy= 0.424476
Thermal correction to Enthalpy= 0.425420
Thermal correction to Gibbs Free Energy= 0.360502
Sum of electronic and ZPE= -885.350407
Sum of electronic and thermal Energies= -885.332702
Sum of electronic and thermal Enthalpies= -885.331758
Sum of electronic and thermal Free Energies= -885.396676

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.362	73.467	136.631

H,2.1118907109,1.2354347051,-2.5665995605
C,2.1901837724,1.2836998256,-1.4738746546
C,2.6671927514,2.7758029486,0.5057358912
C,0.9340734845,0.9585910259,0.6741493736
C,1.3335543264,2.3586205591,1.129441729
C,0.8551807401,0.8908759187,-0.8490426393
C,2.6138430927,2.682952489,-1.0219384519
H,3.4619161347,2.1159928412,0.8784898298
H,1.7207824356,0.245875294,0.9886907001
H,0.5433776687,3.0599206568,0.8292150319
H,0.087012108,1.6227558961,-1.1653962163
H,1.8925306829,3.4186440263,-1.4018680533
H,2.9457789412,0.5466544885,-1.1702677393
H,2.9260410228,3.7932126763,0.8164775395
H,1.3912771153,2.3856231677,2.2241773062
H,3.5870713563,2.9390816434,-1.4531112208
N,0.4998285938,-0.474999993,-1.2264413531
H,0.4656110869,-0.5448655024,-2.2427707985
N,-0.3759358867,0.6030619882,1.2143312817
H,-0.348543771,0.6658724156,2.2313278849
C,-0.8168354109,-0.7537187093,0.8443189263
H,-1.8639586996,-0.8335484893,1.160445893
C,-0.7986164467,-0.916097,-0.6864142224
H,-0.8684753259,-1.990838532,-0.8933601355
C,-0.0528794076,-1.841272256,1.5961845724
C,1.3071828812,-3.7609174558,3.1369173205
C,1.0325761931,-2.5446897053,1.0628044368

C,-0.444063141,-2.1176696713,2.9119888275
C,0.2267979361,-3.0659392248,3.6789115464
C,1.7049392695,-3.4975592693,1.8285393457
H,1.3533093701,-2.3341954457,0.0473885135
H,-1.2923349758,-1.5831418111,3.3352691322
H,-0.0978354919,-3.268201563,4.6952775665
H,2.5449331115,-4.0352328275,1.3984809661
H,1.8321800314,-4.5038818487,3.7295044358
C,-1.9799836972,-0.2600015957,-1.3974793964
C,-4.0857513542,0.8888434516,-2.8653220841
C,-2.6703438967,0.8518071679,-0.902718438
C,-2.3640656257,-0.7849594018,-2.6375041769
C,-3.404787679,-0.2189975384,-3.3682742945
C,-3.71558693,1.4192484651,-1.6320056508
H,-2.3774419036,1.2755983821,0.0527168192
H,-1.8402705228,-1.6548834186,-3.0290680295
H,-3.6894430844,-0.6465280724,-4.3250844876
H,-4.2415631949,2.2815070493,-1.232641378
H,-4.9003483933,1.3324622209,-3.4296018352

2a$^{\textbf{benzene}}$ (Diamine product **2a** in benzene)
trans-dieq-diph-tetrahydroquinoxaline_benzene
M062X/6-31G(d,p)
E(RM062X) = -885.7652427

Zero-point correction= 0.406833 (Hartree/Particle)
Thermal correction to Energy= 0.424553
Thermal correction to Enthalpy= 0.425497
Thermal correction to Gibbs Free Energy= 0.361219
Sum of electronic and ZPE= -885.358410
Sum of electronic and thermal Energies= -885.340690
Sum of electronic and thermal Enthalpies= -885.339746
Sum of electronic and thermal Free Energies= -885.404024

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.411	73.517	135.286

H,1.5118710097,-3.4341216618,-1.9307759498
C,1.8349798797,-3.099119643,-0.9377177384
C,3.8226507333,-2.7546225257,0.5835510104
C,1.8846982022,-1.1513468565,0.6432572188
C,3.3943939733,-1.3009592828,0.7978739127
C,1.4350940066,-1.6419794852,-0.7320350443
C,3.3463585717,-3.2774967395,-0.7752645347
H,3.3932623354,-3.3780479753,1.3789625705

H,1.3788508257,-1.7968022482,1.3882651229
H,3.8840147143,-0.6488711522,0.0630636556
H,1.9612213393,-1.0135879735,-1.4775852747
H,3.8622467063,-2.726853554,-1.5729892693
H,1.2992346404,-3.7123978818,-0.2016740208
H,4.9107336967,-2.8428410017,0.664451318
H,3.7003242946,-0.951502958,1.7913915125
H,3.6162093001,-4.3318654239,-0.8924786823
N,-0.011380271,-1.4813078853,-0.8220573537
H,-0.3451544451,-1.8454284991,-1.7123873613
N,1.4826768851,0.2433353471,0.7827119662
H,1.8122512872,0.6109897164,1.6731542841
C,0.0346908967,0.4211992738,0.7001954114
H,-0.5031272342,-0.1949619342,1.4439635664
C,-0.430826339,-0.0878845663,-0.6896019622
H,0.0610385564,0.5669424302,-1.4321412366
C,-0.3294545855,1.8745555357,0.9060849293
C,-1.0624723737,4.5633551495,1.1920798323
C,0.480902009,2.8888866572,0.3887433348
C,-1.5090685825,2.2223134039,1.5677765004
C,-1.8753349746,3.5574610807,1.710068407
C,0.1162154411,4.2255268861,0.5315265851
H,1.4014469289,2.6158327812,-0.118234242
H,-2.1500652097,1.4367713653,1.9606845443
H,-2.7959166282,3.8123209975,2.2259199525
H,0.7548877705,5.0049359145,0.1268433011
H,-1.3457119852,5.6053443911,1.3042963854
C,-1.930708828,0.0271821658,-0.8456436755
C,-4.712728047,0.2959909955,-1.0376395181
C,-2.4950187815,1.1467898446,-1.4606992618
C,-2.775340821,-0.9583090864,-0.3273854889
C,-4.1583909262,-0.8243756824,-0.4234307945
C,-3.8768528807,1.2825219232,-1.5562434944
H,-1.8429448336,1.9230112481,-1.8539035351
H,-2.3336137195,-1.8314927108,0.1431622324
H,-4.8044523737,-1.5975673885,-0.0185499108
H,-4.3009454464,2.1590924342,-2.0361357846
H,-5.7907451011,0.3993849176,-1.1134533684

2b$^{\textbf{benzene}}$ (Diamine product **2b** in benzene)
cis-diph-tetrahydroquinoxaline_benzene
M062X/6-31G(d,p)
E(RM062X) = -885.7540926

Zero-point correction= 0.407405 (Hartree/Particle)
Thermal correction to Energy= 0.425004

Thermal correction to Enthalpy= 0.425948
Thermal correction to Gibbs Free Energy= 0.361612
Sum of electronic and ZPE= -885.346688
Sum of electronic and thermal Energies= -885.329089
Sum of electronic and thermal Enthalpies= -885.328145
Sum of electronic and thermal Free Energies= -885.392481

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.694	73.504	135.406

H,2.2700610304,-2.9279903813,1.5876541199
C,2.6146037031,-1.9459858371,1.2483274324
C,4.5693768921,-0.6220505192,0.3372059226
C,2.2344386988,-0.1350866107,-0.4556783452
C,3.7079870058,-0.1753938126,-0.846666446
C,1.7737197248,-1.5021315141,0.0567316833
C,4.1015605905,-1.9742971361,0.8843354708
H,4.5045651722,0.1308347536,1.1339947039
H,2.111002644,0.5839289927,0.3797318347
H,3.8239332757,-0.8753228063,-1.6847103589
H,1.9145978993,-2.2166721637,-0.7691674799
H,4.2673673985,-2.7465850528,0.1216269308
H,2.4537673461,-1.2423906833,2.0785520928
H,5.6212148151,-0.6770589515,0.0388617764
H,4.0262644364,0.8114023173,-1.2049878791
H,4.6986843517,-2.257759165,1.7569953354
N,0.3502506511,-1.5098390098,0.3901774465
H,0.2098443146,-0.9235117773,1.2122652541
N,1.4028094301,0.2160500962,-1.6035207162
H,1.7380616616,1.0874316268,-2.0081336677
C,-0.0230949069,0.3543159839,-1.2623554441
H,-0.5408152146,0.5164383202,-2.216093209
C,-0.4768421851,-1.0192000603,-0.7162589363
H,-0.2797861154,-1.7107315345,-1.5484544184
C,-0.3036787236,1.5794518557,-0.3846324262
C,-0.6767389005,3.9443525192,1.1031283012
C,-0.8336287721,1.5395498151,0.9080157768
C,0.0182604272,2.833965984,-0.9193472963
C,-0.1638013655,4.0037507971,-0.1912279133
C,-1.0143888229,2.7098112474,1.6454479298
H,-1.1481211161,0.5988497531,1.3469653926
H,0.408873273,2.8960716105,-1.9335700695
H,0.0891598471,4.9618336771,-0.6348771961
H,-1.4281116319,2.6499356058,2.647362972
H,-0.8208402137,4.8536521212,1.6779301109

C,-1.9582236216,-1.1290653625,-0.3834648405
C,-4.6923549704,-1.4308343447,0.197317889
C,-2.3939867989,-2.0946252889,0.5294923507
C,-2.9152744229,-0.3168555272,-1.0005601667
C,-4.2692215465,-0.4672353988,-0.7141121261
C,-3.7481786871,-2.2436331263,0.8178931594
H,-1.6556503247,-2.727173465,1.0102274711
H,-2.6106372916,0.4521230262,-1.703694946
H,-4.9943877268,0.1770942289,-1.2016241897
H,-4.0647976419,-2.9995872432,1.5302435335
H,-5.7480266285,-1.5450285801,0.4226481709

2c$^{\textbf{benzene}}$ (Diamine product **2c** in benzene)
trans-diax-diph-tetrahydroquinoxaline_benzene
M062X/6-31G(d,p)
E(RM062X) = -885.7572334

Zero-point correction= 0.407381 (Hartree/Particle)
Thermal correction to Energy= 0.425023
Thermal correction to Enthalpy= 0.425968
Thermal correction to Gibbs Free Energy= 0.361760
Sum of electronic and ZPE= -885.349852
Sum of electronic and thermal Energies= -885.332210
Sum of electronic and thermal Enthalpies= -885.331266
Sum of electronic and thermal Free Energies= -885.395473

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	266.706	73.334	135.136

H,2.1144856235,1.2421600689,-2.5677248057
C,2.1918560251,1.2872764176,-1.4745947378
C,2.6701718611,2.7794694353,0.5054826218
C,0.9396751419,0.9598701892,0.6738101853
C,1.3371175049,2.3604555832,1.1296500674
C,0.8562749922,0.8965179983,-0.8493579524
C,2.6174027375,2.6860448016,-1.0223243226
H,3.4659102972,2.1213514604,0.8787169202
H,1.7269340767,0.2467991727,0.9843985133
H,0.5438249267,3.0591427199,0.832912578
H,0.08810415,1.629319468,-1.1618120739
H,1.8976904694,3.4227474085,-1.4029899099
H,2.9446403614,0.546717839,-1.1738977112
H,2.9285409177,3.797016524,0.8157454955
H,1.3979763592,2.3885047311,2.2243940806
H,3.5908306838,2.941747656,-1.4529909937

N,0.4995411516,-0.4684931667,-1.2266489276
H,0.4667419014,-0.5393348857,-2.2422552299
N,-0.3694322078,0.6029805901,1.2139312411
H,-0.3431325431,0.6671039968,2.2301728548
C,-0.8135955235,-0.7526550983,0.8449011979
H,-1.8625097963,-0.8268976011,1.15708601
C,-0.7977346848,-0.9129002582,-0.6873993707
H,-0.8615969326,-1.9888818899,-0.8908142162
C,-0.0543390622,-1.8439260556,1.5939834812
C,1.3041398869,-3.76562785,3.1288891348
C,1.0810373003,-2.486201652,1.0877522441
C,-0.4959351396,-2.1832847766,2.8776319987
C,0.1742933125,-3.1330489728,3.6423006563
C,1.7517013338,-3.4400674662,1.8515568646
H,1.4356465973,-2.2254840258,0.0952320464
H,-1.3848035402,-1.6992967324,3.2779438957
H,-0.189574236,-3.385333156,4.6336944295
H,2.6305911006,-3.9307118355,1.4440169181
H,1.8293097997,-4.5098815745,3.7194102976
C,-1.9823619907,-0.2613149004,-1.3949031595
C,-4.0895680389,0.8864633221,-2.856623389
C,-2.6163225293,0.8992503717,-0.9376835445
C,-2.424164193,-0.8350829419,-2.5922026217
C,-3.4661374012,-0.2695736095,-3.3205345451
C,-3.6623113231,1.4651608422,-1.664801498
H,-2.2768808888,1.3559401712,-0.0130043695
H,-1.9469644884,-1.7445933266,-2.9522753606
H,-3.7967355165,-0.7351255347,-4.2440467574
H,-4.1450786005,2.3652581781,-1.2959811229
H,-4.9052599026,1.3304183314,-3.4187470594

The below coordinates use the 6-31+G(d,p) basis set in acetonitrile.

HF
hf_mecn_6-31+gdp
M062X/6-31+G(d,p)
E(RM062X) = -100.4203466

Zero-point correction= 0.009207 (Hartree/Particle)
Thermal correction to Energy= 0.011568
Thermal correction to Enthalpy= 0.012512
Thermal correction to Gibbs Free Energy= -0.007218
Sum of electronic and ZPE= -100.411139
Sum of electronic and thermal Energies= -100.408779
Sum of electronic and thermal Enthalpies= -100.407835
Sum of electronic and thermal Free Energies= -100.427564

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	7.259	4.968	41.525

F,-1.4028831714,-0.57422968,0.
H,-2.3342596686,-0.57422968,0.

B_2F_4
mecn_b2f4_flat
M062X/6-31+G(d,p)
E(RM062X) = -449.1826894

Zero-point correction= 0.018903 (Hartree/Particle)
Thermal correction to Energy= 0.024889
Thermal correction to Enthalpy= 0.025833
Thermal correction to Gibbs Free Energy= -0.010879
Sum of electronic and ZPE= -449.163786
Sum of electronic and thermal Energies= -449.157801
Sum of electronic and thermal Enthalpies= -449.156856
Sum of electronic and thermal Free Energies= -449.193568

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	15.618	18.194	77.266

B,0.,0.,0.8586809469
B,0.,0.,-0.8586809469
F,-0.0396044168,1.127336663,-1.5581135504
F,0.0396044168,-1.127336663,-1.5581135504
F,0.0396044168,1.127336663,1.5581135504
F,-0.0396044168,-1.127336663,1.5581135504

***E,E*-(18)** (*E,E*-**18** in acetonitrile, see Scheme 4.5)
mecn_edadiim_EE
M062X/6-31+G(d,p)
E(RM062X) = -728.5611576

Zero-point correction= 0.284209 (Hartree/Particle)
Thermal correction to Energy= 0.299812
Thermal correction to Enthalpy= 0.300756
Thermal correction to Gibbs Free Energy= 0.237562
Sum of electronic and ZPE= -728.276949
Sum of electronic and thermal Energies= -728.261346
Sum of electronic and thermal Enthalpies= -728.260401
Sum of electronic and thermal Free Energies= -728.323596

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	188.135	59.755	133.004

C,2.3602461042,-0.6947194916,-0.3278372236
C,2.3602130668,0.6948547879,0.327892545
H,2.3326740211,-0.5782077885,-1.4207964714
H,2.3326286093,0.5783409941,1.420851139
N,1.2319851704,1.4612304756,-0.1703037103
N,1.2320423669,-1.4611404594,0.1703425255
C,0.2220826733,1.5748736279,0.5948593377
H,0.2228924075,1.1603675941,1.6138651661
C,0.2221675647,-1.5748554792,-0.594846171
H,0.2229832548,-1.1603747872,-1.6138625003
C,-1.0256233586,-2.2507767953,-0.1829938424
C,-1.1684824128,-2.8324166004,1.0848089898
C,-2.0941014775,-2.2953830134,-1.0851649239
C,-2.3635263293,-3.450740225,1.4375468959
H,-0.3381777353,-2.7949243085,1.7836578056
C,-3.2929873166,-2.9138049961,-0.7298725191
H,-1.9817085356,-1.8414697584,-2.0669828318
C,-3.4285593721,-3.4920874271,0.5316401954
H,-2.4698227117,-3.9012153154,2.4199195523
H,-4.1177293285,-2.9431843808,-1.4354820961
H,-4.3602643716,-3.9748548159,0.8114253327
C,-1.0257337841,2.250735477,0.1829874731
C,-2.0942520493,2.2952282902,1.0851166771
C,-1.1685787047,2.8324239279,-1.0847943283
C,-3.2931655369,2.9135836822,0.729801754
H,-1.9818688283,1.841279368,2.0669193077
C,-2.363649302,3.4506839223,-1.437553255
H,-0.338243136,2.7950165881,-1.7836110698
C,-3.4287239097,3.4919145177,-0.5316901339
H,-4.1179404374,2.9428720343,1.43537674
H,-2.4699359139,3.9011968479,-2.4199096864
H,-4.3604505042,3.9746300623,-0.8114928093
H,3.2862229236,1.2057405656,0.0478226238
H,3.2862722935,-1.2055675707,-0.0477520279

A (Ionic complex **A**, see Scheme 4.5)
mecn_b2f4_edadiim-EE_sm
M062X/6-31+G(d,p)
E(RM062X) = -1177.8007951

Zero-point correction= 0.308786 (Hartree/Particle)

Thermal correction to Energy= 0.329557
Thermal correction to Enthalpy= 0.330501
Thermal correction to Gibbs Free Energy= 0.257878
Sum of electronic and ZPE= -1177.492009
Sum of electronic and thermal Energies= -1177.471238
Sum of electronic and thermal Enthalpies= -1177.470294
Sum of electronic and thermal Free Energies= -1177.542917

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.800	80.909	152.848

C,-0.7134777051,2.1050772493,0.0852494819
C,0.6929597717,2.0179705924,-0.5240353021
H,-0.675507583,2.5573898217,1.077378439
H,0.6244369273,1.9568070301,-1.611437378
N,1.4314684289,0.8352203584,-0.033462663
N,-1.3273543468,0.7779970981,0.2516764183
C,2.1655059864,0.2125159768,-0.8822215924
H,2.2576289347,0.6584989022,-1.8752397266
C,-2.2193044765,0.4128658679,-0.5986352343
H,-2.4035674764,1.0766305296,-1.4469738905
B,1.0593606955,0.5091564003,1.522224835
B,-0.5916750351,-0.0627356207,1.472204641
F,1.2541329191,1.7734398951,2.1645132938
F,2.0287810545,-0.367135168,2.0509465676
F,-1.3768308068,0.1897523729,2.6303652088
F,-0.6929334166,-1.4379830972,1.1428720548
C,-3.048255564,-0.7928767532,-0.5460021485
C,-3.4436012499,-1.3895121794,0.6601148902
C,-3.5275069187,-1.2946694957,-1.7646000737
C,-4.2821956,-2.4985792489,0.6370672801
H,-3.1096697058,-0.9727685811,1.6040324916
C,-4.3466374749,-2.4200060121,-1.7828580073
H,-3.2474248507,-0.8044278192,-2.6933019874
C,-4.723317388,-3.0215562963,-0.5813656655
H,-4.5968778605,-2.9548476822,1.5703129247
H,-4.7015811772,-2.8171968339,-2.7284368836
H,-5.3744044564,-3.8906050595,-0.5920325653
C,2.899761382,-1.0480139009,-0.6969315103
C,4.1412773498,-1.1608387428,-1.3378548793
C,2.3590357614,-2.1505852269,-0.0222494852
C,4.8694999193,-2.3440822084,-1.2472089328
H,4.5362377322,-0.3158661738,-1.8959618352
C,3.0784800466,-3.3403347511,0.0390675729
H,1.3773186971,-2.0777789861,0.4335051328

C,4.337418792,-3.4347415299,-0.5583510298
H,5.8407856883,-2.419734746,-1.7257637199
H,2.6547598711,-4.1973113946,0.5534225731
H,4.8962048181,-4.364010074,-0.4996431833
H,1.2482399787,2.9178629173,-0.247491777
H,-1.3336806922,2.7297914398,-0.5596976642

B (Ionic complex **B**, see Scheme 4.5)
zwit-hf_b2f4_edadiim_EE_sm_6-31+gdp-acn
M062X/6-31+G(d,p)
E(RM062X) = -1278.2523465

Zero-point correction= 0.323435 (Hartree/Particle)
Thermal correction to Energy= 0.346308
Thermal correction to Enthalpy= 0.347252
Thermal correction to Gibbs Free Energy= 0.268776
Sum of electronic and ZPE= -1277.928911
Sum of electronic and thermal Energies= -1277.906039
Sum of electronic and thermal Enthalpies= -1277.905095
Sum of electronic and thermal Free Energies= -1277.983571

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	217.311	87.029	165.167

C,1.5880335878,-2.1239896278,-0.3525611285
C,1.8979727059,-1.0189927093,0.6739453646
H,1.8200287512,-1.7871454253,-1.3624814317
H,1.7133182494,-1.380579223,1.6878419145
N,1.0570391603,0.1540104832,0.3998047937
N,0.1648783886,-2.4570825405,-0.2950731996
C,-0.0151732951,0.2596861514,1.1100128069
H,-0.1490806008,-0.4956527383,1.8877607315
C,-0.7268836385,-1.818162076,-0.9767690671
H,-0.3486773456,-1.1045126155,-1.7108181699
B,1.5655609998,1.1448048461,-0.8104053076
B,2.1164568239,2.6872359324,-0.1752664791
F,0.4728420722,1.1503241855,-1.7378174553
F,2.6081125745,0.4014914195,-1.4447146606
F,1.5819763981,3.8180306741,-0.8969694061
F,3.5472358285,2.8188836194,-0.2454039535
C,-2.1614653593,-1.9106168269,-0.8015896708
C,-2.7829466435,-2.8232980942,0.0691864193
C,-2.9267639027,-0.9560180984,-1.4908914221
C,-4.1580218365,-2.767904287,0.2446856045
H,-2.2067998963,-3.575911757,0.6001881562

C,-4.3040944109,-0.901983466,-1.3017733178
H,-2.4317361293,-0.2533165479,-2.1560577794
C,-4.9160170243,-1.8058740048,-0.4339914115
H,-4.6452556579,-3.4710620122,0.9120152072
H,-4.8949031573,-0.1575446708,-1.8250978854
H,-5.9905296431,-1.7660574168,-0.2828178019
C,-1.1425105209,1.1901014542,1.0137352187
C,-2.278132074,0.7929019215,1.7442767466
C,-1.1935994291,2.3776709473,0.264169211
C,-3.4498133466,1.5419503789,1.7051022447
H,-2.2402194029,-0.1169418194,2.3385207288
C,-2.3617885115,3.1320193106,0.2448445195
H,-0.3355245165,2.7211830038,-0.2955849925
C,-3.4923588843,2.7145507441,0.9519055353
H,-4.3212422218,1.214017543,2.2628881672
H,-2.3911005153,4.0515245877,-0.3313273773
H,-4.4015249701,3.3074954775,0.919161116
H,-0.1235521842,-3.1099927548,0.4351292056
F,1.7733251178,2.9081912002,1.2083768142
H,2.9479648345,-0.7448367385,0.572418734
H,2.1626226257,-3.0189554297,-0.1137273222

C (Ionic transition state **C**, see Scheme 4.5)
zwit-hf_loaded-geom_b2f4_edadiim_EE_ts-guess
M062X/6-31+G(d,p)
E(RM062X) = -1278.2154898

Zero-point correction= 0.321524 (Hartree/Particle)
Thermal correction to Energy= 0.343857
Thermal correction to Enthalpy= 0.344801
Thermal correction to Gibbs Free Energy= 0.269103
Sum of electronic and ZPE= -1277.893966
Sum of electronic and thermal Energies= -1277.871633
Sum of electronic and thermal Enthalpies= -1277.870688
Sum of electronic and thermal Free Energies= -1277.946386

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	215.774	85.803	159.320

C,1.5106163922,-1.8201385667,-1.0917909247
C,1.8824524733,-0.9881702541,0.1494670387
H,1.6357344226,-1.2218331555,-1.9981784269
H,1.6752747009,-1.559790782,1.0584386095
N,1.1079209401,0.2616892811,0.1735209131
N,0.1296209672,-2.2531618249,-0.9950048473

C,-0.1744102903,0.1210014382,0.5898360472
H,-0.3327282105,-0.6560037533,1.3366283351
C,-0.8320697585,-1.3531952244,-1.1009065123
H,-0.643955096,-0.529235557,-1.7872232222
B,1.8767103478,1.4952889236,-0.0794988852
B,2.3651591438,1.5524615704,1.8611361673
F,1.2290487499,2.6902953972,-0.2860268917
F,3.0036472171,1.3507221295,-0.8705094441
F,1.1919107315,1.7305388128,2.5697012155
F,3.153984657,2.6971604229,1.8474110344
C,-2.2158603269,-1.6090413578,-0.7093144312
C,-2.5487360629,-2.5036774133,0.3195886163
C,-3.2252854597,-0.8778086212,-1.3521173775
C,-3.8801374562,-2.6740863881,0.6830604388
H,-1.7738111501,-3.0445287666,0.8570471053
C,-4.5564811877,-1.0536927152,-0.984843345
H,-2.9589278746,-0.1764331422,-2.1381057558
C,-4.8840355598,-1.9514070528,0.0319803549
H,-4.1360639029,-3.3613985483,1.4830523301
H,-5.3349464482,-0.4876801892,-1.4866725519
H,-5.9211983643,-2.0835713159,0.3249105581
C,-1.2264070542,1.1221757131,0.4592995854
C,-2.2316086008,1.1488988727,1.4439734122
C,-1.3764645596,1.9432404085,-0.6729127596
C,-3.3296480077,1.9949213467,1.3209902011
H,-2.1407035009,0.497503964,2.3102166604
C,-2.4724792786,2.7950302829,-0.7881493094
H,-0.6467696559,1.8965928509,-1.47537091
C,-3.4514391998,2.8290980794,0.2068072338
H,-4.0915903356,2.0038135024,2.0950671081
H,-2.5705263225,3.4232416382,-1.6688337845
H,-4.307405032,3.4900161898,0.1092652801
H,-0.0434109897,-3.0963657599,-0.452670585
F,3.079665726,0.4427967086,2.2774949255
H,2.9445566961,-0.7586247981,0.1051566909
H,2.1564491004,-2.6967190764,-1.1422405576

D (Sigmatropic transition state **D**, see Scheme 4.5)
acetonitrile_6-31+gdp_m062x_b2f4_edadiim_EE_ts-guess_hf
M062X/6-31+G(d,p)
E(RM062X) = -1177.7767617

Zero-point correction= 0.309168 (Hartree/Particle)
Thermal correction to Energy= 0.328889
Thermal correction to Enthalpy= 0.329833
Thermal correction to Gibbs Free Energy= 0.261517

Sum of electronic and ZPE= -1177.467594
Sum of electronic and thermal Energies= -1177.447873
Sum of electronic and thermal Enthalpies= -1177.446929
Sum of electronic and thermal Free Energies= -1177.515245

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	206.381	78.536	143.784

C,2.3538222227,0.808006789,-0.2830796865
C,2.2932282981,-0.6940355582,-0.727625425
H,3.0991072977,0.9415089615,0.4991993797
H,2.1989723998,-0.7763178267,-1.80941343
N,1.1086454307,-1.3143588086,-0.1065475626
N,1.0410397326,1.1993409758,0.2555111408
C,0.0211369625,-1.240413083,-0.8716977484
H,0.2263906162,-1.1114773306,-1.9306514039
C,0.0885442649,1.2495727916,-0.6750793973
H,0.4287719391,1.1873527378,-1.7066256354
B,1.2155079934,-1.304198987,1.3754072045
B,0.8976458959,0.7322124219,1.6749380455
F,2.5029261773,-1.5141884521,1.8429399723
F,0.2826372463,-2.0032916625,2.104498846
F,1.9265211919,1.12380421,2.5111455927
F,-0.3317335332,0.8120796086,2.2861328185
C,-1.290016823,1.6940029604,-0.4791031257
C,-1.7070868381,2.4889534995,0.599589412
C,-2.2270326901,1.3455546909,-1.4690248729
C,-3.0417104365,2.8754861825,0.7092482856
H,-0.9868059081,2.8250249194,1.336672304
C,-3.557668528,1.7286322741,-1.3540338368
H,-1.9022630885,0.7532500939,-2.3210602201
C,-3.9721590695,2.4861266079,-0.2548273939
H,-3.3528171128,3.4917878654,1.5473676114
H,-4.2716470098,1.4374097154,-2.1186799283
H,-5.0114604488,2.786392654,-0.1609462006
C,-1.3649891716,-1.6132764531,-0.5647062108
C,-2.0972646999,-2.1636810397,-1.6311684443
C,-2.0364057874,-1.3211949241,0.6335036559
C,-3.4501049922,-2.4603881149,-1.4923311035
H,-1.5954496256,-2.3567402805,-2.576188715
C,-3.3927837076,-1.6073784146,0.7643215298
H,-1.5140954238,-0.8432431516,1.4510725082
C,-4.1030549677,-2.1835096382,-0.2905506994
H,-3.9947004255,-2.8965301015,-2.3242063208
H,-3.8998333225,-1.3661221833,1.6938689483

H,-5.1608513079,-2.4029296467,-0.1803659389
H,3.1916402235,-1.2143014802,-0.4000992243
H,2.5995858353,1.4450075374,-1.1334009107

REFERENCES

REFERENCES

(1) Carter, C. A. G.; John, K. D.; Mann, G.; Martin, R. L.; Cameron, T. M.; Baker, R. T.; Bishop, K. L.; Broene, R. D.; Wescott, S. A. Bifunctional Lewis Acid Reactivity of Diol-Derived Diboron Reagents. *ACS Symposium Series: Group 13 Chemistry* **2002**, *822*, 70–87.

(2) Chen, D.; Xu, G.; Zhou, Q.; Chung, L. W.; Tang, W. Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. *J. Am. Chem. Soc.* **2017**, *139*, 9767–9770.

(3) Zhou, M.; Li, K.; Chen, D.; Xu, R.; Xu, G.; Tang, W. Enantioselective Reductive Coupling of Imines Templated by Chiral Diboron. *J. Am. Chem. Soc.* **2020**, *142*, 10337–10342.

(4) Zhang, L.; Jiao, L. Super electron donors derived from diboron. *Chem. Sci.* **2018**, *9*, 2711–2722.

(5) Alam, R.; Das, A.; Huang, G.; Eriksson, L.; Himo, F.; Szabó, K. J. Stereoselective allylboration of imines and indoles under mild conditions. An *in situ E*/*Z* isomerization of imines by allylboroxines. *Chem. Sci.* **2014**, *5*, 2732–2738.

(6) Cade, I. A. Chau, W. Y.; Vitorica-Yrezabal, I.; Ingleson, M. J. 1,1/1,2 Isomerisation in Lewis base adducts of B_2cat_2. *Dalton Trans.* **2015**, ***44***, 7506–7511.

(7) Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

(8) Zhao, Y.; Schultz, N. E.; Truhlar, D. G. Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions *J. Chem. Theory. Comput.* **2006**, *2*, 364–382.

(9) Zhao, Y.; Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.* **2006**, *125*, 194101–194118.

(10) Zhao, Y.; Truhlar, D. G. Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. *J. Phys. Chem. A* **2006**, *110*, 13126–13130.

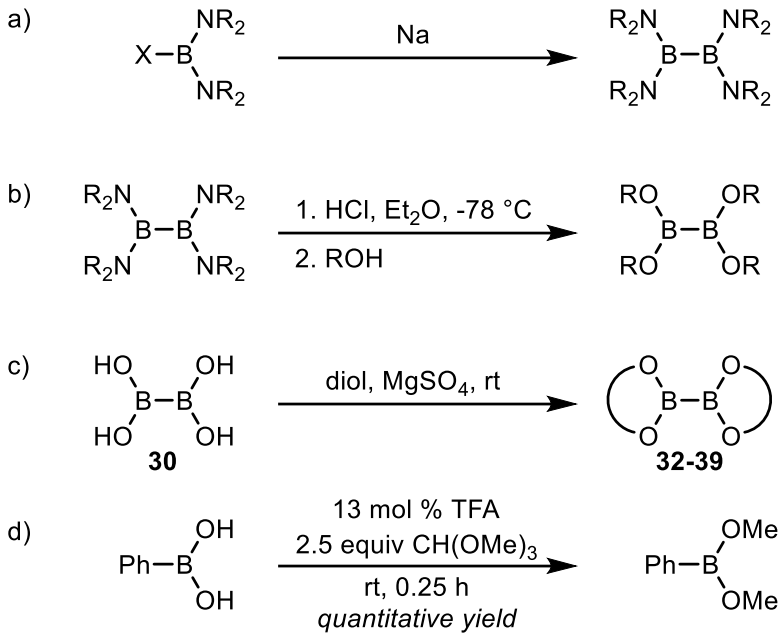
(11) Lawlor, F. J.; Norman, N. C.; Pickett, N. L.; Robins, E. G.; Nguyen, P.; Lesley, G.; Marder, T. B.; Ashmore, J. A.; Green, J. C. Bis-Catecholate, Bis-Dithiocatecholate, and Tetraalkoxy Diborane(4) Compounds: Aspects of Synthesis and Electronic Structure. *Inorg. Chem.* **1998**, *37*, 5282–5288.

Chapter 5. An Improved Preparation of Tetraalkoxydiborons and Diboron Diolates from Tetrahydroxydiboron

Introduction.

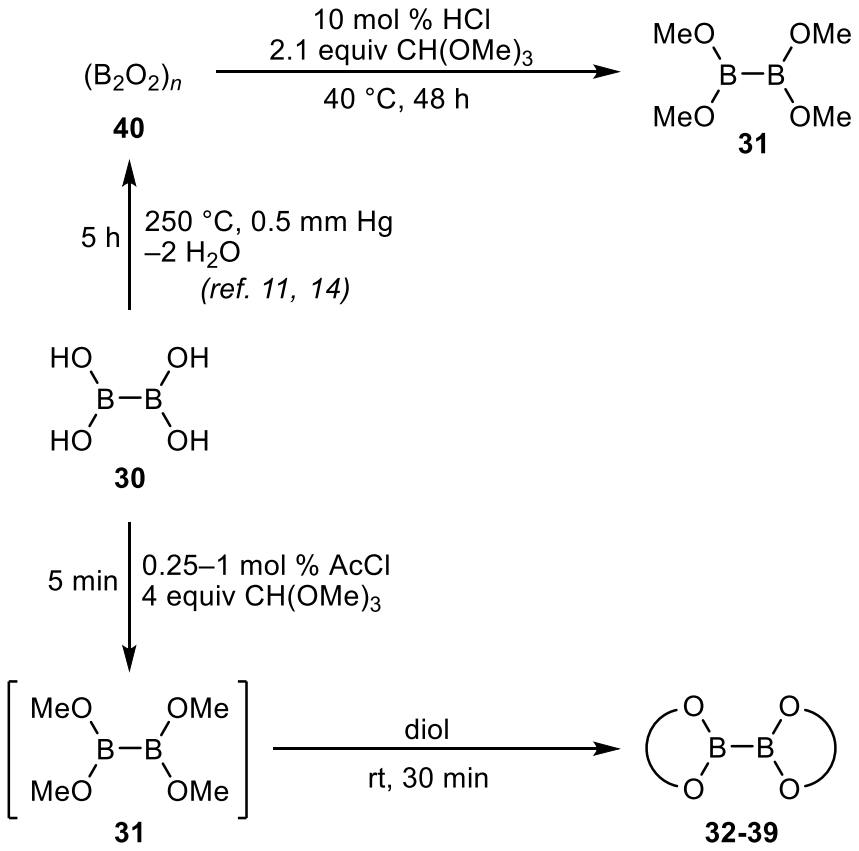
As detailed in previous chapters, diboron diolates (and other diborons) have broad applications in many reactions,[1-5] and while they are generally bench stable compounds, their preparation can be tedious. Boron-boron bonds are commercially prepared via the Wurtz coupling of halobis(dialkylamino)boranes (Scheme 5.1a).[6-7] While tetrakis(dialkylamino)diborons of this type do have applications in synthesis,[8-10] diboron diolates are far more widely used.[1-5] Their direct preparation from tetracids(dialkylamino)diborons requires the use of a dry solution of HCl in Et_2O at -78 °C, followed by tedious filtration of dialkylammonium hydrochloride salts, then distillation, sublimation, or crystallization of the diboron diolate (Scheme 5.1b).[6-7] However, $B_2(OH)_4$ is also readily prepared via hydrolysis of tetrakis(dialkylamino)diboron.[11] Diboron diolates can be synthesized by stirring a heterogeneous mixture of $B_2(OH)_4$ with a diol and $MgSO_4$ for 24 hours (Scheme 5.1c).[12]

Scheme 5.1. Previously reported syntheses of diboron diolates and similar compounds.

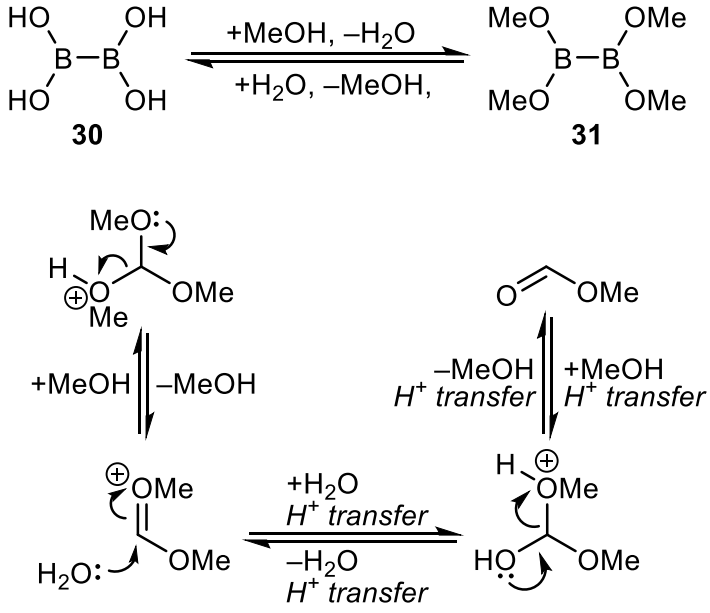


Inspired by a previous report for the preparation of $PhB(OMe)_2$ from $PhB(OH)_2$ by reaction with trimethyl orthoformate in the presence of an acid catalyst (Scheme 5.1d),[13] we have developed an exceptionally fast and convenient method for the preparation of diboron diolates and tetraalkoxydiborons (Scheme 5.2). The use of this method is much easier and more practical than the previously reported methods.

Scheme 5.2. This work.



Proposed mechanism:

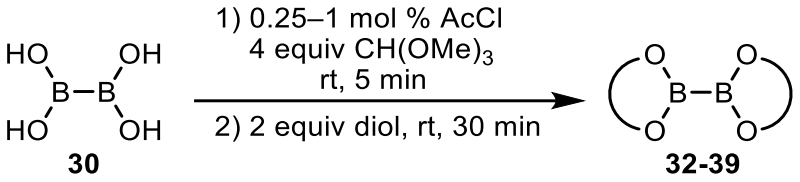


Scope of the Reaction.

The AcCl-catalyzed reaction of $B_2(OH)_4$ (**30**) with $CH(OMe)_3$ is complete within minutes at room temperature, is not particularly air sensitive, and offers a visual indicator of completion, producing a homogenous solution [containing $B_2(OMe)_4$ (**31**), MeOH, and methyl formate] after consumption of starting material. The diol is then added, the solution stirred briefly, and the solvent removed in vacuo to afford the desired diboron in high yield, typically without a need for further purification (Scheme 2, bottom).

A variety of diboron diolates (compounds **32**-**39**) were prepared on gram scale (Table 5.1) using this methodology. Reactions with aliphatic 1,2-diols (Entries 1-3), aliphatic 1,3-diols (Entries 4-6) and phenols such as catechol or 2-hydroxybenzyl alcohol (Entries 7-8) were successful. Conversion was low with diisopropyl tartrate, and perfluoropinacol failed to afford any product, likely due to diminished nucleophilicity relative to the other substrates. Attempts to separate $B_2(OMe)_4$ (**31**) from the MeOH byproduct by distillation were unsuccessful. Interestingly, the anhydride of $B_2(OH)_4$ can be prepared quantitatively by heating under vacuum for several hours, generating $(B_2O_2)_n$ (**40**) as a hard white solid.[11,14] This material failed to react with $CH(OMe)_3$ in the presence of catalytic AcCl, but did so with dry HCl in Et_2O (Scheme 5.2, top). These reactions are much slower than those with $B_2(OH)_4$ (48 hours instead of 5 minutes) and require gentle heating (40 °C instead of room temperature). Removal of residual $(B_2O_2)_n$ (**40**) by filtration, and Et_2O and methyl formate by distillation (which is trivial, given the wide separation in boiling points vs. $B_2(OMe)_4$) (**31**), afforded $B_2(OMe)_4$ (**31**) (Scheme 5.3) in high yield, containing a small amount of residual $B(OMe)_3$.

Table 5.1. Scope of the reaction: diboron diolates (**32-39**) prepared from **30**.

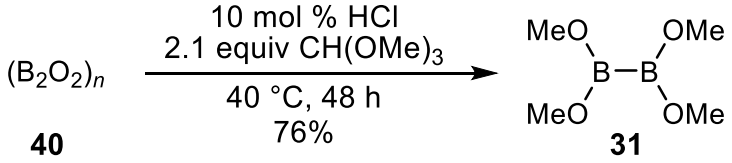


Entry (diboron)	Diol	Yield (%)[a]
1 (32)	Ethylene glycol	92
2 (33)	Propylene glycol	99
3 (34)	(1*S*,2*S*)-1,2-Diphenylethylene glycol	97
4 (35)	1,3-Butanediol	99
5 (36)[b]	Neopentyl glycol	95
6 (37)	Hexylene glycol	94
7 (38)	Catechol	98
8 (39)[b]	2-Hydroxybenzyl alcohol	97

[a] Isolated yield. [b] Dichloromethane was added after addition of the diol to improve the homogeneity of the reaction mixture.

We also attempted to prepare $B_2(OEt)_4$ (**41**) via this method, and obtained a mixture whose primary spectral features were consistent with its structure. However, our assignment is not secure due to the complexity of the spectra. *(Caution: unlike $B_2(OMe)_4$, the reaction of $B_2(OEt)_4$ with air is spontaneous and is very exothermic!)* This is a simple alternative to previous methods for their synthesis from tetrakis(dialkylamino)diborons.[6]

Scheme 5.3. Synthesis of tetramethoxydiboron (**31**).



Conclusions.

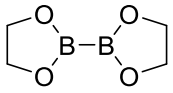
To summarize, we have developed a simple, convenient, and high yielding method for the preparation of both diboron diolates and tetraalkoxydiborons using bench stable $B_2(OH)_4$ as a universal precursor. Diboron diolates were prepared via pre-treatment with acetyl chloride and trimethyl orthoformate, followed by addition of the diol. This method was largely substrate tolerant with respect to the diol. Tetraalkoxydiborons were prepared by thermal/vacuum dehydration of $B_2(OH)_4$ to yield $(B_2O_2)_n$, followed by treatment with a trialkyl orthoformate in the presence of acid.

Experimental Section.

General. All reactions were carried out under a nitrogen atmosphere in flame-dried glassware unless otherwise noted. All reagents were obtained from commercial sources and were used as obtained unless otherwise noted. Dichloromethane was obtained from commercial sources and used without further purification. Boron monoxide was prepared as previously described in the literature.[11,14] Yields refer to isolated yields of compounds estimated to be ≥95% pure as determined by ^{1}H NMR analysis unless otherwise noted. The yields reported here are the results of a single experiment.

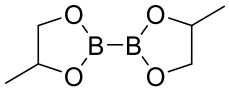
General Procedure: Preparation and Characterization of Diboron Diolates. A flask was charged with $B_2(OH)_4$ (**30**, 1.0 equiv) and $CH(OMe)_3$ (4.0 equiv), and a stir bar. AcCl was added (0.0025–0.01 equiv), the vessel flushed with N_2 and sealed with a silicone septum, and the mixture stirred rapidly at room temperature until all solid material had dissolved (5 minutes or less, determined by stir rate and the grain size of the $B_2(OH)_4$).

The diol was then added and stirred for 30 minutes. Solvent was removed in vacuo via rotary evaporation to afford the title compound.



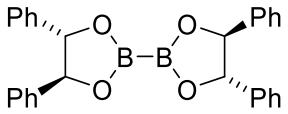
32

2,2′-Bi(1,3,2-dioxaborolane) (32). The title compound was prepared from $B_2(OH)_4$ (**30**, 2.24 g, 25 mmol), $CH(OMe)_3$ (10.94 mL, 100 mmol), 1 mol % AcCl (18 µL, 0.25 mmol), and ethylene glycol (2.8 mL, 50 mmol) according to the general procedure. The solid material was then washed twice with cold dichloromethane. This procedure afforded 3.24 g (92%) of the title compound as a white solid: mp = 133–149 °C (lit. mp[12] = 159-160 °C, lit. mp[22] = 168-170 °C). ^{1}H, ^{13}C, and ^{11}B NMR data[12] were consistent with literature values: ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.21 (s, 8H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 65.5; ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.8.



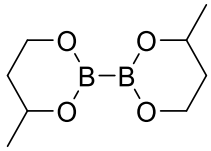
33

4,4′-Dimethyl-2,2′-bi(1,3,2-dioxaborolane) (33). The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 1 mol % AcCl (7.1 µL, 0.1 mmol), and propylene glycol (1.47 mL, 20 mmol) according to the general procedure. This procedure afforded 1.7 g (99%) of the title compound as a colorless oil: ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.59–4.50 (m, 2H), 4.27 (dd, J = 9.0, 8.0 Hz, 2H), 3.70 (dd, J = 9.0, 7.5 Hz, 2H), 1.31 (d, J = 6.2 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 73.5, 72.0, 21.7; ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.8.



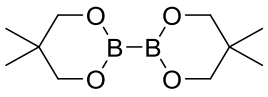
34

(4*S*,4*S′*,5*S*,5*S′*)-4,4′,5,5′-Tetraphenyl-2,2′-bi(1,3,2-dioxaborolane) (34). The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 1 mol % AcCl (7.1 µL, 0.1 mmol), and (1*S*,2*S*)-1,2-diphenylethylene glycol (4.29 g, 20 mmol) according to the general procedure. This procedure afforded 4.33 g (97%) of the title compound as a very pale pink-white solid: mp = 136–140 °C. ^{1}H and ^{13}C NMR data[15-16] were consistent with literature values: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45–7.35 (m, 20H), 5.30 (s, 4H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 139.8, 128.8, 128.4, 126.0, 86.7; ^{11}B NMR (160 MHz, $CDCl_3$) δ 31.9.



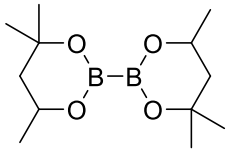
35

4,4′-Dimethyl-2,2′-bi(1,3,2-dioxaborinane) (35). The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 1 mol % AcCl (7.1 µL, 0.1 mmol), and 1,3-butanediol (1.79 mL, 20 mmol) according to the general procedure. This procedure afforded 1.98 g (99%) of the title compound as a colorless viscous oil. ^{1}H NMR data[17] were consistent with reported values. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.14–4.06 (m, 2H), 3.98–4.03 (m, 2H), 3.89–3.96 (m, 2H), 1.88–1.95 (m, 2H), 1.74–1.65 (m, 2H), 1.27 (d, *J* = 6.3 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 66.7, 60.5, 34.2, 22.8; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.3.



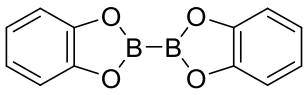
36

5,5,5′,5′-Tetramethyl-2,2′-bi(1,3,2-dioxaborinane) (36). The title compound was prepared from $B_2(OH)_4$ (**30**, 2.24 g, 25 mmol), $CH(OMe)_3$ (10.94 mL, 100 mmol), 0.25 mol % AcCl (4.4 µL, 0.0625 mmol), and neopentyl glycol (5.21 g, 50 mmol) according to the general procedure. Dichloromethane (5 mL) was added after addition of the neopentyl glycol to improve the homogeneity of the reaction mixture. This procedure afforded 5.35 g (95%) of the title compound as a white solid: mp = 128–147 °C (lit. mp[20] = 182.5–184.5 °C). ^{1}H and ^{13}C NMR data[18], and ^{11}B NMR data[19] were consistent with reported values. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.55 (s, 8H), 0.91 (s, 12H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 71.5, 31.6, 22.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 27.8.



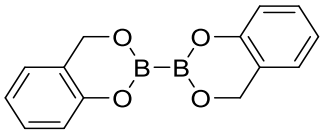
37

4,4,4′,4′,6,6′-Hexamethyl-2,2′-bi(1,3,2-dioxaborinane) (37). The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 1 mol % AcCl (7.1 µL, 0.1 mmol), and hexylene glycol (2.57 mL, 20 mmol) according to the general procedure. This procedure afforded 2.38 g (94%) of the title compound as a white solid: mp = 96–99 °C (lit. mp[20] = 99–101.6 °C). ^{1}H and ^{13}C NMR data[18] were consistent with reported values: ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.17–4.08 (m, 2H), 1.73–1.68 (m, 2H), 1.44–1.52 (m, 2H), 1.27–1.24 (m, 12H), 1.24–1.21 (m, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 70.0, 64.0, 46.2, 31.2, 28.4, 23.2; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.1.



38

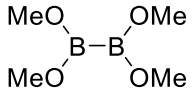
2,2′-Bibenzo[*d*][1,3,2]dioxaborole (38). The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 0.5 mol % AcCl (3.6 µL, 0.05 mmol), and catechol (2.20 g, 20 mmol) according to general procedure. This procedure afforded 2.34 g (98%) of the title compound as an off-white solid, consisting of 5% catechol by mass: mp = 172–176 °C (lit. mp[22] = 195–198°C). ^{1}H data and ^{11}B data[21] were consistent with reported values: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 5.9, 3.3 Hz, 4H), 7.19 (dd, *J* = 5.9, 3.3 Hz, 4H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 147.7, 123.4, 113.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 31.0.



39

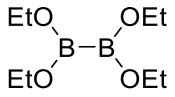
***4H*,4*H′*-2,2′-Bibenzo[*d*][1,3,2]dioxaborinine (39).** The title compound was prepared from $B_2(OH)_4$ (**30**, 0.90 g, 10 mmol), $CH(OMe)_3$ (4.38 mL, 40 mmol), 0.5 mol % AcCl (3.6 µL, 0.05 mmol), and 2-hydroxybenzyl alcohol (2.48 g, 20 mmol) according to general procedure. Dichloromethane (10 mL) was added after addition of the 2-hydroxybenzyl alcohol to improve the homogeneity of the reaction mixture. This procedure afforded 2.57 g (97%) of the title compound as an orange solid: mp = 110–126 °C. ^{1}H NMR data[17] were consistent with reported values: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23–7.18 (m, 2H), 7.01–7.09 (m, 4H), 6.91–6.95 (m, 2H), 5.12 (s, 4H); ^{13}C{^{1}H} NMR (126

MHz, $CDCl_3$) δ 147.8, 128.7, 124.8, 123.5, 122.7, 118.0, 61.9; ^{11}B NMR (160 MHz, $CDCl_3$) δ 27.9.



31

Tetramethoxydiboron (31). A 1-dram vial was charged with a stir bar, B_2O_2 (**40**, 268 mg, 5 mmol), $CH(OMe)_3$ (1.15 mL, 10.5 mmol), and 2 M HCl in Et_2O (0.25 mL, 0.5 mmol). The vial was flushed with N_2 and capped, then stirred at 40 °C for 48 h. The cap was replaced with a septum, and connected to a water aspirator by a length of PTFE tubing. HCO_2Me and Et_2O were removed via vacuum distillation (400 mmHg) at room temperature, gradually raising the temperature over an hour to 40 °C. The remaining liquid was then filtered through glass wool under a N_2 atmosphere. This procedure afforded 608 mg of the title compound in 91% purity (containing 4% methyl formate, 2% methanol, 3% diethyl ether) as a colorless oil, for an overall yield of 553 mg (76%). $B(OMe)_3$ content was judged by ^{11}B NMR to be <1%. The relative proportions of each component were estimated via spectral deconvolution using the line fitting protocol in MNova 14.2.0 (Mestrelab Research, S.L.; Santiago de Compostela, Spain) using Gaussian/Lorentzian peak shapes and simulated annealing. ^1H NMR (500 MHz, $CDCl_3$) δ 3.61 (s, 12H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 51.9; ^{11}B NMR (160 MHz, $CDCl_3$) δ 31.2.



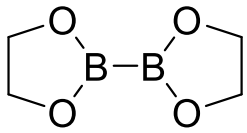
41

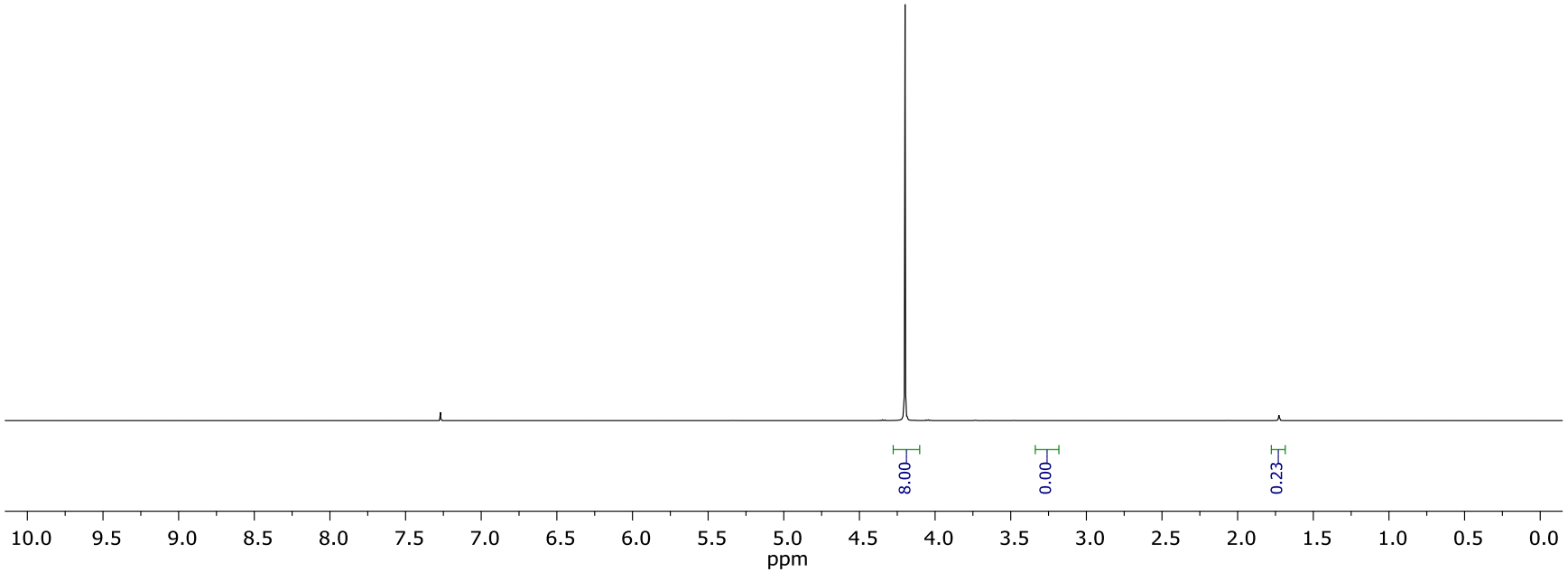
Tetraethoxydiboron (41). A 1-dram vial was charged with a stir bar, B_2O_2 (**40**, 268 mg, 5 mmol), $CH(OEt)_3$ (1.75 mL, 10.5 mmol), and 2 M HCl in Et_2O (0.25 mL, 0.5 mmol). The vial was flushed with N_2 and capped, then stirred at 40 °C for 48 h. The cap was replaced with a septum, and connected to a water aspirator by a length of PTFE tubing. Et_2O was removed via vacuum distillation (400 mmHg) at room temperature, and the temperature was then gradually raised over an hour to 40 °C to remove HCO_2Et. The remaining liquid was then filtered through glass wool under a N_2 atmosphere. This procedure afforded 810 mg of an impure colorless oil. Its spectral features were consistent with $B_2(OEt)_4$ being the primary component, although our assignment is not secure, and we were unable to easily assess its purity based on spectral data due to the complexity of its spectra. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.23–3.97 (m, 4H), 3.93 (q, *J* = 7.1 Hz, 4H), 1.25 (t, *J* = 7.1 Hz, 6H), 1.20 (t, *J* = 7.1 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 60.0, 17.6; ^{11}B NMR (160 MHz, $CDCl_3$) δ 31.0.

APPENDIX

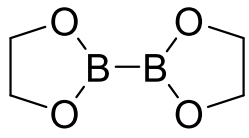
Spectral Data.

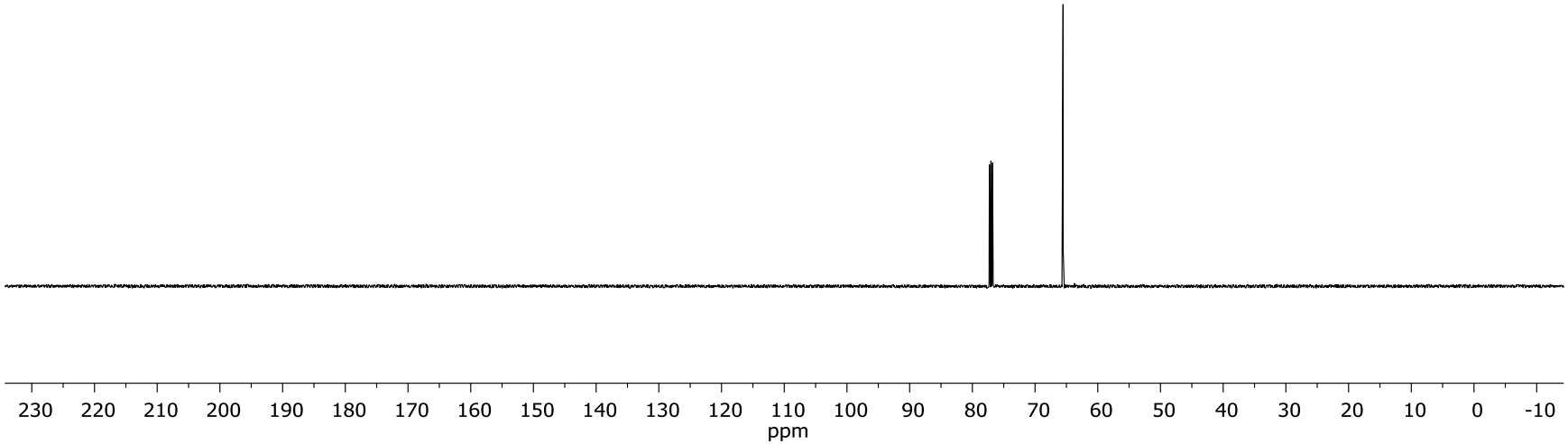
^{1}H 500 MHz, $CDCl_3$



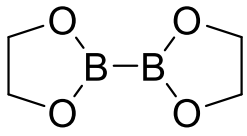


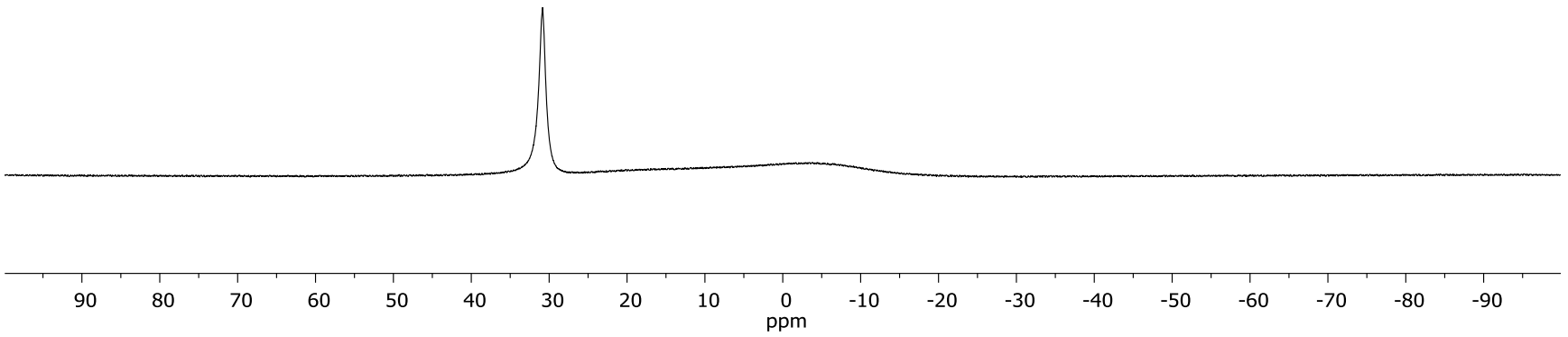
^{13}C 126 MHz, $CDCl_3$



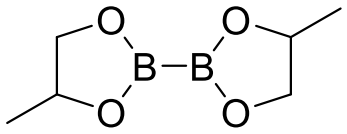


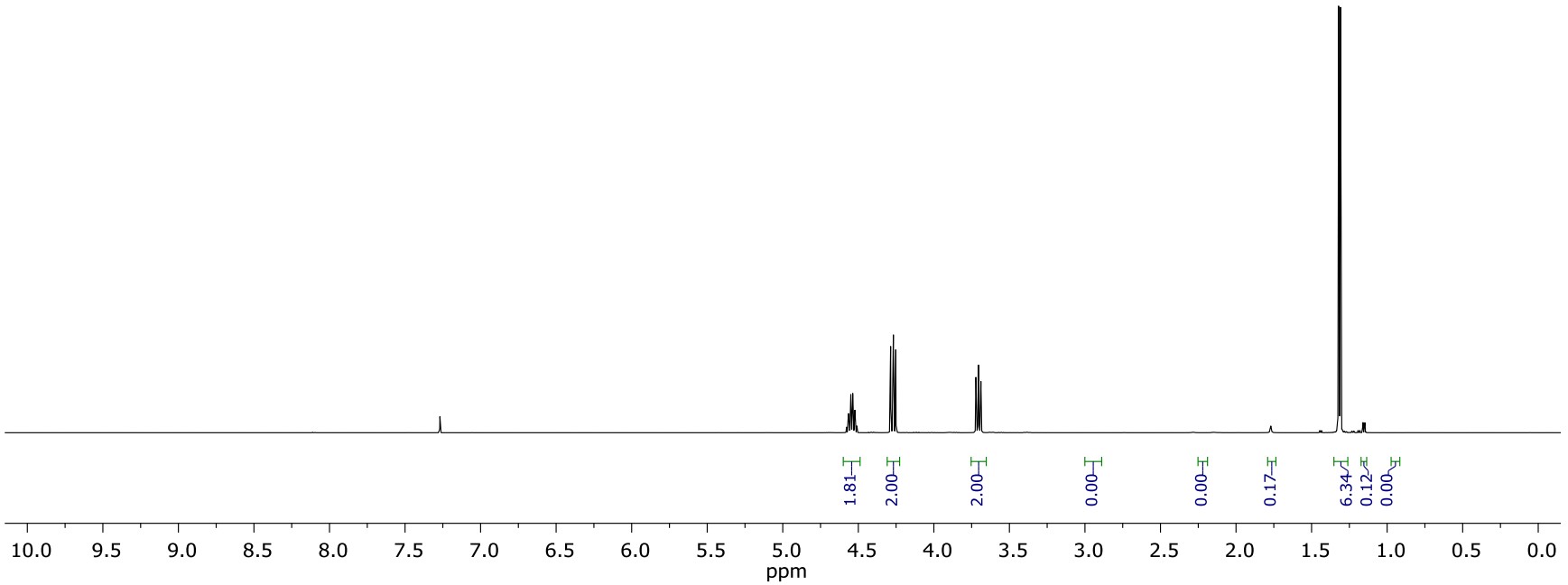
^{11}B 160 MHz, $CDCl_3$



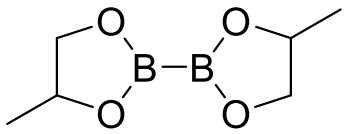


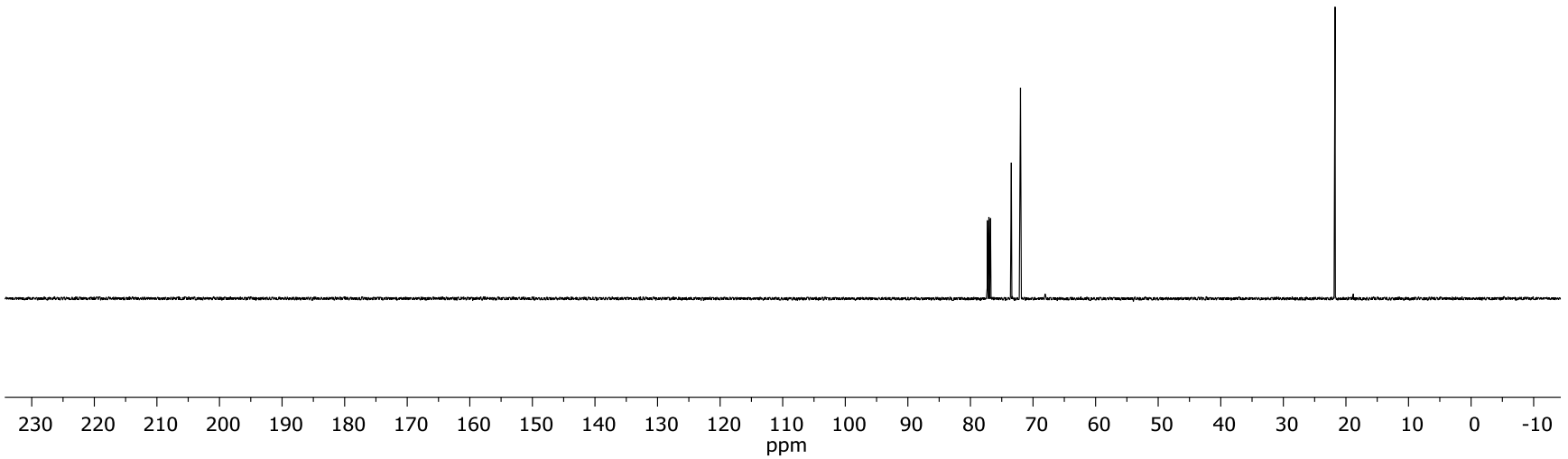
^{1}H 500 MHz, $CDCl_3$



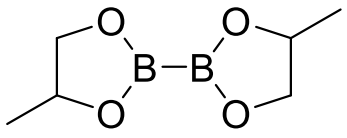


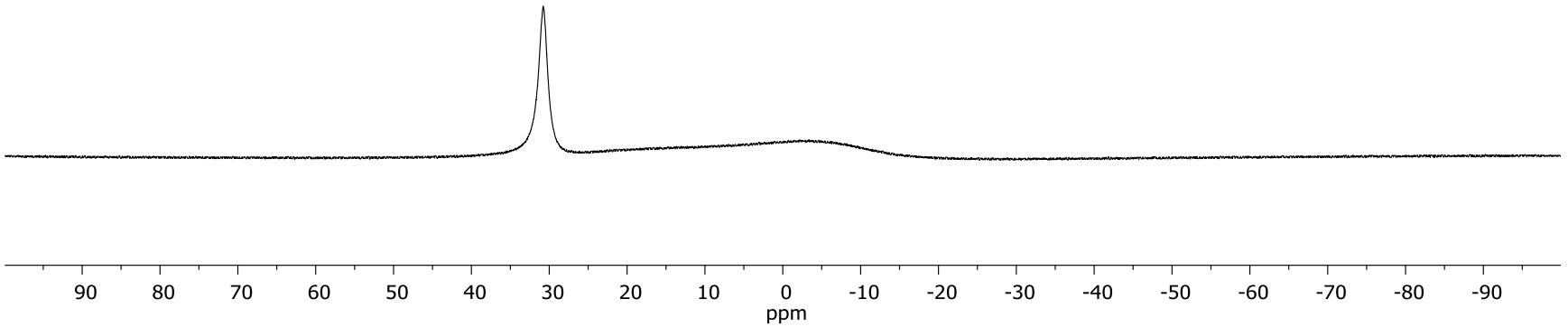
^{13}C 126 MHz, $CDCl_3$



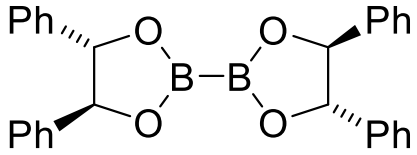


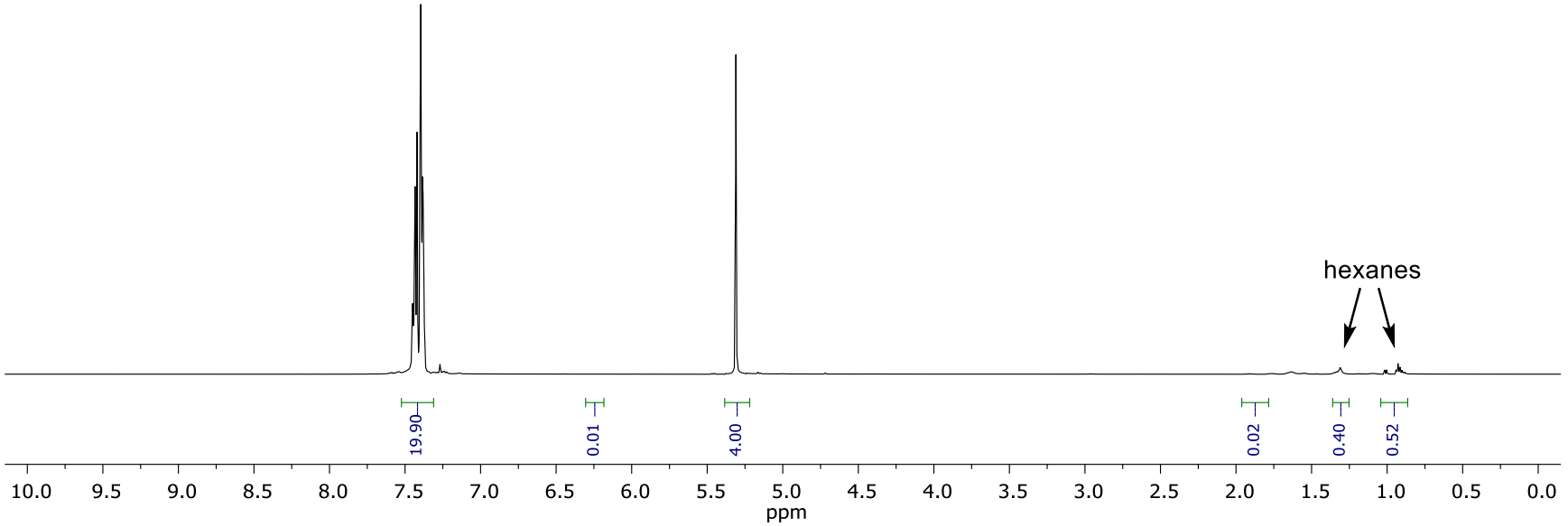
^{11}B 160 MHz, $CDCl_3$



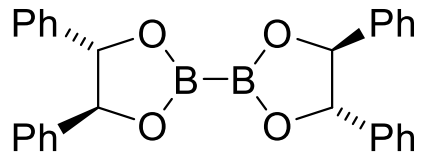


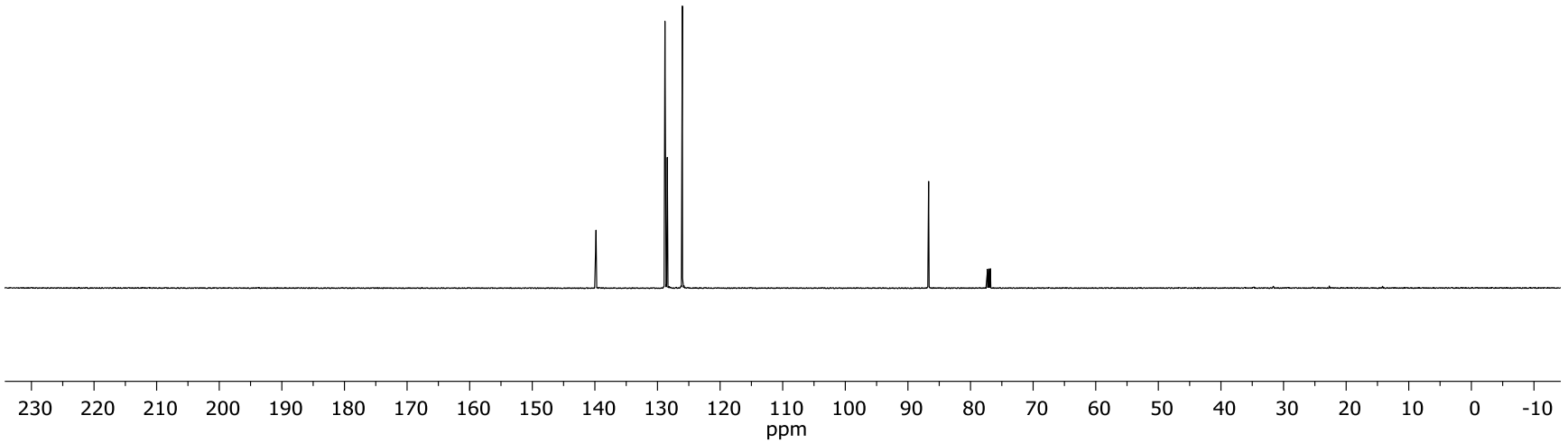
^{1}H 500 MHz, $CDCl_3$



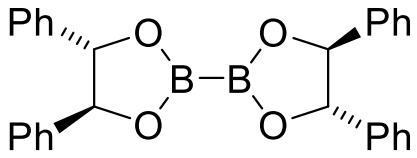


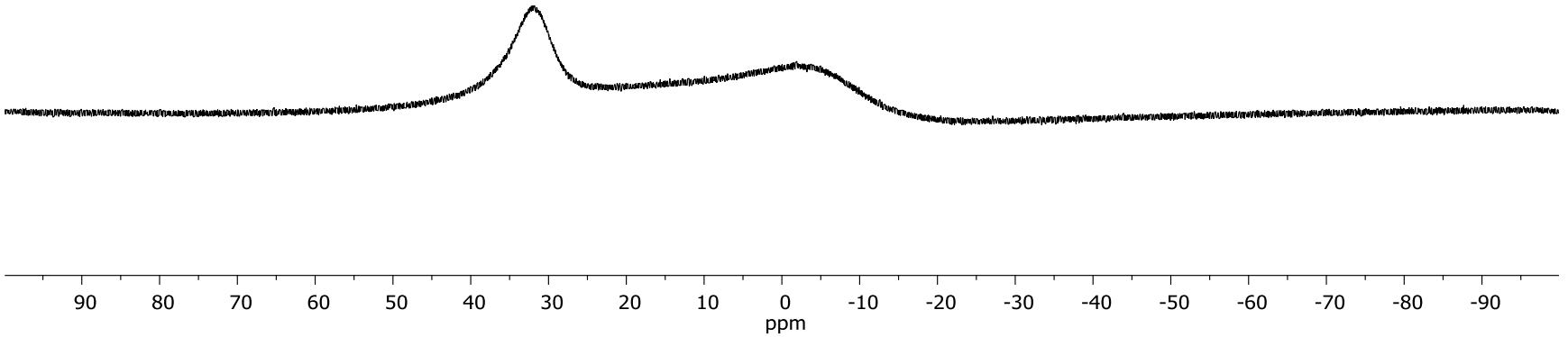
^{13}C 126 MHz, $CDCl_3$



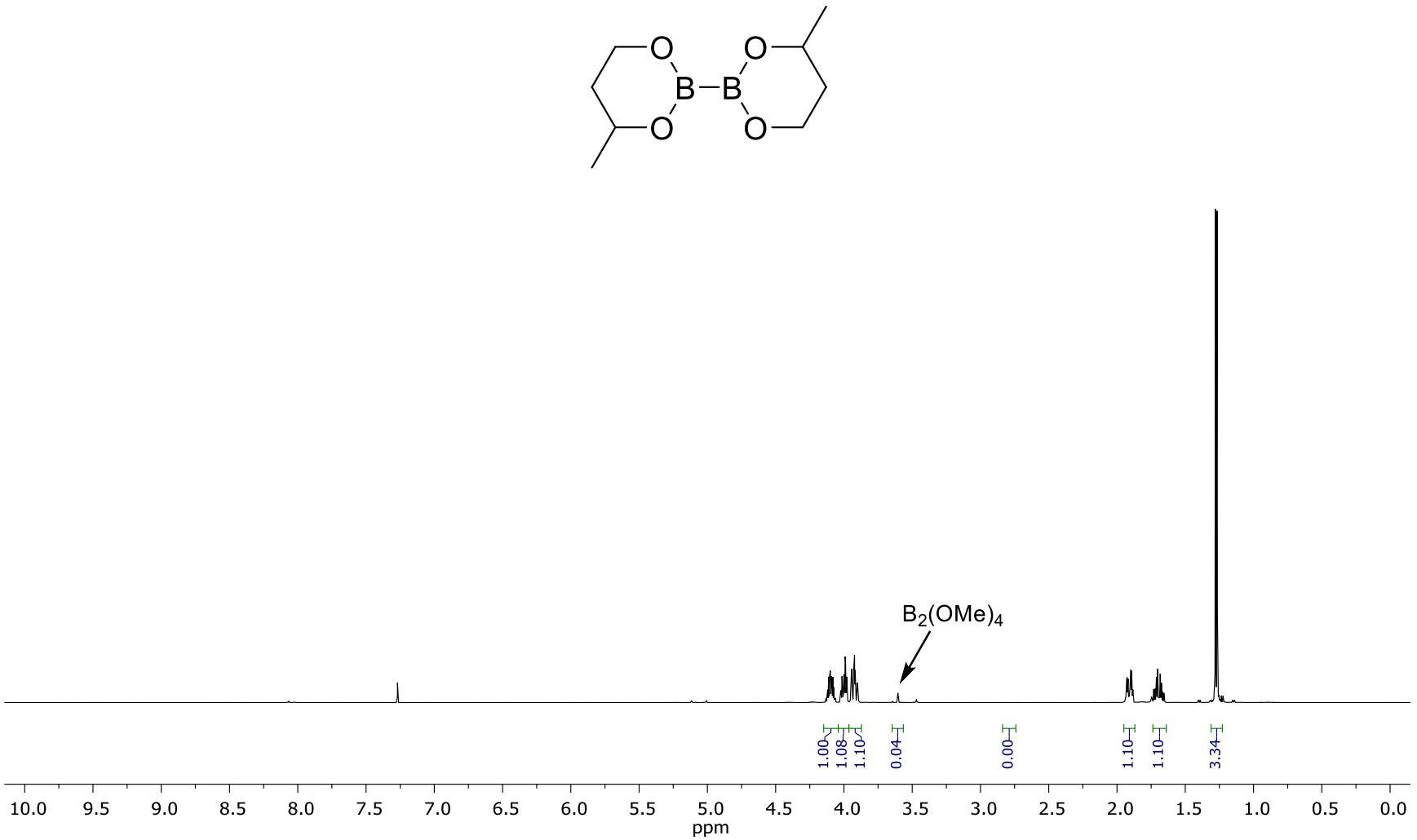


^{11}B 160 MHz, $CDCl_3$

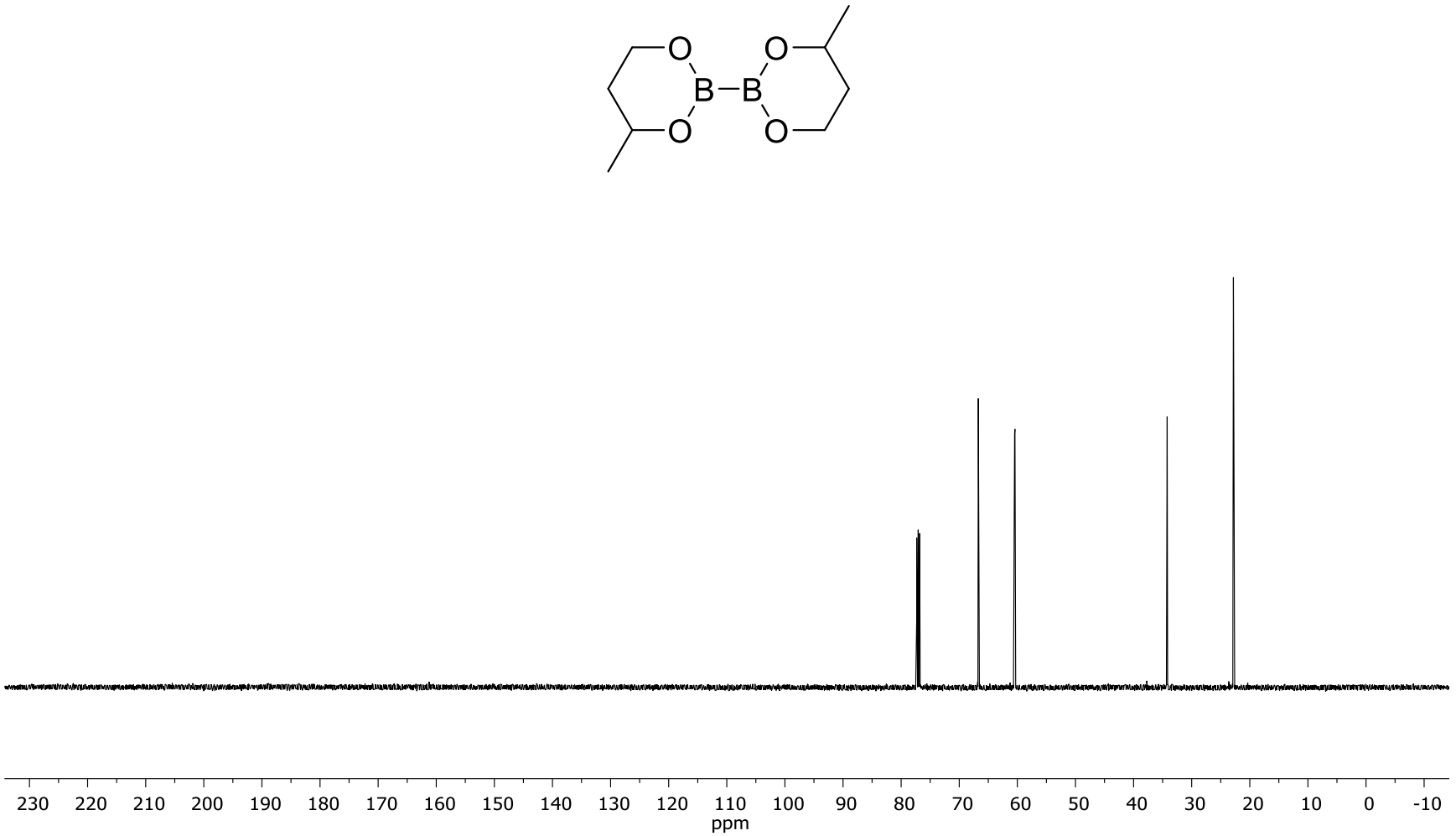




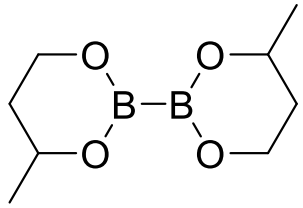
^{1}H 500 MHz, $CDCl_3$

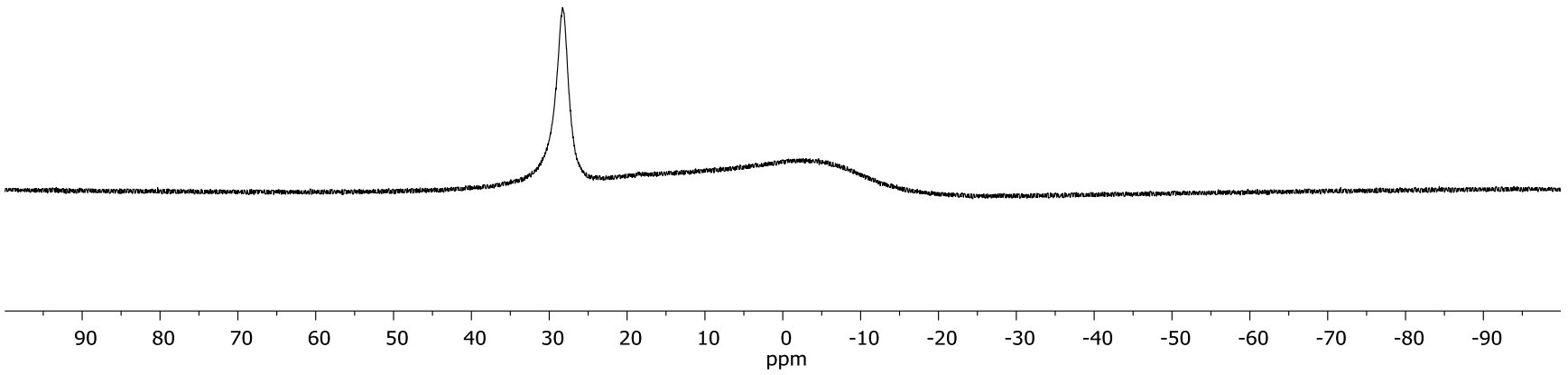


^{13}C 126 MHz, $CDCl_3$

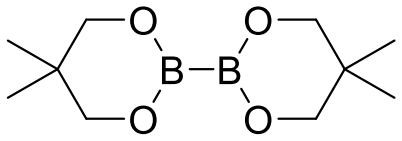


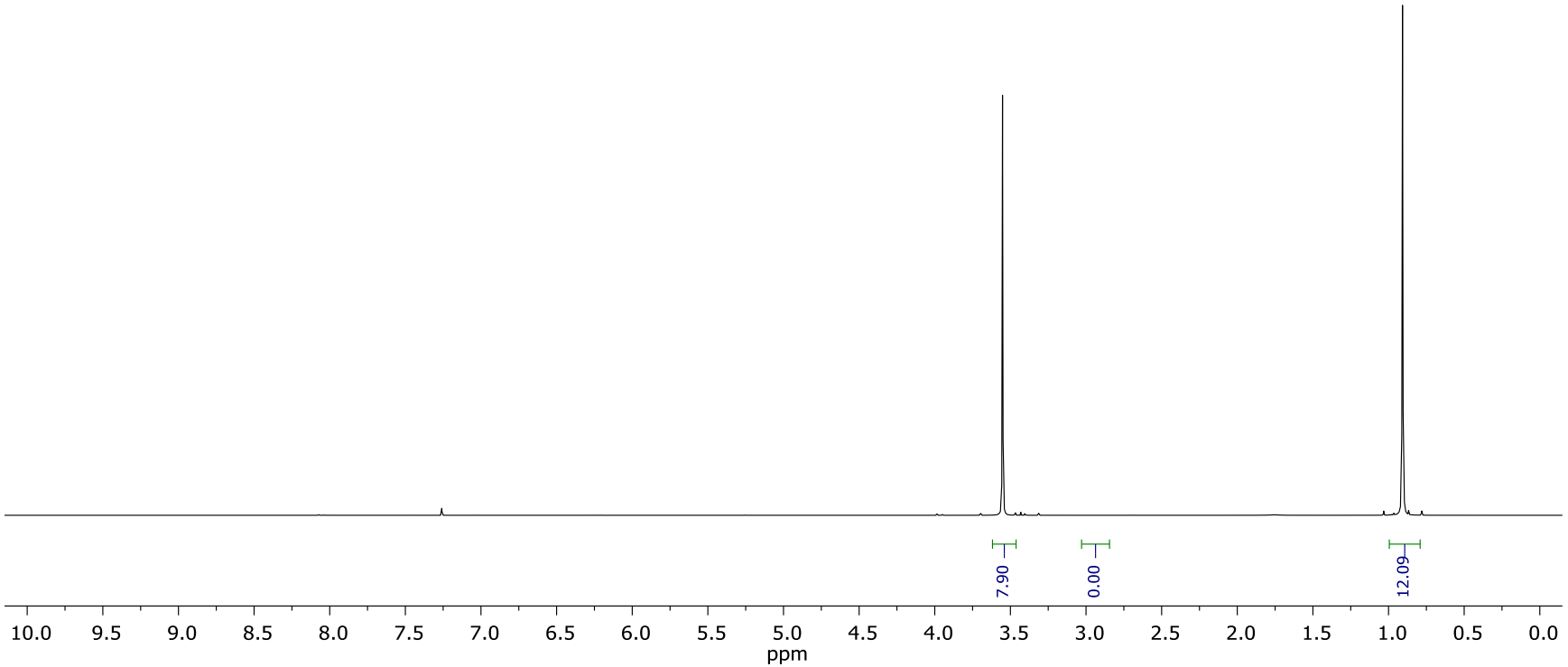
^{11}B 160 MHz, $CDCl_3$



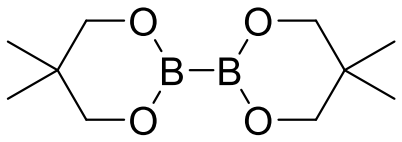


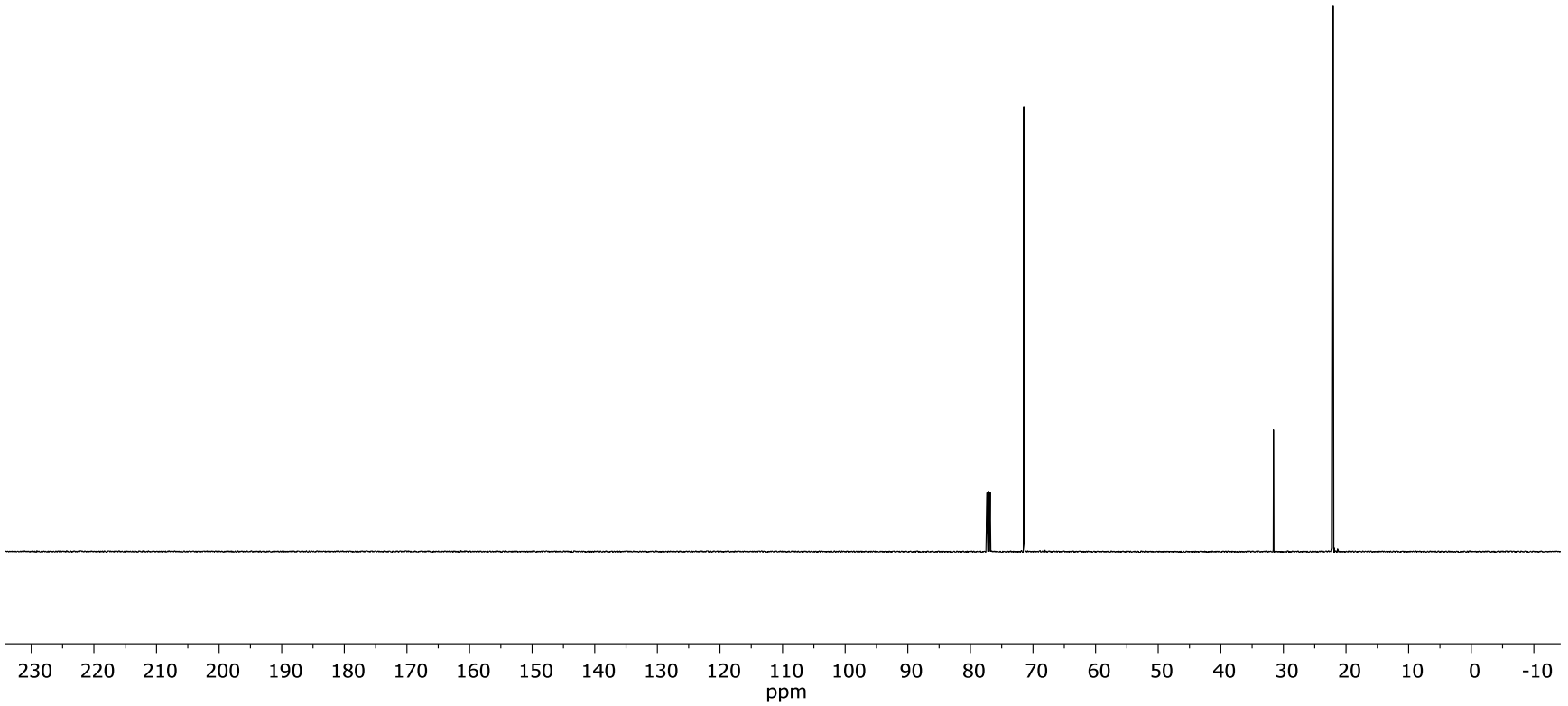
^{1}H 500 MHz, $CDCl_3$



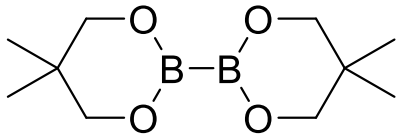


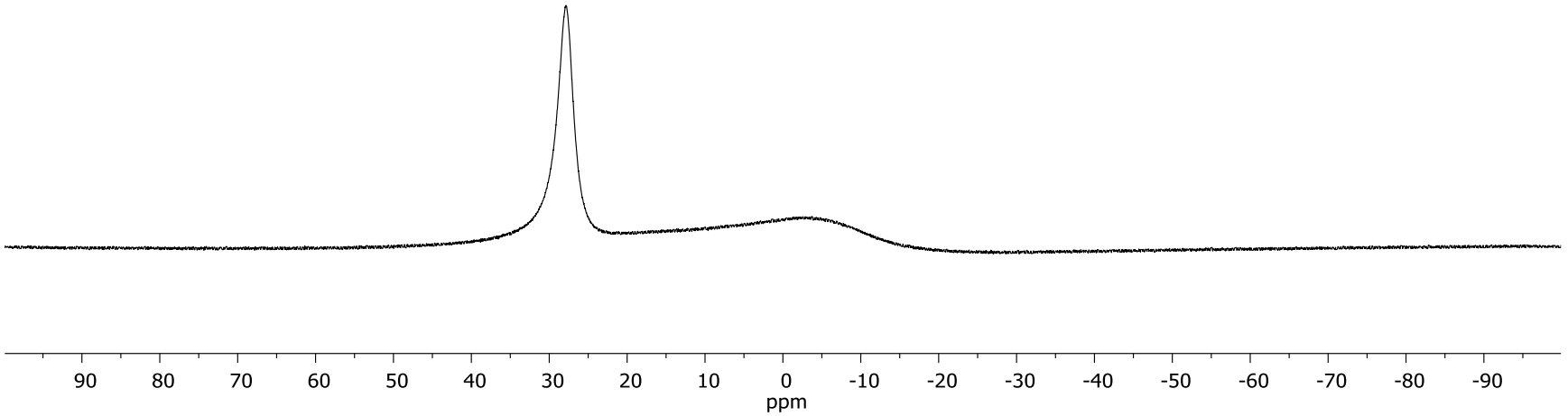
^{13}C 126 MHz, $CDCl_3$



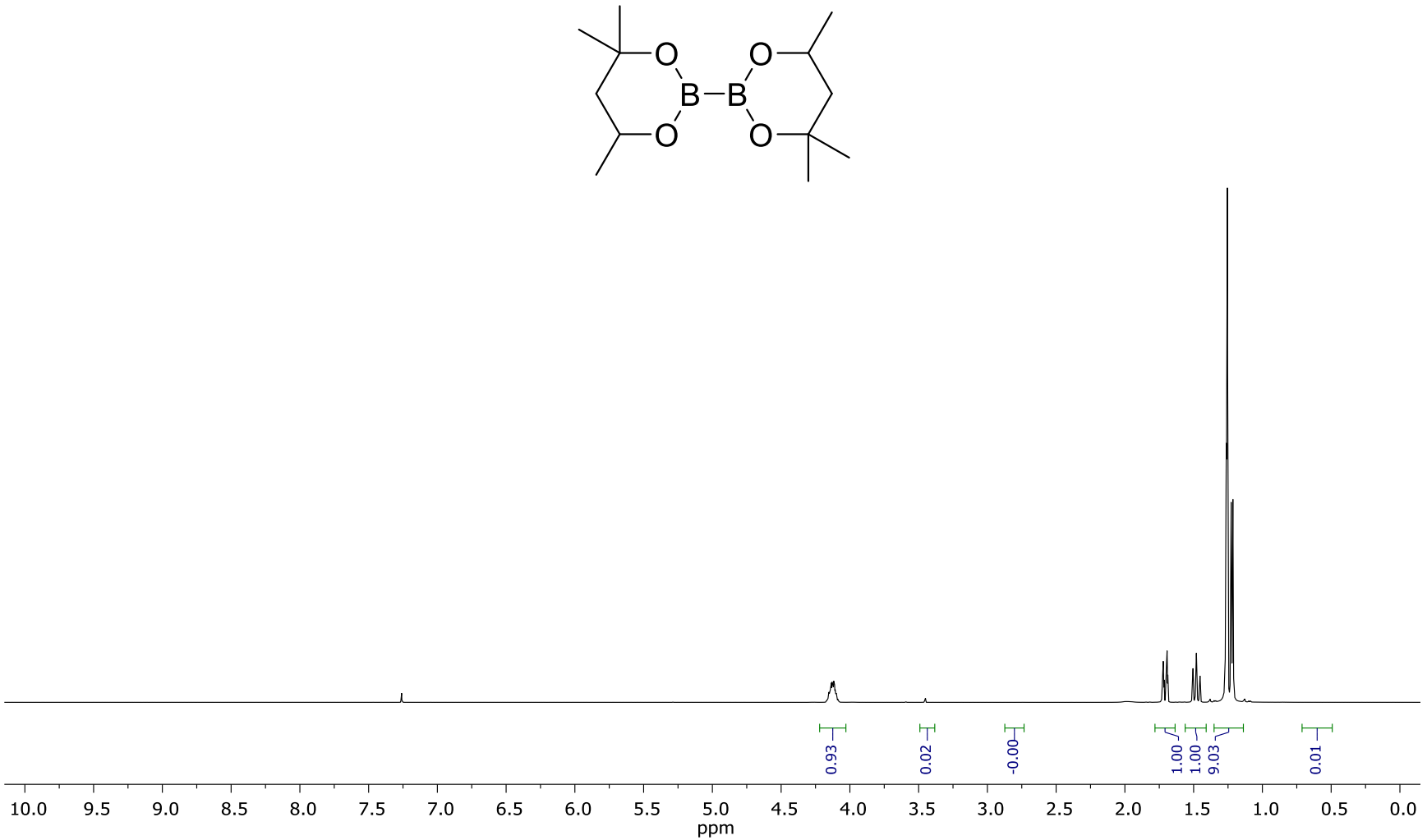


^{11}B 160 MHz, $CDCl_3$

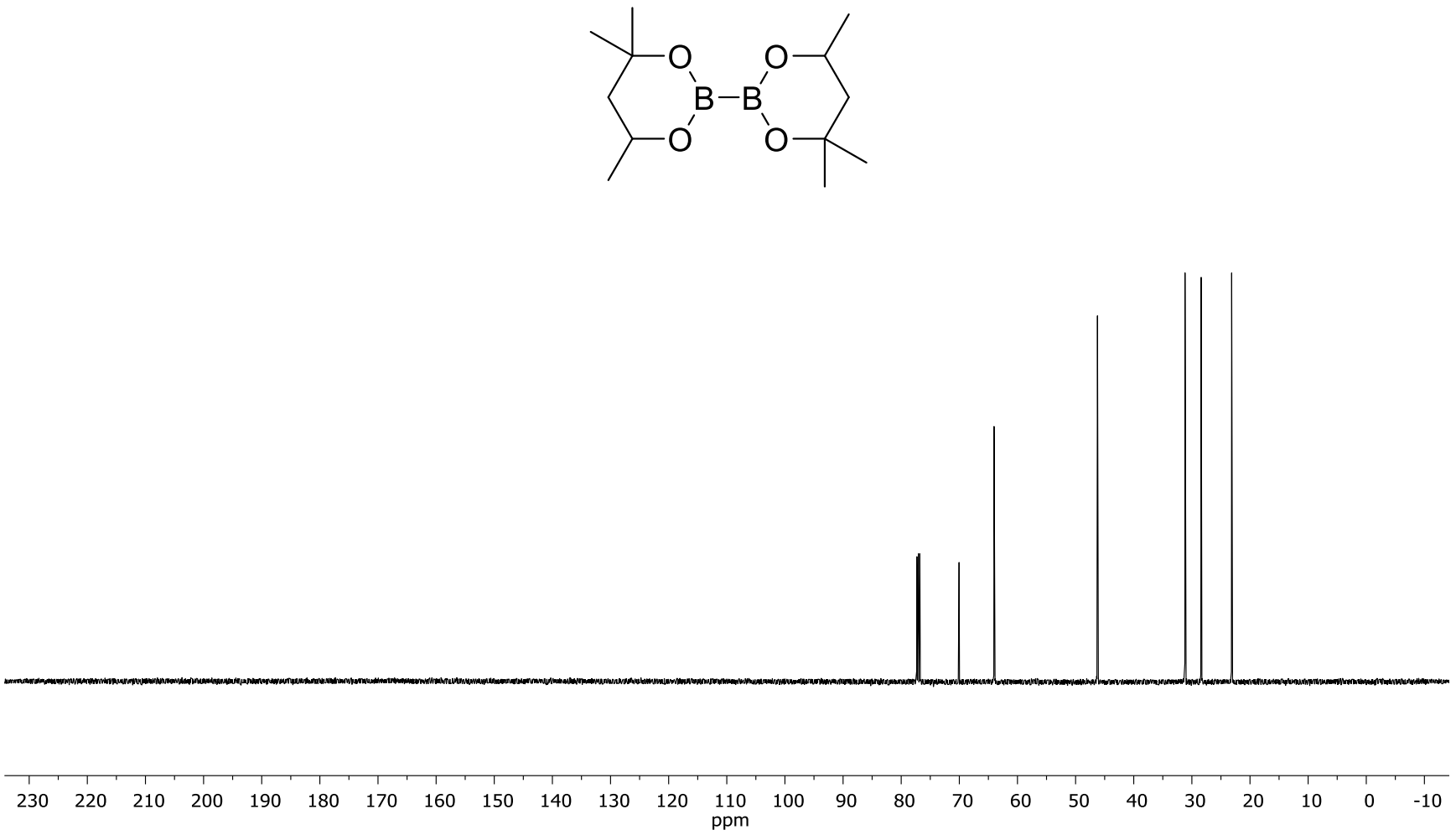




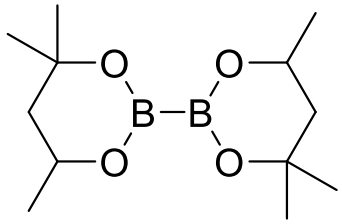
^{1}H 500 MHz, $CDCl_3$

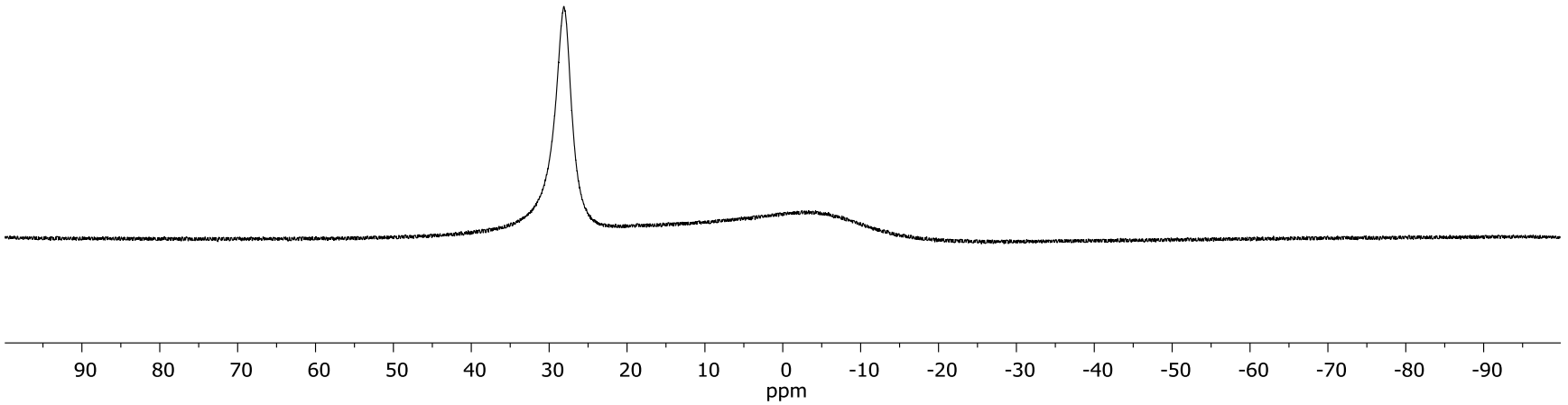


^{13}C 126 MHz, $CDCl_3$

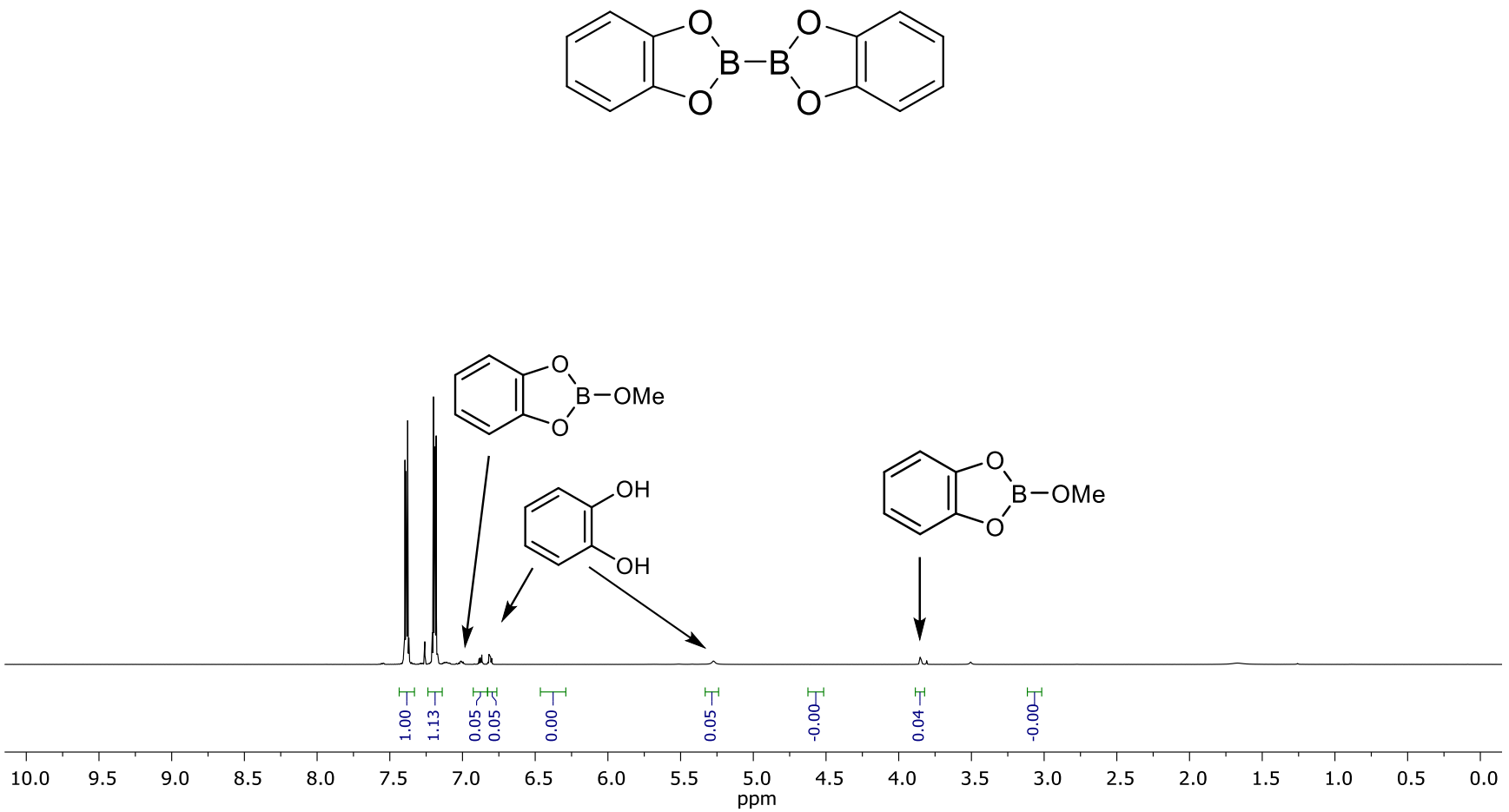


^{11}B 160 MHz, $CDCl_3$

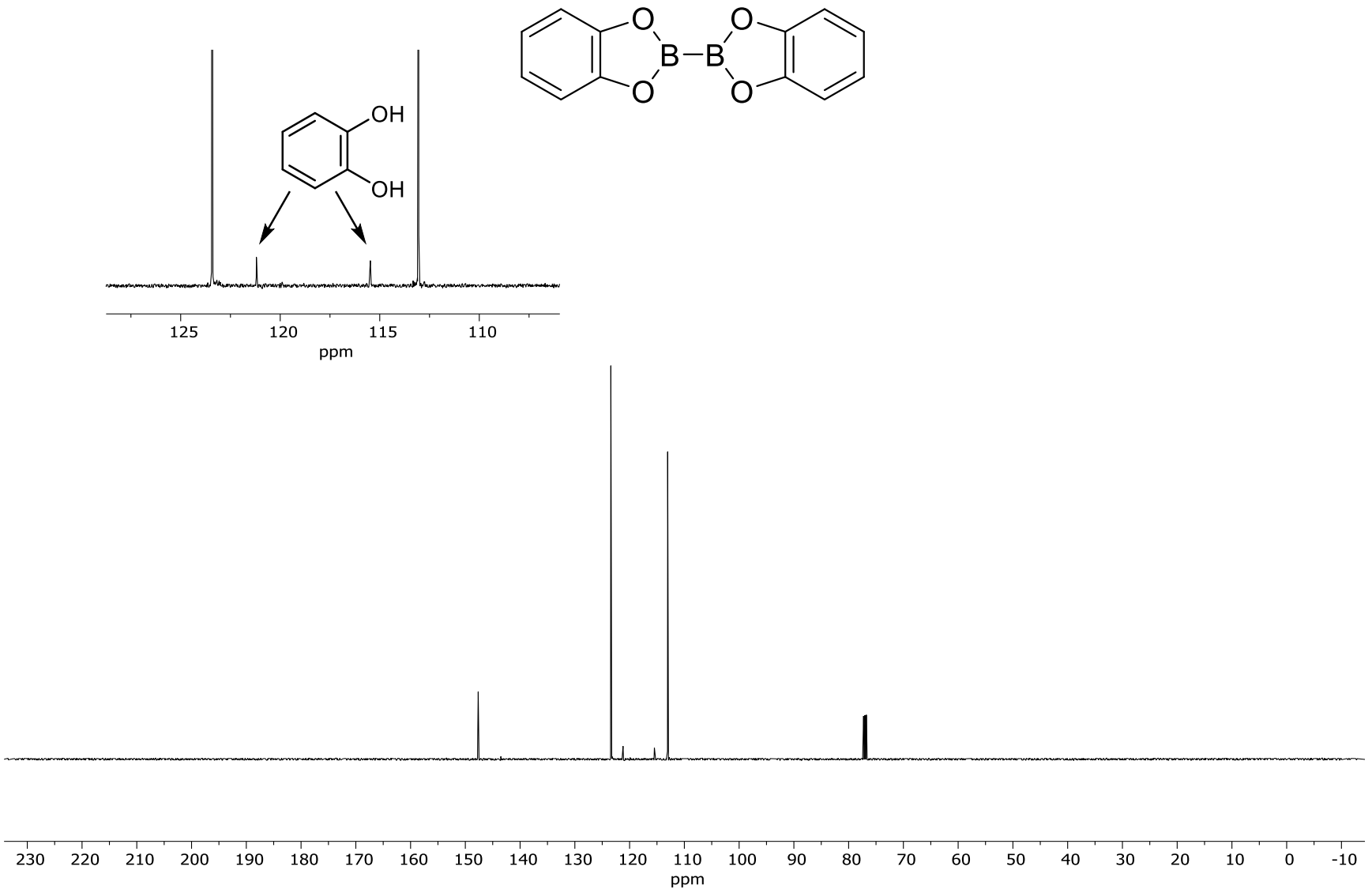




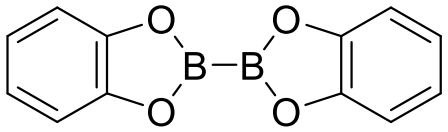
^{1}H 500 MHz, $CDCl_3$

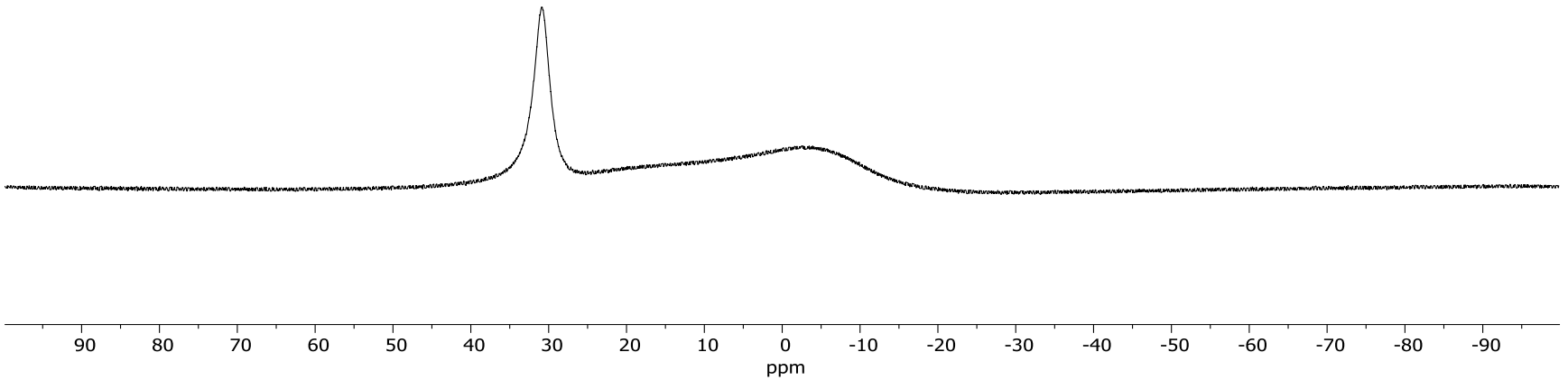


^{13}C 126 MHz, $CDCl_3$

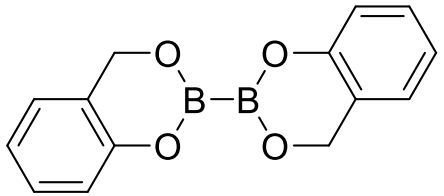


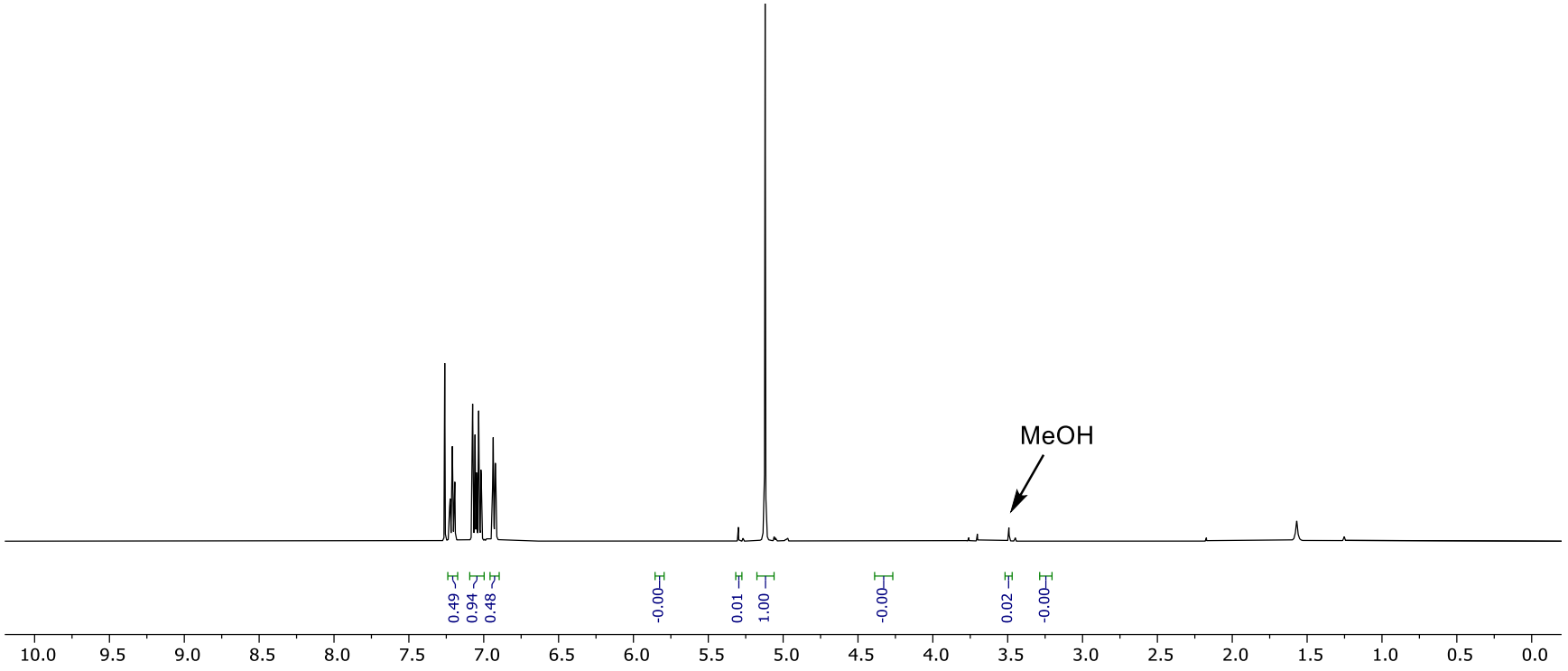
^{11}B 160 MHz, $CDCl_3$



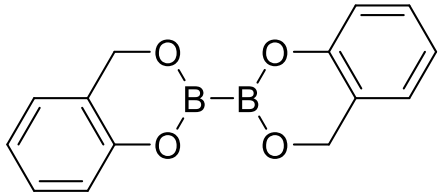


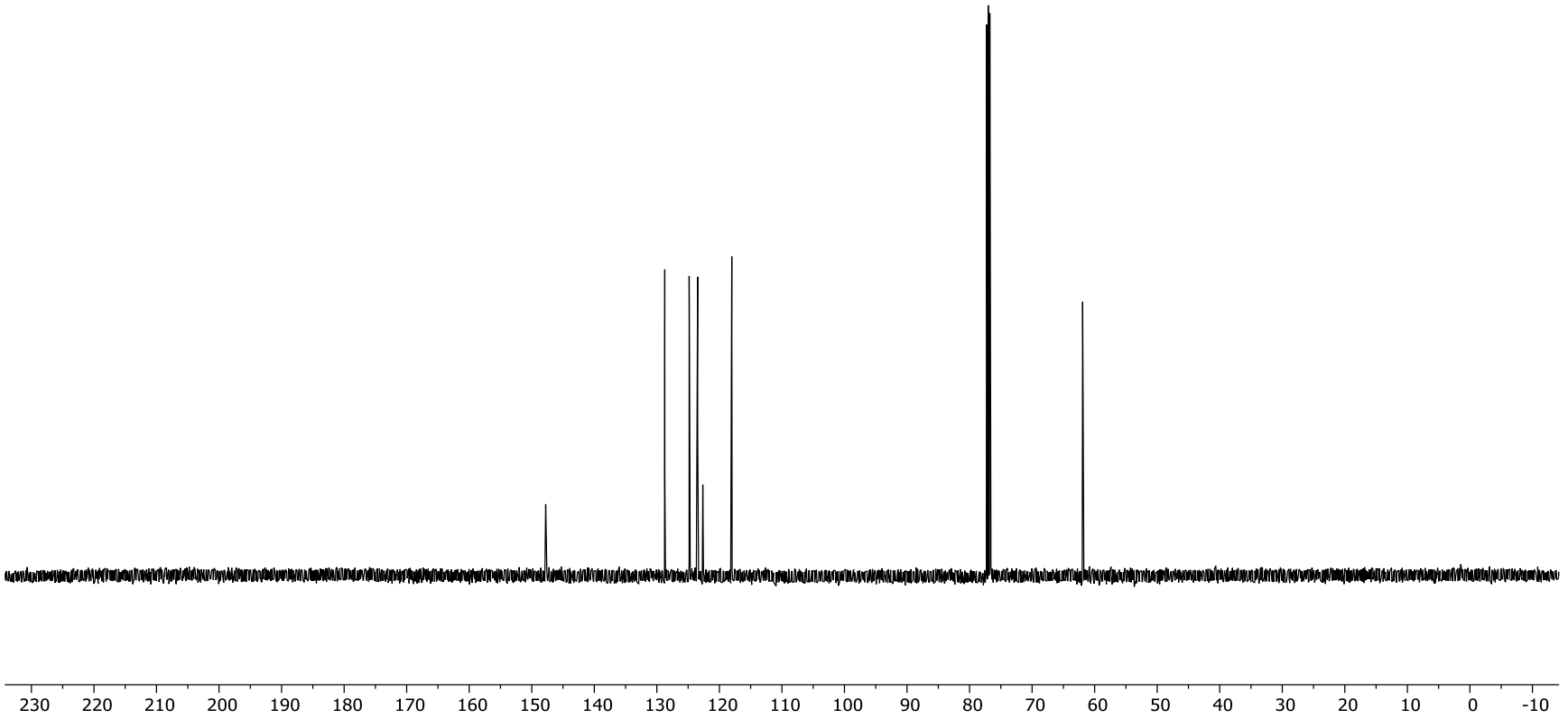
^{1}H 500 MHz, $CDCl_3$



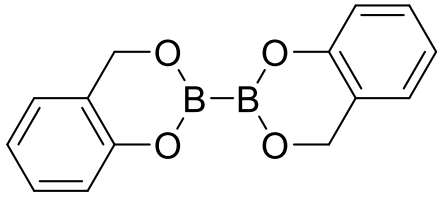


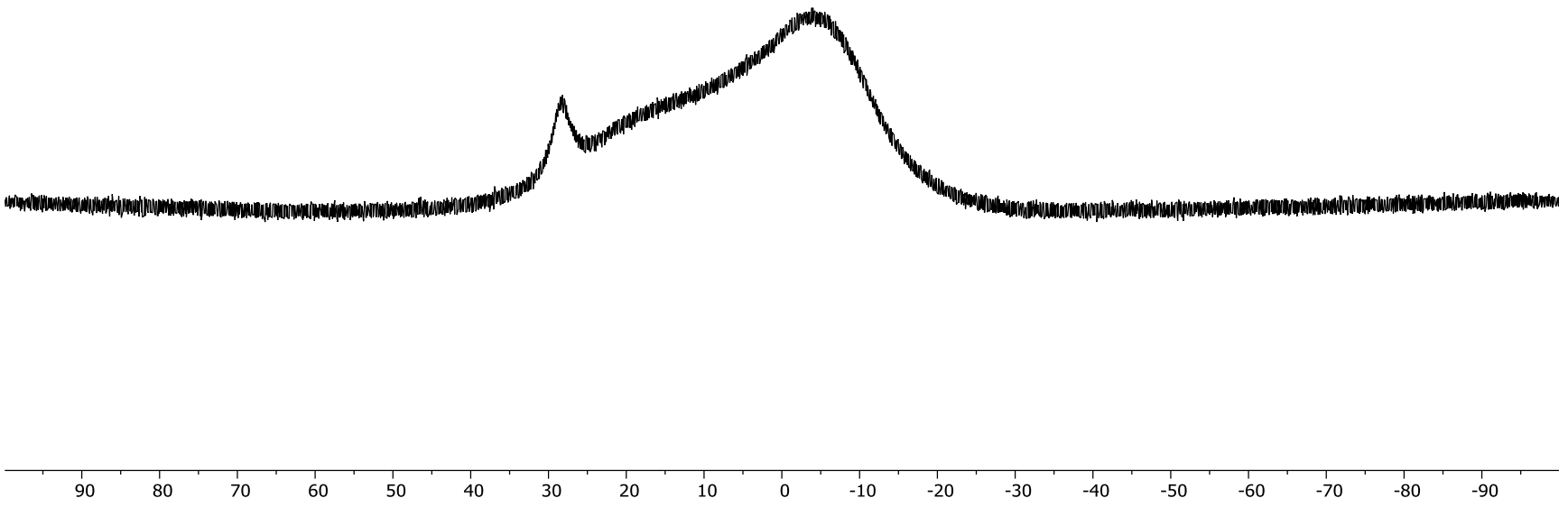
^{13}C 126 MHz, $CDCl_3$



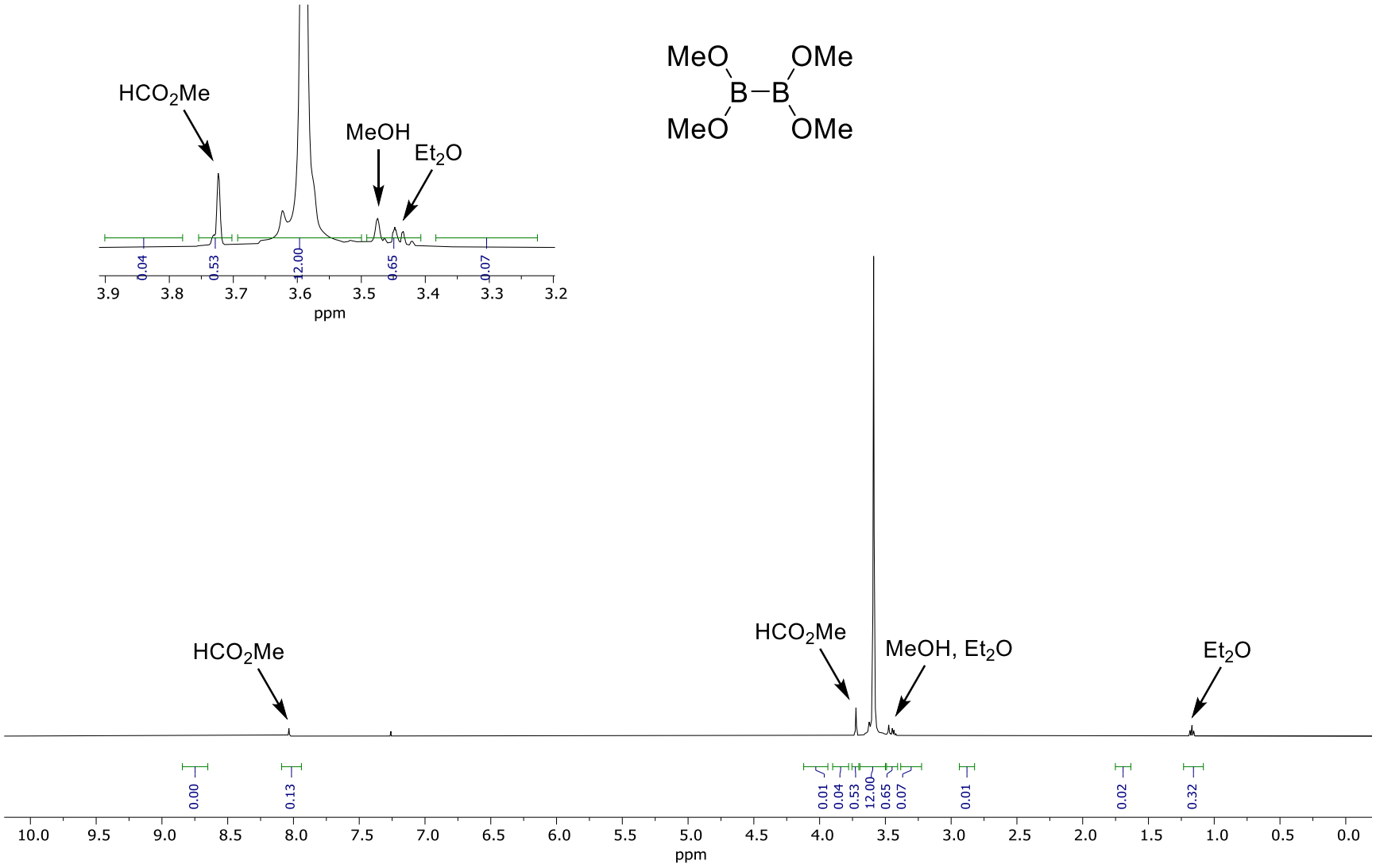


^{11}B 160 MHz, $CDCl_3$

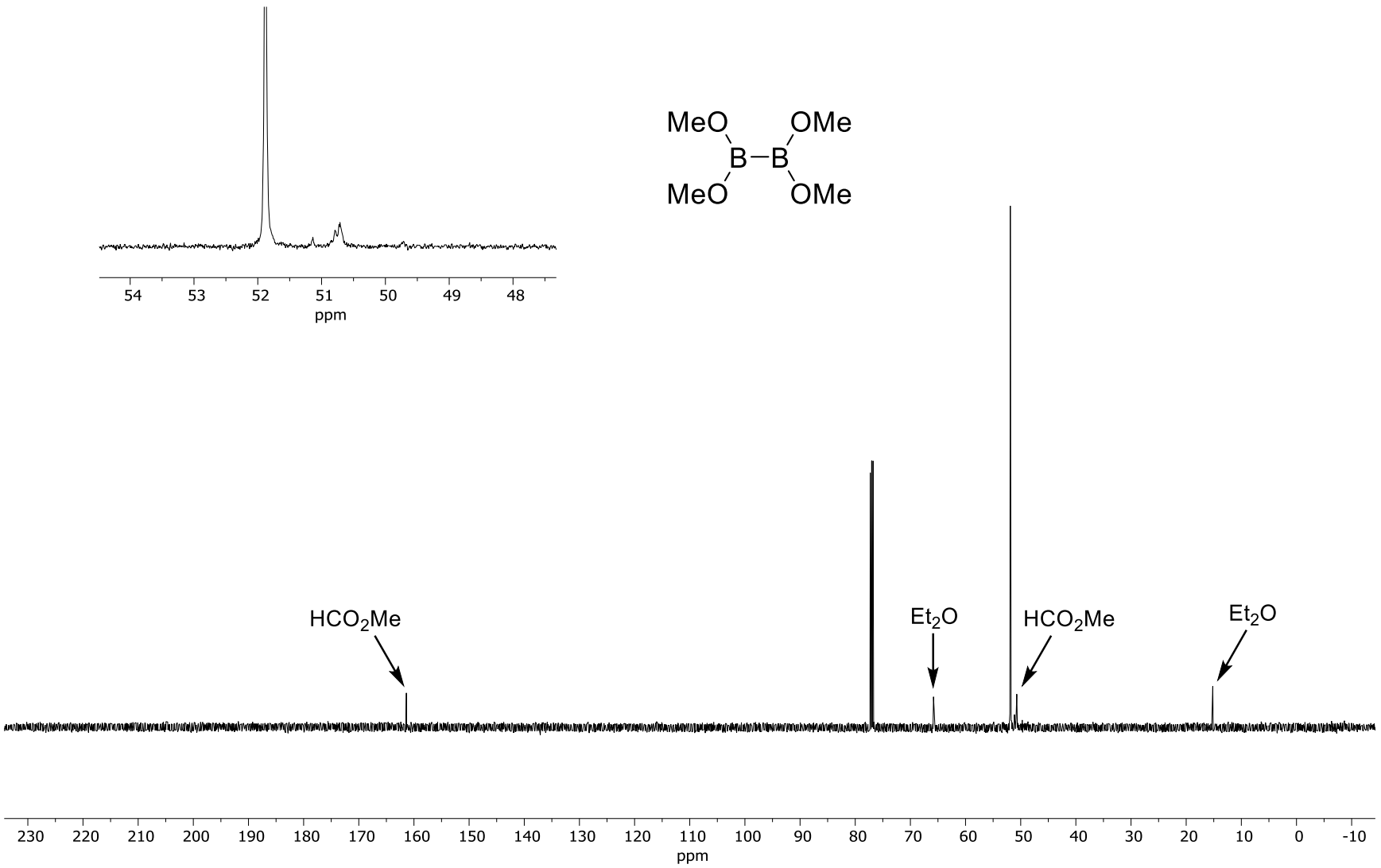




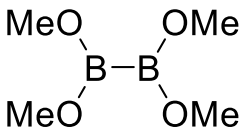
^{1}H 500 MHz, $CDCl_3$

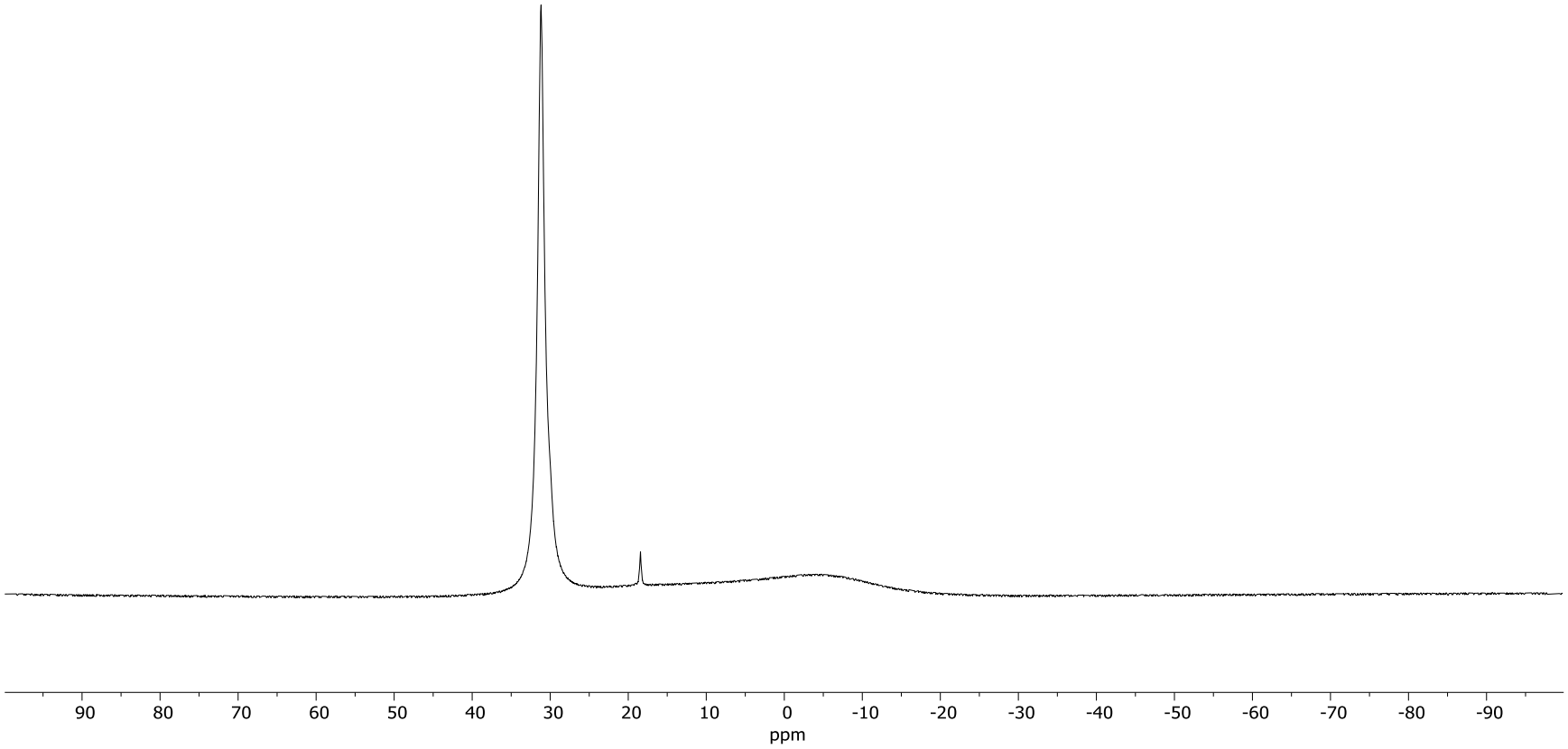


^{13}C 126 MHz, $CDCl_3$

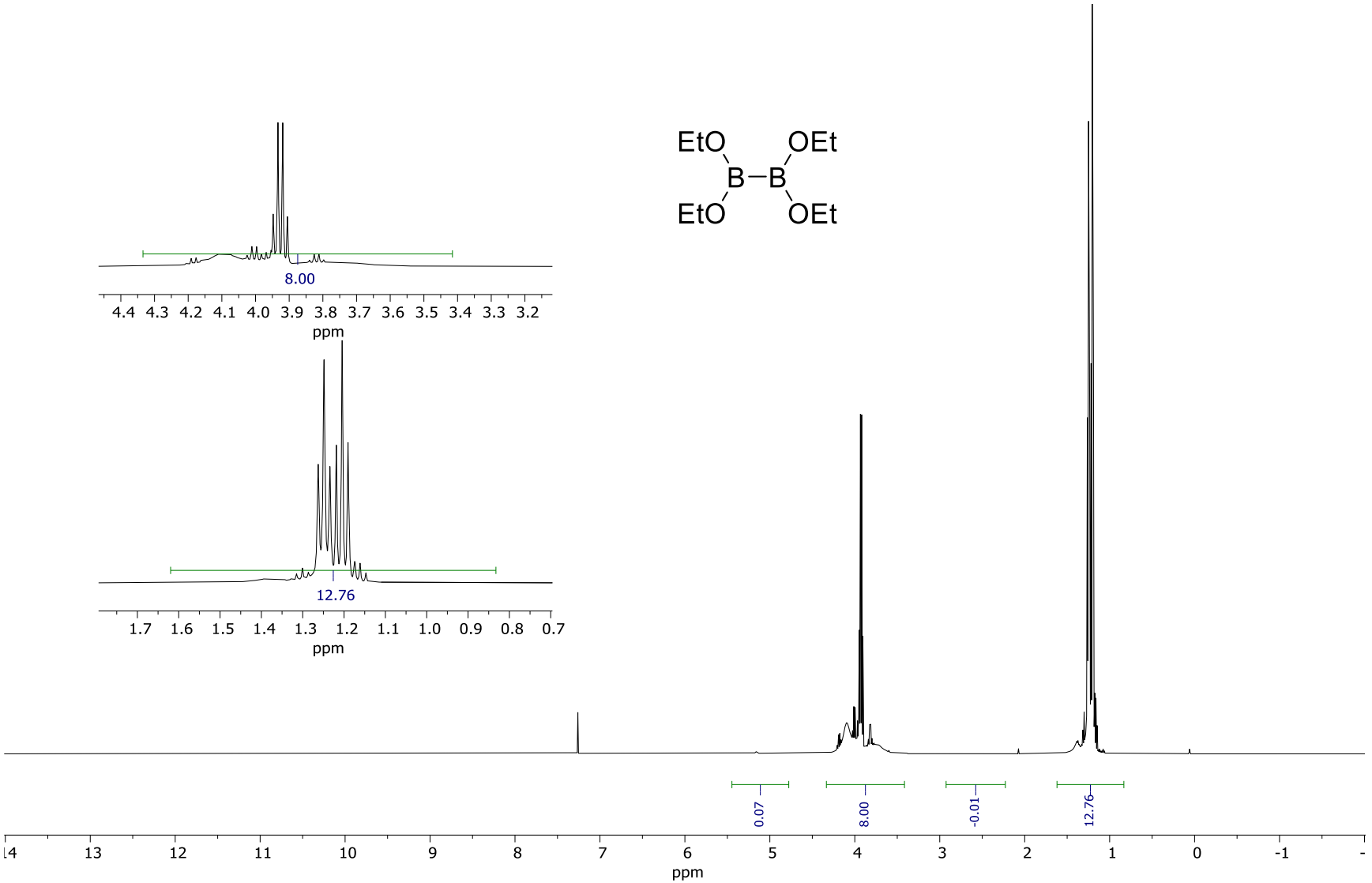


^{11}B 160 MHz, $CDCl_3$

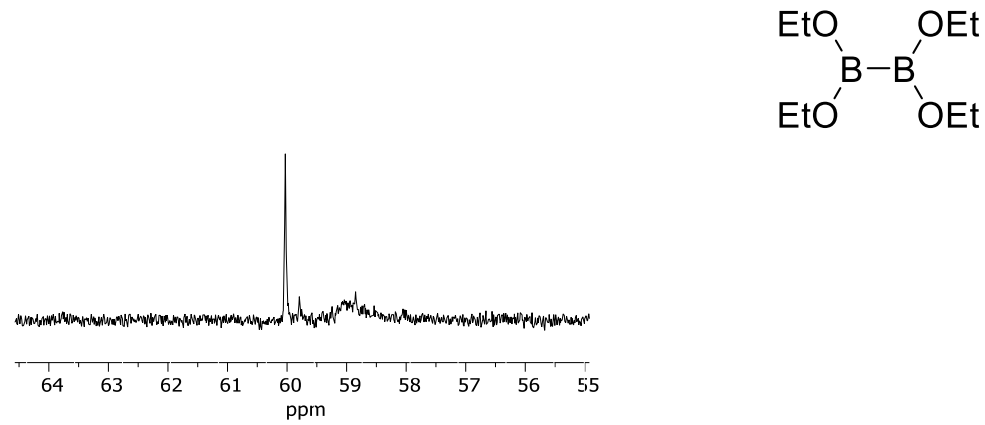




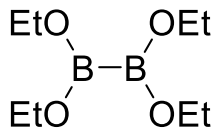
^{1}H 500 MHz, $CDCl_3$

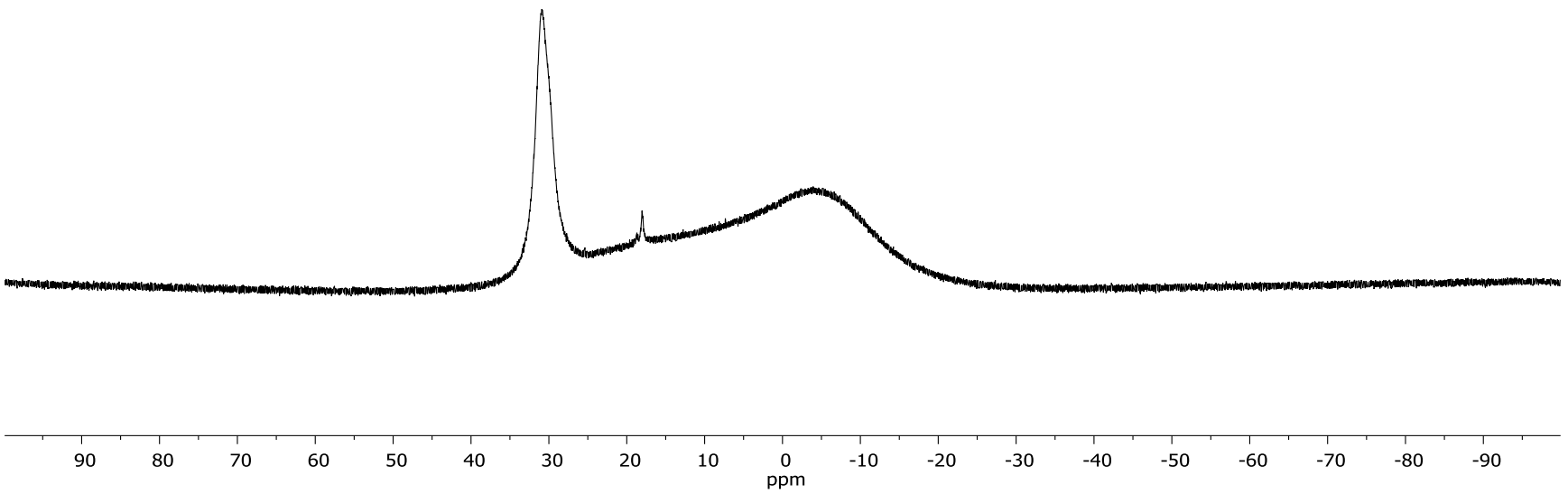


^{13}C 126 MHz, $CDCl_3$



^{11}B 160 MHz, $CDCl_3$





REFERENCES

REFERENCES

(1) Neeve, E. C.; Geier, S. J.; Mkhalid, I. A. I.; Westcott, S. A.; Marder, T. B. Diboron(4) Compounds: From Structural Curiosity to Synthetic Workhorse. *Chem. Rev.* **2016**, *116*, 9091–9161.

(2) Ishiyama, T.; Murata, M.; Miyaura, N. Palladium(0)-Catalyzed Cross-Coupling Reaction of Alkoxydiboron with Haloarenes: A Direct Procedure for Arylboronic Esters. *J. Org. Chem.* **1995**, *60*, 7508–7510.

(3) Dudnik, A. S.; Fu, G. C. Nickel-Catalyzed Coupling Reactions of Alkyl Electrophiles, Including Unactivated Tertiary Halides, To Generate Carbon-Boron Bonds. *J. Am. Chem. Soc.* **2012**, *134*, 10693–10697.

(4) Cheng, Y.; Mück-Lichtenfeld, C.; Studer, A. Metal-Free Radical Borylation of Alkyl and Aryl Iodides. *Angew. Chem. Int. Ed.* **2018**, *57*, 16832–16836.

(5) Tian, Y.-M.; Guo, X.-N.; Braunschweig, H.; Radius, U.; Marder, T. B. Photoinduced Borylation for the Synthesis of Organoboron Compounds. *Chem. Rev.* **2021**, *121*, 3561–3597.

(6) Brotherton, R. J.; McCloskey, A. L. Tetra-(amino)-diborons. *J. Am. Chem. Soc.* **1960**, *82*, 6242–6245.

(7) Ishiyama, T.; Murata, M.; Ahiko, T.; Miyuara, N. Bis(pinacolato)diboron. *Org. Synth.* **2000**, *77*, 176–180.

(8) Bello, C. S.; Schmidt-Leithoff, J. Borylation of organo halides and triflates using tetrakis(dimethylamino)diboron. *Tetrahedron Lett*. **2012**, *53*, 6230–6235.

(9) Molander, G. A.; Trice, S. L. J.; Kennedy, S. M. Palladium-Catalyzed Borylation of Aryl and Heteroaryl Halides Utilizing Tetrakis(dimethylamino)diboron: One Step Greener. *Org. Lett.* **2012**, *14*, 4814–4817.

(10) Molander, G. A.; Wisniewski, S. R.; Hosseini-Sarvari, M. Synthesis and Suzuki–Miyaura Cross-Coupling of Enantioenriched Secondary Potassium β-Trifluoroboratoamides: Catalytic, Asymmetric Conjugate Addition of Bisboronic Acid and Tetrakis(dimethylamino)diboron to α,β-Unsaturated Carbonyl Compounds. *Adv. Synth. Catal.* **2013**, *355*, 3037–3057.

(11) McCloskey, A. L.; Brotherton, R. J.; Boone, J. L. The Preparation of Boron Monoxide and its Conversion to Diboron Tetrachloride. *J. Am. Chem. Soc.* **1961**, *83*, 4750–4754.

(12) Chattopadhyay, B.; Dannatt, J. E.; Andujar-De Sanctis, I. L.; Gore, K. A.; Maleczka, R. E.; Singleton, D. A.; Smith, M. R. Ir-Catalyzed ortho-Borylation of Phenols Directed by Substrate–Ligand Electrostatic Interactions: A Combined Experimental/in Silico Strategy for Optimizing Weak Interactions. *J. Am. Chem. Soc.* **2017**, *139*, 7864–7871.

(13) Elkin, P. K.; Levin, V. V.; Dilman, A. D.; Struchkova, M. I.; Belyakov, P. A.; Arkhipov, D. E.; Korlyukov, A. A.; Tartakovsky, V. A. Reactions of CF_3-substituted boranes with a-diazocarbonyl compounds. *Tetrahedron Lett.* **2011**, *52*, 5259–5263.

(14) Wartik, T.; Apple, E. F. A New Modification of Boron Monoxide. *J. Am. Chem. Soc.* **1955**, *77*, 6400–6401.

(15) Clegg, W.; Johann, T. R. F.; Marder, T. B.; Norman, N. C.; Orpen, A. G.; Peakman, T. M.; Quayle, M. J.; Rice, C. R.; Scott, A. J. Platinum-catalysed 1,4-diboration of 1,3-dienes. *J. Chem. Soc., Dalton Trans.* **1998**, 1431–1438.

(16) Chen, D.; Xu, G.; Zhou, Q.; Chung, L. W.; Tang, W. Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. *J. Am. Chem. Soc.* **2017**, *139*, 9767–9770.

(17) The Commonwealth of Australia Commonwealth Scientific and Industrial Research Organization. Boronic compounds. US6346639, **2002**, B1.

(18) Luna-Herrera, J. C.; Sampedro, D.; Jiménez, M. C.; Pérez-Ruiz, R. Rapid Access to Borylated Thiophenes Enabled by Visible Light. *Org. Lett.* **2020**, *22*, 3273–3278.

(19) Lawlor, F. J.; Norman, N. C.; Pickett, N. L.; Robins, E. G. Bis-Catecholate, Bis-Dithiocatecholate, and Tetraalkoxy Diborane(4) Compounds: Aspects of Synthesis and Electronic Structure. *Inorg. Chem.* **1998**, *37*, 5282–5288.

(20) Boron Molecular Pty Ltd. Preparation of Diboronic Esters. WO2004/76467, **2004**, A1

(21) Clegg, W.; Dai, C.; Lawlor, F. J.; Marder, T. B.; Nguyen, P.; Norman, N. C.; Pickett, N. L.; Power, W. P.; Scott, A. J. Lewis-base adducts of the diborane(4) compounds $B_2(1,2\text{-}E_2C_6H_4)_2$ (E = O or S). *J. Chem. Soc., Dalton Trans.* **1997**, 839–846.

(22) Welch, S. Boron Heterocycles. V. Preparation and Characterization of Selected Heteronuclear Diboron Ring Systems. *Inorg. Chem.* **1968**, *7*, 225–230.