

Supplemental Information for
ULTRAFAST DYNAMICS OF IRON(II)-BASED COMPLEXES IN SOLUTION AND
SEMICONDUCTOR-CHROMOPHORE ASSEMBLIES

By

Jennifer Nicole Miller

A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

Chemistry – Doctor of Philosophy

2018

Chapter 3: Outer-sphere effects on the excited state dynamics of ligand field states in Fe(II) polypyridyl complexes

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[Fe(5,5'-dmb) ₃] ²⁺ singlet in ethanol, applied by CPCM	115
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[Fe(bpy)₃]²⁺ singlet in gas phase

Fe	-0.00070200	0.00000000	4.07637100
N	1.54484000	0.77715700	3.02296300
C	1.45675100	1.59847900	1.96072200
H	0.45624500	1.82780600	1.61550200
C	2.57101600	2.13217400	1.32001700
H	2.44026100	2.78749700	0.46618400
C	3.83795900	1.80676600	1.80149500
H	4.73119600	2.20542600	1.33188700
C	3.94058700	0.95847800	2.90103600
H	4.91672500	0.69816100	3.29127900
C	2.77909100	0.45439100	3.49422600
C	2.77909100	-0.45439100	4.65851500
N	1.54484000	-0.77715800	5.12977800
N	-1.44624200	0.95038100	3.02303700
C	-2.11436100	0.46317600	1.96146900
H	-1.81427100	-0.51880400	1.61730200
C	-3.13272900	1.16209000	1.32008300
H	-3.63565000	0.72094200	0.46683300
C	-3.48242300	2.42310000	1.80012100
H	-4.27340100	2.99803200	1.32986600
C	-2.79843500	2.93621500	2.89920700
H	-3.05971700	3.91247600	3.28849100
C	-1.78232200	2.18147100	3.49327900
C	-0.99542000	2.63543900	4.65783400
N	-0.10027500	1.72697200	5.13013400
N	-0.10027500	-1.72697200	3.02260700
C	0.65431300	-2.06057900	1.95959700
H	1.35197300	-1.30806200	1.61350300
C	0.56006400	-3.29258400	1.31912300
H	1.19224100	-3.50635600	0.46458800
C	-0.35357400	-4.22811100	1.80173100
H	-0.45430400	-5.20118500	1.33235400
C	-1.13874000	-3.89363700	2.90207300
H	-1.85104800	-4.60960600	3.29311400
C	-0.99542000	-2.63543900	3.49490700
C	-1.78232200	-2.18147100	4.65946200
N	-1.44624200	-0.95038100	5.12970400
C	-2.11436100	-0.46317600	6.19127200
H	-1.81427100	0.51880400	6.53543900
C	-3.13272900	-1.16208900	6.83265800
H	-3.63565000	-0.72094200	7.68590800
C	-3.48242300	-2.42310000	6.35262000
H	-4.27340200	-2.99803200	6.82287500
C	-2.79843500	-2.93621500	5.25353400
H	-3.05971700	-3.91247600	4.86425000

C	0.65431300	2.06057900	6.19314400
H	1.35197300	1.30806200	6.53923800
C	0.56006400	3.29258400	6.83361800
H	1.19224100	3.50635600	7.68815300
C	-0.35357300	4.22811100	6.35101000
H	-0.45430400	5.20118500	6.82038700
C	-1.13874000	3.89363700	5.25066800
H	-1.85104700	4.60960600	4.85962700
C	1.45675000	-1.59847900	6.19201900
H	0.45624500	-1.82780600	6.53723900
C	2.57101600	-2.13217400	6.83272400
H	2.44026100	-2.78749700	7.68655700
C	3.83795900	-1.80676600	6.35124600
H	4.73119600	-2.20542600	6.82085400
C	3.94058700	-0.95847800	5.25170500
H	4.91672500	-0.69816100	4.86146200

[Fe(bpy)₃]²⁺ quintet in gas phase, <S²> = 6.0105

Fe	0.00961900	0.00000400	4.07636800
N	1.78390600	0.72784100	2.94248600
C	1.71811200	1.52417700	1.86236700
H	0.72308400	1.71772600	1.47457200
C	2.84279400	2.08076000	1.25948000
H	2.73703100	2.71517700	0.38662500
C	4.09148500	1.80285900	1.81269000
H	4.99488700	2.22249100	1.38188200
C	4.16855300	0.97976600	2.93477100
H	5.13341300	0.77201900	3.38011200
C	2.99566600	0.44625800	3.48028600
C	2.99565500	-0.44629500	4.67248700
N	1.78388300	-0.72789600	5.21025400
N	-1.53746200	1.16985100	2.95960300
C	-2.19627600	0.70811000	1.88436700
H	-1.87641700	-0.25834300	1.50798900
C	-3.23229800	1.40700400	1.27017300
H	-3.73129900	0.99118900	0.40202700
C	-3.60293200	2.63992700	1.80367400
H	-4.40896900	3.21653000	1.36152600
C	-2.92526300	3.12557700	2.92036000
H	-3.21402600	4.07711100	3.34889300
C	-1.88879700	2.36999500	3.47934800
C	-1.11281000	2.81631600	4.66807300
N	-0.23879700	1.91658600	5.18153600
N	-0.23878500	-1.91656100	2.97118100
C	0.49185500	-2.25357200	1.89473400
H	1.17685200	-1.49595700	1.52847500
C	0.39430000	-3.49372600	1.27063700

H	1.00348400	-3.71708400	0.40204400
C	-0.49709800	-4.42719400	1.79687300
H	-0.60056200	-5.40968800	1.34762600
C	-1.25578100	-4.08604600	2.91491700
H	-1.94144800	-4.81001200	3.33683000
C	-1.11280000	-2.81629000	3.48464600
C	-1.88877700	-2.36997900	4.67338200
N	-1.53742900	-1.16984900	5.19315200
C	-2.19623900	-0.70812600	6.26839800
H	-1.87636800	0.25831400	6.64480000
C	-3.23227100	-1.40702000	6.88257600
H	-3.73126800	-0.99121800	7.75073000
C	-3.60291800	-2.63992800	6.34904900
H	-4.40896200	-3.21653200	6.79118400
C	-2.92525300	-3.12556200	5.23235500
H	-3.21402600	-4.07708400	4.80380200
C	0.49185800	2.25360000	6.25797100
H	1.17685100	1.49598100	6.62423200
C	0.39432100	3.49376200	6.88205600
H	1.00351700	3.71712300	7.75064000
C	-0.49707700	4.42723200	6.35582300
H	-0.60053000	5.40973000	6.80506400
C	-1.25577700	4.08607900	5.23779100
H	-1.94144600	4.81004400	4.81588000
C	1.71807000	-1.52422800	6.29037400
H	0.72303300	-1.71779400	6.67813700
C	2.84274400	-2.08078600	6.89329900
H	2.73696600	-2.71520000	7.76615600
C	4.09144600	-1.80287100	6.34012200
H	4.99484200	-2.22248700	6.77095800
C	4.16853300	-0.97978500	5.21803700
H	5.13340300	-0.77202800	4.77272100

[Fe(bpy)₃]²⁺ singlet in water, applied by CPCM

Fe	0.01627000	0.00000000	4.07637100
N	1.52005500	0.75060800	3.01704400
C	1.41201900	1.51349600	1.91789600
H	0.40486300	1.74009300	1.59669400
C	2.52167900	1.97556900	1.22223300
H	2.38766200	2.58530800	0.34192500
C	3.79036100	1.63349700	1.68175100
H	4.67457800	1.97275000	1.16116400
C	3.91049900	0.84171300	2.81767500
H	4.88298400	0.55282800	3.18893200
C	2.75439400	0.41564800	3.46955100
C	2.75439400	-0.41564800	4.68319000
N	1.52005500	-0.75060800	5.13569700

N	-1.41902100	0.92865500	3.04101200
C	-2.06375500	0.45889000	1.96086800
H	-1.73356600	-0.49948200	1.58409100
C	-3.09705900	1.15727100	1.34645100
H	-3.58903700	0.74094400	0.47967100
C	-3.47944400	2.38932800	1.86973600
H	-4.28088400	2.95781900	1.42017300
C	-2.81195900	2.88410900	2.98259600
H	-3.08152300	3.83713100	3.41390800
C	-1.78439000	2.13260400	3.54898700
C	-1.00559200	2.57296400	4.71588200
N	-0.06322500	1.68830900	5.12679500
N	-0.06322500	-1.68830900	3.02594600
C	0.73252900	-2.01960700	1.99727400
H	1.47668700	-1.28780900	1.71749700
C	0.61495800	-3.22604400	1.32059800
H	1.28312900	-3.44197200	0.50002900
C	-0.36307200	-4.13038200	1.72461100
H	-0.47998200	-5.07980200	1.21928200
C	-1.18269200	-3.80077500	2.79812100
H	-1.93932900	-4.49031800	3.14459800
C	-1.00559300	-2.57296400	3.43685900
C	-1.78439000	-2.13260300	4.60375400
N	-1.41902200	-0.92865500	5.11172900
C	-2.06375600	-0.45889000	6.19187300
H	-1.73356600	0.49948200	6.56865000
C	-3.09706000	-1.15727100	6.80629000
H	-3.58903800	-0.74094400	7.67307000
C	-3.47944500	-2.38932800	6.28300500
H	-4.28088500	-2.95781800	6.73256800
C	-2.81196000	-2.88410800	5.17014500
H	-3.08152400	-3.83713100	4.73883300
C	0.73252900	2.01960700	6.15546800
H	1.47668700	1.28780900	6.43524500
C	0.61495800	3.22604400	6.83214400
H	1.28312900	3.44197200	7.65271200
C	-0.36307200	4.13038200	6.42813000
H	-0.47998200	5.07980200	6.93345900
C	-1.18269100	3.80077500	5.35462000
H	-1.93932900	4.49031900	5.00814200
C	1.41201900	-1.51349700	6.23484500
H	0.40486300	-1.74009300	6.55604700
C	2.52167900	-1.97556900	6.93050800
H	2.38766100	-2.58530900	7.81081600
C	3.79036100	-1.63349800	6.47099100
H	4.67457800	-1.97275100	6.99157700

C	3.91049900	-0.84171300	5.33506600
H	4.88298400	-0.55282800	4.96381000

[Fe(bpy)₃]²⁺ quintet in water, applied by CPCM, <S²> = 6.0122

Fe	-0.02558400	-0.00000400	4.07637200
N	1.70020200	0.63373700	2.90104600
C	1.62095800	1.29804300	1.74002900
H	0.61973200	1.47639800	1.37011200
C	2.74322200	1.74505600	1.05418100
H	2.63242700	2.28325800	0.12387800
C	3.99737100	1.46613800	1.58958900
H	4.89614700	1.78860600	1.08316100
C	4.08642600	0.77040600	2.79099500
H	5.05257100	0.54506100	3.21648000
C	2.91397200	0.36747000	3.43225700
C	2.91397000	-0.36745700	4.72050700
N	1.70019600	-0.63372100	5.25171200
N	-1.44402200	1.20966000	2.91202400
C	-2.01237300	0.81245000	1.76467700
H	-1.70194700	-0.15603900	1.38983700
C	-2.95145000	1.58204800	1.08639900
H	-3.38877500	1.22346400	0.16603200
C	-3.31586500	2.81095200	1.62818600
H	-4.05088600	3.43483900	1.13912900
C	-2.72435700	3.23111000	2.81343700
H	-2.99903800	4.17638600	3.25768900
C	-1.78240000	2.40962800	3.43312200
C	-1.10619600	2.77832500	4.69907600
N	-0.30511500	1.83284000	5.23735900
N	-0.30512400	-1.83284800	2.91538300
C	0.30668500	-2.07673500	1.74708400
H	0.93130600	-1.28017300	1.36324000
C	0.16516400	-3.27732600	1.06228700
H	0.67328300	-3.42442300	0.12008000
C	-0.62809600	-4.27018300	1.63017200
H	-0.74913600	-5.22824500	1.14174200
C	-1.27456300	-4.01857000	2.83588300
H	-1.89225500	-4.77943400	3.29061600
C	-1.10621300	-2.77833100	3.45365500
C	-1.78242500	-2.40963100	4.71960500
N	-1.44404400	-1.20966400	5.24070400
C	-2.01239300	-0.81245000	6.38804900
H	-1.70196300	0.15603800	6.76288900
C	-2.95147400	-1.58204500	7.06632600
H	-3.38879900	-1.22345900	7.98669400
C	-3.31589600	-2.81094600	6.52453700
H	-4.05092200	-3.43482800	7.01359200

C	-2.72438900	-3.23110700	5.33928700
H	-2.99907300	-4.17638200	4.89503400
C	0.30668100	2.07672800	6.40566500
H	0.93129600	1.28016600	6.78951700
C	0.16515600	3.27732000	7.09046000
H	0.67326500	3.42441700	8.03267200
C	-0.62809400	4.27017900	6.52256400
H	-0.74913700	5.22824300	7.01099000
C	-1.27454700	4.01856600	5.31684600
H	-1.89222900	4.77943300	4.86210400
C	1.62094600	-1.29803700	6.41272300
H	0.61971700	-1.47638900	6.78263600
C	2.74320600	-1.74506000	7.09857200
H	2.63240500	-2.28326800	8.02887100
C	3.99735800	-1.46613900	6.56317300
H	4.89613100	-1.78861200	7.06960300
C	4.08642000	-0.77040000	5.36177100
H	5.05256800	-0.54505700	4.93629100

[Fe(bpy)₃]²⁺ singlet in dimethyl sulfoxide, applied by CPCM

Fe	0.01105200	0.00000000	4.07637000
N	1.53261500	0.76071400	3.01975500
C	1.43212500	1.53967200	1.92976200
H	0.42817000	1.77180400	1.60094300
C	2.54391400	2.01464600	1.24354600
H	2.40914700	2.63566700	0.36858200
C	3.81226400	1.67179500	1.70564600
H	4.70044600	2.01988800	1.19366000
C	3.92586200	0.86726700	2.83476800
H	4.89973900	0.58349700	3.20934500
C	2.76726200	0.42755200	3.47662400
C	2.76726200	-0.42755200	4.67611800
N	1.53261500	-0.76071400	5.13298600
N	-1.42794100	0.93881200	3.03439300
C	-2.08229600	0.46209000	1.96193200
H	-1.76874400	-0.50774300	1.59957400
C	-3.10445400	1.16457400	1.33243400
H	-3.59933700	0.73626100	0.47097800
C	-3.46775000	2.41216300	1.83380500
H	-4.26013200	2.98703500	1.37153200
C	-2.79518800	2.91324300	2.94285600
H	-3.05758300	3.87803300	3.35455500
C	-1.77825100	2.15557400	3.52516700
C	-0.99976200	2.59711500	4.69498900
N	-0.07926300	1.70040700	5.13283500
N	-0.07926300	-1.70040700	3.01990600
C	0.69105400	-2.02503900	1.96838700

H	1.41273500	-1.28176600	1.65819500
C	0.57746800	-3.23874600	1.30043400
H	1.22455600	-3.44739800	0.45890200
C	-0.37320400	-4.15758400	1.73787600
H	-0.49062900	-5.11326800	1.24156600
C	-1.16980300	-3.83334300	2.83133500
H	-1.90854800	-4.53413500	3.19605200
C	-0.99976200	-2.59711500	3.45775200
C	-1.77825100	-2.15557400	4.62757300
N	-1.42794200	-0.93881200	5.11834800
C	-2.08229600	-0.46209000	6.19080900
H	-1.76874300	0.50774400	6.55316700
C	-3.10445400	-1.16457300	6.82030700
H	-3.59933700	-0.73626000	7.68176300
C	-3.46775000	-2.41216300	6.31893600
H	-4.26013200	-2.98703400	6.78120900
C	-2.79518800	-2.91324300	5.20988500
H	-3.05758300	-3.87803300	4.79818600
C	0.69105500	2.02503900	6.18435300
H	1.41273500	1.28176600	6.49454600
C	0.57746900	3.23874600	6.85230700
H	1.22455600	3.44739800	7.69383900
C	-0.37320400	4.15758400	6.41486500
H	-0.49062900	5.11326800	6.91117500
C	-1.16980300	3.83334300	5.32140600
H	-1.90854700	4.53413500	4.95668900
C	1.43212500	-1.53967200	6.22297900
H	0.42817000	-1.77180400	6.55179800
C	2.54391400	-2.01464600	6.90919500
H	2.40914700	-2.63566700	7.78415900
C	3.81226400	-1.67179500	6.44709500
H	4.70044600	-2.01988800	6.95908100
C	3.92586100	-0.86726700	5.31797300
H	4.89973900	-0.58349700	4.94339600

[Fe(bpy)₃]²⁺ quintet in dimethyl sulfoxide, applied by CPCM, <S²> = 6.0119

Fe	-0.01510500	0.00000300	4.07637300
N	1.72901800	0.67675300	2.91968100
C	1.65422100	1.37442900	1.77676200
H	0.65482300	1.57792900	1.41120800
C	2.78001300	1.82028600	1.09262500
H	2.67091300	2.37994200	0.17323500
C	4.03318200	1.52111000	1.62122400
H	4.93597500	1.84680200	1.11971800
C	4.11764600	0.80030800	2.80913600
H	5.08474100	0.56645500	3.23129500
C	2.94267300	0.38639400	3.44184100

C	2.94266800	-0.38641000	4.71092100
N	1.72900800	-0.67676400	5.23307400
N	-1.48429800	1.19641300	2.93223200
C	-2.08718800	0.77607400	1.81043300
H	-1.78496400	-0.19821600	1.44255700
C	-3.04618200	1.53229100	1.14307800
H	-3.50702600	1.15279300	0.24066200
C	-3.39194600	2.77465500	1.66853300
H	-4.13718700	3.39304700	1.18385000
C	-2.76965900	3.21592400	2.83226300
H	-3.03349700	4.17314600	3.25997500
C	-1.81287100	2.40355600	3.44526500
C	-1.10777300	2.79078800	4.69332500
N	-0.28535900	1.85651800	5.22272200
N	-0.28535000	-1.85650700	2.93001800
C	0.36102600	-2.12017700	1.78419400
H	1.00416000	-1.33312200	1.40853200
C	0.22846300	-3.32783300	1.10735700
H	0.76576400	-3.49185500	0.18260100
C	-0.59754500	-4.30410200	1.65854200
H	-0.71924200	-5.26477600	1.17245500
C	-1.27389200	-4.03451100	2.84520700
H	-1.91625800	-4.78571800	3.28374800
C	-1.10776800	-2.79077600	3.45941100
C	-1.81287300	-2.40354600	4.70746800
N	-1.48430300	-1.19640400	5.22050600
C	-2.08720100	-0.77606700	6.34230000
H	-1.78497900	0.19822200	6.71018100
C	-3.04620000	-1.53228400	7.00964600
H	-3.50705200	-1.15278700	7.91206000
C	-3.39196100	-2.77464800	6.48418700
H	-4.13720500	-3.39304100	6.96886500
C	-2.76966500	-3.21591400	5.32046100
H	-3.03350000	-4.17313600	4.89274700
C	0.36101500	2.12018800	6.36854600
H	1.00414500	1.33313200	6.74421200
C	0.22845400	3.32784600	7.04538000
H	0.76575300	3.49187000	7.97013700
C	-0.59755200	4.30411600	6.49419200
H	-0.71924900	5.26479000	6.98027700
C	-1.27389700	4.03452400	5.30752700
H	-1.91626200	4.78573000	4.86898200
C	1.65420200	-1.37444000	6.37599200
H	0.65480000	-1.57793600	6.74153900
C	2.77998800	-1.82030400	7.06013400
H	2.67088000	-2.37996100	7.97952200

C	4.03316100	-1.52113800	6.53153900
H	4.93595000	-1.84683900	7.03304700
C	4.11763500	-0.80033400	5.34362900
H	5.08473300	-0.56648900	4.92147200

[Fe(bpy)₃]²⁺ singlet in ethylene glycol, applied by CPCM

Fe	0.01212400	0.00000000	4.07637100
N	1.53121800	0.75874600	3.01910000
C	1.42934800	1.53411100	1.92686900
H	0.42479800	1.76591200	1.59981800
C	2.54060100	2.00519400	1.23746300
H	2.40565800	2.62387300	0.36119600
C	3.80908700	1.66070700	1.69764300
H	4.69658800	2.00530500	1.18263300
C	3.92394100	0.85914600	2.82859400
H	4.89792900	0.57263100	3.20043600
C	2.76593100	0.42449300	3.47456000
C	2.76593100	-0.42449300	4.67818100
N	1.53121800	-0.75874600	5.13364200
N	-1.42666800	0.93797500	3.03572000
C	-2.07972300	0.46280500	1.96192700
H	-1.76376800	-0.50521700	1.59690500
C	-3.10358200	1.16492100	1.33494100
H	-3.59794000	0.73862200	0.47245500
C	-3.46977500	2.41003400	1.84016400
H	-4.26359100	2.98417300	1.38003100
C	-2.79799800	2.90960200	2.95011900
H	-3.06169200	3.87242100	3.36525500
C	-1.77933900	2.15261500	3.52969000
C	-1.00066500	2.59350000	4.69924200
N	-0.07655000	1.69854400	5.13245200
N	-0.07655000	-1.69854300	3.02028900
C	0.69775600	-2.02376000	1.97209200
H	1.42362100	-1.28233600	1.66758800
C	0.58326800	-3.23588500	1.30190000
H	1.23376400	-3.44528800	0.46347800
C	-0.37222300	-4.15242800	1.73342300
H	-0.49004800	-5.10676700	1.23499700
C	-1.17214300	-3.82798600	2.82427000
H	-1.91386100	-4.52720000	3.18568300
C	-1.00066500	-2.59349900	3.45349900
C	-1.77933900	-2.15261500	4.62305100
N	-1.42666800	-0.93797500	5.11702100
C	-2.07972300	-0.46280500	6.19081400
H	-1.76376800	0.50521700	6.55583700
C	-3.10358300	-1.16492100	6.81780000
H	-3.59794100	-0.73862200	7.68028600

C	-3.46977600	-2.41003300	6.31257700
H	-4.26359200	-2.98417200	6.77270900
C	-2.79799800	-2.90960200	5.20262200
H	-3.06169200	-3.87242100	4.78748600
C	0.69775600	2.02376100	6.18064900
H	1.42362100	1.28233700	6.48515300
C	0.58326700	3.23588600	6.85084100
H	1.23376300	3.44528900	7.68926400
C	-0.37222300	4.15242800	6.41931800
H	-0.49004900	5.10676800	6.91774400
C	-1.17214400	3.82798700	5.32847100
H	-1.91386100	4.52720100	4.96705800
C	1.42934800	-1.53411100	6.22587200
H	0.42479800	-1.76591200	6.55292300
C	2.54060100	-2.00519500	6.91527700
H	2.40565800	-2.62387400	7.79154400
C	3.80908700	-1.66070900	6.45509800
H	4.69658800	-2.00530700	6.97010700
C	3.92394100	-0.85914700	5.32414600
H	4.89792900	-0.57263300	4.95230400

[Fe(bpy)₃]²⁺ quintet in ethylene glycol, applied by CPCM, <S²> = 6.0118

Fe	-0.01920800	-0.00000800	4.07636900
N	1.72188300	0.66762100	2.91548600
C	1.64593600	1.35795000	1.76838600
H	0.64581500	1.55554100	1.40180800
C	2.77103200	1.80344000	1.08326200
H	2.66151100	2.35799700	0.16102300
C	4.02452500	1.50923500	1.61378500
H	4.92658700	1.83427200	1.11107500
C	4.11006500	0.79452300	2.80520600
H	5.07712100	0.56367700	3.22873500
C	2.93565100	0.38249200	3.43971800
C	2.93564900	-0.38246900	4.71304800
N	1.72187800	-0.66759300	5.23727400
N	-1.47725700	1.20179100	2.92826400
C	-2.07520800	0.78588300	1.80225600
H	-1.77288600	-0.18790800	1.43310300
C	-3.02968400	1.54563400	1.13271000
H	-3.48708200	1.16995500	0.22721600
C	-3.37645900	2.78661000	1.66049100
H	-4.11885200	3.40712600	1.17466700
C	-2.75885300	3.22354000	2.82808400
H	-3.02325400	4.17932100	3.25829600
C	-1.80598900	2.40819400	3.44274200
C	-1.10602600	2.79099600	4.69465000
N	-0.28876700	1.85352200	5.22590000

N	-0.28878700	-1.85354000	2.92684500
C	0.35177400	-2.11302800	1.77689800
H	0.99144700	-1.32403600	1.39980900
C	0.21848000	-3.31934900	1.09812400
H	0.75069600	-3.47951200	0.16996700
C	-0.60072600	-4.29951900	1.65228100
H	-0.72170700	-5.25966900	1.16533400
C	-1.27148700	-4.03419400	2.84291000
H	-1.90844900	-4.78816200	3.28432400
C	-1.10605400	-2.79101100	3.45808300
C	-1.80602700	-2.40820100	4.70998500
N	-1.47729600	-1.20179500	5.22445300
C	-2.07524500	-0.78587500	6.35045600
H	-1.77292400	0.18791900	6.71960000
C	-3.02972000	-1.54562200	7.02000900
H	-3.48711800	-1.16993600	7.92550100
C	-3.37649600	-2.78660100	6.49223700
H	-4.11889100	-3.40711200	6.97806500
C	-2.75889200	-3.22354100	5.32464700
H	-3.02329300	-4.17932500	4.89444100
C	0.35177800	2.11301200	6.37585600
H	0.99144700	1.32402100	6.75295200
C	0.21847800	3.31933200	7.05462900
H	0.75068100	3.47949400	7.98279300
C	-0.60071700	4.29950500	6.50045900
H	-0.72170000	5.25965700	6.98740300
C	-1.27146000	4.03418000	5.30982200
H	-1.90841200	4.78815200	4.86839700
C	1.64592400	-1.35793500	6.38436600
H	0.64580100	-1.55552100	6.75094200
C	2.77101600	-1.80344000	7.06948700
H	2.66148900	-2.35800800	7.99171900
C	4.02451200	-1.50923300	6.53897300
H	4.92657100	-1.83427700	7.04168500
C	4.11005900	-0.79450900	5.34756000
H	5.07711700	-0.56366200	4.92403600

[Fe(bpy)₃]²⁺ singlet in 1,3-propanediol, applied by CPCM

Fe	0.01096100	0.00000000	4.07637000
N	1.53274200	0.76087000	3.01979900
C	1.43237900	1.54011400	1.92997600
H	0.42845800	1.77227700	1.60104200
C	2.54420600	2.01540700	1.24401300
H	2.40948200	2.63662200	0.36915300
C	3.81254900	1.67270900	1.70628300
H	4.70078100	2.02110600	1.19455400
C	3.92603300	0.86794400	2.83526400

H	4.89991000	0.58441900	3.21006400
C	2.76738900	0.42779600	3.47678300
C	2.76738900	-0.42779600	4.67595800
N	1.53274200	-0.76087000	5.13294200
N	-1.42805700	0.93889300	3.03427500
C	-2.08251900	0.46207200	1.96190200
H	-1.76917100	-0.50793000	1.59979300
C	-3.10451700	1.16459900	1.33218100
H	-3.59946300	0.73616300	0.47079800
C	-3.46757700	2.41239200	1.83324500
H	-4.25983300	2.98732900	1.37079200
C	-2.79495700	2.91356300	2.94224100
H	-3.05725600	3.87850900	3.35366900
C	-1.77817300	2.15583000	3.52479400
C	-0.99971800	2.59742000	4.69466000
N	-0.07949500	1.70057700	5.13287300
N	-0.07949500	-1.70057700	3.01986800
C	0.69049900	-2.02519500	1.96808300
H	1.41187000	-1.28177800	1.65746900
C	0.57697700	-3.23902100	1.30029900
H	1.22379300	-3.44765100	0.45852800
C	-0.37331900	-4.15803900	1.73821300
H	-0.49070400	-5.11383200	1.24207600
C	-1.16964600	-3.83378900	2.83188100
H	-1.90814600	-4.53471700	3.19686600
C	-0.99971800	-2.59742000	3.45808100
C	-1.77817300	-2.15583000	4.62794700
N	-1.42805700	-0.93889300	5.11846600
C	-2.08251900	-0.46207200	6.19083900
H	-1.76917100	0.50793000	6.55294800
C	-3.10451800	-1.16459800	6.82056000
H	-3.59946300	-0.73616300	7.68194300
C	-3.46757700	-2.41239200	6.31949600
H	-4.25983300	-2.98732900	6.78194900
C	-2.79495700	-2.91356300	5.21050000
H	-3.05725700	-3.87850900	4.79907200
C	0.69049900	2.02519400	6.18465800
H	1.41187000	1.28177800	6.49527200
C	0.57697800	3.23902100	6.85244200
H	1.22379300	3.44765000	7.69421300
C	-0.37331900	4.15803900	6.41452800
H	-0.49070300	5.11383200	6.91066500
C	-1.16964600	3.83378900	5.32086000
H	-1.90814500	4.53471800	4.95587500
C	1.43237900	-1.54011400	6.22276500
H	0.42845800	-1.77227700	6.55169900

C	2.54420500	-2.01540700	6.90872900
H	2.40948200	-2.63662200	7.78358800
C	3.81254900	-1.67270900	6.44645800
H	4.70078100	-2.02110600	6.95818800
C	3.92603300	-0.86794400	5.31747800
H	4.89991000	-0.58441800	4.94267700

[Fe(bpy)₃]²⁺ quintet in 1,3-propanediol, applied by CPCM, <S²> = 6.0119

Fe	-0.01488900	0.00000200	4.07637300
N	1.72947700	0.67720600	2.91987800
C	1.65476400	1.37525900	1.77715700
H	0.65539000	1.57905300	1.41166000
C	2.78058300	1.82114400	1.09305900
H	2.67152300	2.38107500	0.17381500
C	4.03374500	1.52171800	1.62156000
H	4.93657900	1.84745100	1.12011500
C	4.11813700	0.80059300	2.80929300
H	5.08525400	0.56658800	3.23135300
C	2.94313900	0.38659100	3.44193600
C	2.94313400	-0.38659400	4.71082700
N	1.72946700	-0.67720100	5.23287900
N	-1.48458900	1.19623500	2.93234900
C	-2.08762300	0.77575300	1.81066500
H	-1.78534700	-0.19853900	1.44281900
C	-3.04683300	1.53177700	1.14338500
H	-3.50776900	1.15213600	0.24105400
C	-3.39267900	2.77414800	1.66880100
H	-4.13807400	3.39242200	1.18416700
C	-2.77026700	3.21556900	2.83242800
H	-3.03420200	4.17282100	3.26004500
C	-1.81326700	2.40337300	3.44537100
C	-1.10799200	2.79081300	4.69330300
N	-0.28527000	1.85673100	5.22260800
N	-0.28527500	-1.85673000	2.93013600
C	0.36136100	-2.12066700	1.78450300
H	1.00473800	-1.33374900	1.40892900
C	0.22877500	-3.32837600	1.10774500
H	0.76632600	-3.49265100	0.18316000
C	-0.59764900	-4.30440800	1.65876200
H	-0.71943800	-5.26509800	1.17270500
C	-1.27424100	-4.03455700	2.84524100
H	-1.91691400	-4.78561000	3.28362300
C	-1.10800000	-2.79081300	3.45943200
C	-1.81328200	-2.40337200	4.70736000
N	-1.48460900	-1.19623300	5.22037900
C	-2.08764800	-0.77574800	6.34206000
H	-1.78537600	0.19854700	6.70990400

C	-3.04685800	-1.53177300	7.00933800
H	-3.50779900	-1.15213100	7.91166600
C	-3.39270000	-2.77414600	6.48392400
H	-4.13809500	-3.39242000	6.96855800
C	-2.77028200	-3.21556900	5.32030100
H	-3.03421300	-4.17282300	4.89268500
C	0.36136200	2.12067400	6.36824200
H	1.00473800	1.33375800	6.74382100
C	0.22877200	3.32838500	7.04499600
H	0.76631900	3.49266300	7.96958300
C	-0.59764800	4.30441600	6.49397000
H	-0.71943700	5.26510800	6.98002100
C	-1.27423300	4.03456000	5.30748900
H	-1.91690000	4.78561400	4.86910000
C	1.65474500	-1.37525800	6.37559700
H	0.65536800	-1.57904500	6.74109100
C	2.78055800	-1.82115300	7.05969900
H	2.67149100	-2.38108700	7.97894100
C	4.03372400	-1.52173600	6.53120300
H	4.93655400	-1.84747800	7.03265000
C	4.11812700	-0.80060800	5.34347200
H	5.08524700	-0.56661000	4.92141600

[Fe(bpy)₃]²⁺ singlet in 1,4-butanediol, applied by CPCM

Fe	0.00993500	0.00000000	4.07637100
N	1.53363100	0.76265900	3.02047400
C	1.43436200	1.54570000	1.93312300
H	0.43091200	1.77735600	1.60225900
C	2.54660500	2.02602000	1.25108400
H	2.41205400	2.64961500	0.37765000
C	3.81484900	1.68638300	1.71615200
H	4.70361900	2.03961700	1.20829900
C	3.92733200	0.87837900	2.84302200
H	4.90107100	0.59897200	3.22152100
C	2.76821300	0.43130800	3.47920200
C	2.76821300	-0.43130800	4.67353900
N	1.53363100	-0.76266000	5.13226700
N	-1.42915700	0.93913700	3.03289600
C	-2.08457600	0.46074900	1.96169300
H	-1.77312900	-0.51082200	1.60209300
C	-3.10516200	1.16338600	1.32969200
H	-3.60052900	0.73312600	0.46925900
C	-3.46590700	2.41330700	1.82725400
H	-4.25696900	2.98867900	1.36286900
C	-2.79268500	2.91604500	2.93536800
H	-3.05388400	3.88271200	3.34370100
C	-1.77735000	2.15794400	3.52041600

C	-0.99901800	2.60047500	4.69031200
N	-0.08175100	1.70235300	5.13253800
N	-0.08175200	-1.70235300	3.02020300
C	0.68522100	-2.02691700	1.96603400
H	1.40321000	-1.28210400	1.65071500
C	0.57260500	-3.24230400	1.30058300
H	1.21679800	-3.45071200	0.45653400
C	-0.37368800	-4.16308300	1.74360200
H	-0.49050200	-5.12020800	1.24962600
C	-1.16755700	-3.83854600	2.83906100
H	-1.90358500	-4.54065400	3.20697500
C	-0.99901800	-2.60047500	3.46242900
C	-1.77735000	-2.15794400	4.63232500
N	-1.42915800	-0.93913700	5.11984500
C	-2.08457600	-0.46074900	6.19104800
H	-1.77312900	0.51082200	6.55064800
C	-3.10516200	-1.16338600	6.82304900
H	-3.60052900	-0.73312600	7.68348200
C	-3.46590700	-2.41330700	6.32548700
H	-4.25696900	-2.98867800	6.78987200
C	-2.79268500	-2.91604500	5.21737300
H	-3.05388500	-3.88271200	4.80904000
C	0.68522100	2.02691700	6.18670700
H	1.40321100	1.28210400	6.50202600
C	0.57260500	3.24230400	6.85215800
H	1.21679800	3.45071200	7.69620700
C	-0.37368700	4.16308300	6.40913900
H	-0.49050100	5.12020800	6.90311500
C	-1.16755700	3.83854600	5.31368000
H	-1.90358500	4.54065400	4.94576600
C	1.43436200	-1.54570000	6.21961800
H	0.43091200	-1.77735600	6.55048200
C	2.54660500	-2.02602000	6.90165700
H	2.41205300	-2.64961500	7.77509100
C	3.81484900	-1.68638300	6.43658900
H	4.70361900	-2.03961700	6.94444200
C	3.92733200	-0.87837900	5.30972000
H	4.90107100	-0.59897300	4.93122000

[Fe(bpy)₃]²⁺ quintet in 1,4-butanediol, applied by CPCM, <S²> = 6.0118

Fe	-0.01245700	0.00000200	4.07637100
N	1.73410800	0.68261500	2.92242500
C	1.65996000	1.38515300	1.78226900
H	0.66091800	1.59168800	1.41716000
C	2.78610700	1.83183200	1.09895200
H	2.67719800	2.39493300	0.18146800
C	4.03913900	1.52975800	1.62636800

H	4.94238900	1.85626700	1.12578300
C	4.12300600	0.80459100	2.81176900
H	5.09026300	0.56889000	3.23285400
C	2.94774300	0.38910200	3.44328400
C	2.94773700	-0.38912600	4.70947300
N	1.73409700	-0.68263700	5.23032400
N	-1.48903200	1.19368100	2.93535800
C	-2.09427000	0.77114400	1.81558000
H	-1.79163100	-0.20314300	1.44800800
C	-3.05629300	1.52496300	1.14967800
H	-3.51858300	1.14335400	0.24867400
C	-3.40258000	2.76752500	1.67452600
H	-4.14988700	3.38445600	1.19074500
C	-2.77803500	3.21107600	2.83639000
H	-3.04241800	4.16881200	3.26291500
C	-1.81834000	2.40084200	3.44810200
C	-1.10990600	2.79094200	4.69368300
N	-0.28300500	1.85929000	5.22110400
N	-0.28299100	-1.85927900	2.93163300
C	0.36810500	-2.12638500	1.78918300
H	1.01462000	-1.34126200	1.41504400
C	0.23574900	-3.33482600	1.11347100
H	0.77732700	-3.50194100	0.19158600
C	-0.59630000	-4.30776500	1.66164700
H	-0.71889000	-5.26864000	1.17590100
C	-1.27708900	-4.03480900	2.84511900
H	-1.92399900	-4.78375400	3.28105600
C	-1.10989900	-2.79092800	3.45905200
C	-1.81833700	-2.40082900	4.70463100
N	-1.48902700	-1.19367100	5.21738300
C	-2.09427200	-0.77113900	6.33715900
H	-1.79163200	0.20314400	6.70473900
C	-3.05630600	-1.52495600	7.00304900
H	-3.51860200	-1.14334900	7.90405100
C	-3.40259300	-2.76751500	6.47819300
H	-4.14990700	-3.38444500	6.96196500
C	-2.77803900	-3.21106200	5.31633200
H	-3.04242400	-4.16879500	4.88980200
C	0.36809300	2.12639300	6.36355200
H	1.01460200	1.34126700	6.73769500
C	0.23574400	3.33483700	7.03926200
H	0.77732300	3.50195100	7.96114600
C	-0.59630100	4.30777800	6.49108400
H	-0.71888800	5.26865500	6.97683000
C	-1.27709200	4.03482500	5.30761300
H	-1.92400100	4.78377000	4.87167600

C	1.65993900	-1.38517100	6.37048200
H	0.66089300	-1.59170400	6.73558300
C	2.78607900	-1.83184800	7.05381100
H	2.67716300	-2.39494500	7.97129600
C	4.03911600	-1.52978000	6.52640100
H	4.94236200	-1.85629200	7.02699300
C	4.12299400	-0.80461700	5.34099900
H	5.09025400	-0.56892200	4.91991900

[Fe(bpy)₃]²⁺ singlet in 1,5-pentanediol, applied by CPCM

Fe	0.00924200	0.00000000	4.07637100
N	1.53442000	0.76412400	3.02115800
C	1.43568900	1.55074700	1.93622900
H	0.43250300	1.78141900	1.60376800
C	2.54800900	2.03641900	1.25794400
H	2.41338000	2.66228500	0.38596100
C	3.81625200	1.70024400	1.72568100
H	4.70531300	2.05862100	1.22165400
C	3.92830000	0.88907500	2.85040500
H	4.90220000	0.61420000	3.23197900
C	2.76904600	0.43465500	3.48147700
C	2.76904600	-0.43465500	4.67126400
N	1.53442000	-0.76412400	5.13158300
N	-1.42998200	0.93905800	3.03166400
C	-2.08612800	0.45922900	1.96145900
H	-1.77604200	-0.51358200	1.60397300
C	-3.10573100	1.16172500	1.32762800
H	-3.60144200	0.72989600	0.46802400
C	-3.46481400	2.41331400	1.82231000
H	-4.25504800	2.98884400	1.35638900
C	-2.79110300	2.91752400	2.92960800
H	-3.05152700	3.88556800	3.33537000
C	-1.77676900	2.15936400	3.51665900
C	-0.99844400	2.60295200	4.68640100
N	-0.08338700	1.70399400	5.13186100
N	-0.08338700	-1.70399400	3.02088000
C	0.68143700	-2.02889100	1.96511900
H	1.39691100	-1.28313200	1.64612300
C	0.56961300	-3.24567800	1.30182700
H	1.21191500	-3.45423900	0.45621300
C	-0.37361800	-4.16768200	1.74895500
H	-0.48986100	-5.12600400	1.25696200
C	-1.16578500	-3.84253900	2.84553700
H	-1.89992900	-4.54545600	3.21583500
C	-0.99844400	-2.60295200	3.46634000
C	-1.77677000	-2.15936400	4.63608200
N	-1.42998300	-0.93905800	5.12107700

C	-2.08612800	-0.45922900	6.19128200
H	-1.77604200	0.51358200	6.54876800
C	-3.10573100	-1.16172500	6.82511300
H	-3.60144200	-0.72989600	7.68471700
C	-3.46481500	-2.41331400	6.33043100
H	-4.25504900	-2.98884400	6.79635200
C	-2.79110300	-2.91752400	5.22313300
H	-3.05152700	-3.88556800	4.81737100
C	0.68143700	2.02889100	6.18762200
H	1.39691100	1.28313200	6.50661800
C	0.56961300	3.24567800	6.85091400
H	1.21191500	3.45423900	7.69652800
C	-0.37361800	4.16768200	6.40378600
H	-0.48986000	5.12600400	6.89577900
C	-1.16578500	3.84253900	5.30720400
H	-1.89992900	4.54545600	4.93690600
C	1.43568900	-1.55074800	6.21651200
H	0.43250300	-1.78141900	6.54897300
C	2.54800900	-2.03641900	6.89479700
H	2.41338000	-2.66228500	7.76678000
C	3.81625200	-1.70024400	6.42706000
H	4.70531300	-2.05862100	6.93108700
C	3.92830000	-0.88907500	5.30233600
H	4.90220000	-0.61420000	4.92076300

[Fe(bpy)₃]²⁺ quintet in 1,5-pentanediol, applied by CPCM, <S²> = 6.0118

Fe	-0.01065900	0.00000300	4.07637200
N	1.73755100	0.68633200	2.92420200
C	1.66376100	1.39212900	1.78591300
H	0.66489600	1.60035500	1.42106900
C	2.79009200	1.83965100	1.10325300
H	2.68126800	2.40510000	0.18707600
C	4.04306700	1.53580700	1.62990800
H	4.94659200	1.86304400	1.12999900
C	4.12660600	0.80761300	2.81355600
H	5.09400900	0.57077000	3.23389000
C	2.95119000	0.39091400	3.44425300
C	2.95118500	-0.39092900	4.70850500
N	1.73754100	-0.68634400	5.22854900
N	-1.49229100	1.19193400	2.93770800
C	-2.09913800	0.76797200	1.81928700
H	-1.79609700	-0.20621100	1.45174800
C	-3.06343000	1.52004200	1.15456500
H	-3.52668400	1.13702700	0.25450400
C	-3.41031900	2.76257000	1.67922900
H	-4.15921800	3.37840800	1.19623300
C	-2.78422200	3.20762900	2.83982500

H	-3.04915700	4.16560100	3.26568700
C	-1.82230200	2.39898000	3.45044000
C	-1.11144200	2.79110100	4.69420700
N	-0.28106000	1.86144400	5.21996500
N	-0.28104800	-1.86143600	2.93277300
C	0.37376600	-2.13118200	1.79299800
H	1.02298600	-1.34761100	1.42015300
C	0.24156900	-3.34017300	1.11808000
H	0.78652000	-3.50964300	0.19848900
C	-0.59520900	-4.31053300	1.66375800
H	-0.71847700	-5.27151700	1.17820300
C	-1.27946800	-4.03502900	2.84471600
H	-1.92987400	-4.78222600	3.27859000
C	-1.11143400	-2.79109200	3.45852800
C	-1.82230000	-2.39897300	4.70229200
N	-1.49229100	-1.19192900	5.21503000
C	-2.09914500	-0.76796900	6.33344700
H	-1.79610600	0.20621300	6.70099100
C	-3.06344400	-1.52003900	6.99816100
H	-3.52670400	-1.13702500	7.89821900
C	-3.41033000	-2.76256500	6.47349100
H	-4.15923300	-3.37840400	6.95648100
C	-2.78422500	-3.20762200	5.31289900
H	-3.04915800	-4.16559300	4.88703400
C	0.37375200	2.13119000	6.35974200
H	1.02296800	1.34761700	6.73259000
C	0.24155700	3.34018200	7.03465700
H	0.78650500	3.50965200	7.95425000
C	-0.59521800	4.31054300	6.48897600
H	-0.71848600	5.27152800	6.97452900
C	-1.27947400	4.03503800	5.30801600
H	-1.92987800	4.78223600	4.87413900
C	1.66374400	-1.39213800	6.36683900
H	0.66487500	-1.60036200	6.73167600
C	2.79006900	-1.83966100	7.04950600
H	2.68123800	-2.40510800	7.96568400
C	4.04304800	-1.53582300	6.52285800
H	4.94656900	-1.86306200	7.02277200
C	4.12659600	-0.80763100	5.33920900
H	5.09400200	-0.57079200	4.91888000

[Fe(bpy)₃]²⁺ singlet in propylene carbonate, applied by CPCM

Fe	0.01017200	0.00000000	4.07637100
N	1.53337000	0.76223300	3.02031900
C	1.43383500	1.54435700	1.93238500
H	0.43030900	1.77613400	1.60191100
C	2.54601200	2.02344300	1.24943200

H	2.41138400	2.64644500	0.37564700
C	3.81426400	1.68304300	1.71383200
H	4.70292500	2.03507200	1.20504200
C	3.92697900	0.87582200	2.84120600
H	4.90070600	0.59537100	3.21888600
C	2.76794800	0.43047000	3.47863900
C	2.76794800	-0.43047000	4.67410200
N	1.53337000	-0.76223400	5.13242200
N	-1.42887600	0.93905000	3.03324300
C	-2.08405400	0.46099100	1.96179200
H	-1.77213700	-0.51016400	1.60152800
C	-3.10500700	1.16358600	1.33037000
H	-3.60023300	0.73369100	0.46972400
C	-3.46630300	2.41299300	1.82875700
H	-4.25766200	2.98825500	1.36484100
C	-2.79322000	2.91541000	2.93705000
H	-3.05465700	3.88167300	3.34611100
C	-1.77752500	2.15740500	3.52147100
C	-0.99913900	2.59971100	4.69132400
N	-0.08119700	1.70187900	5.13260000
N	-0.08119800	-1.70187900	3.02014100
C	0.68649200	-2.02638400	1.96653200
H	1.40523200	-1.28188900	1.65227100
C	0.57367200	-3.24140600	1.30053400
H	1.21847900	-3.44978300	0.45700200
C	-0.37354400	-4.16178100	1.74234600
H	-0.49050800	-5.11858200	1.24784300
C	-1.16800300	-3.83736900	2.83738500
H	-1.90462700	-4.53918100	3.20459900
C	-0.99913900	-2.59971100	3.46141700
C	-1.77752500	-2.15740500	4.63127000
N	-1.42887600	-0.93905000	5.11949800
C	-2.08405400	-0.46099100	6.19094900
H	-1.77213700	0.51016400	6.55121300
C	-3.10500700	-1.16358600	6.82237100
H	-3.60023300	-0.73369100	7.68301700
C	-3.46630300	-2.41299300	6.32398400
H	-4.25766300	-2.98825500	6.78790000
C	-2.79322000	-2.91541000	5.21569100
H	-3.05465700	-3.88167300	4.80663000
C	0.68649200	2.02638400	6.18620900
H	1.40523200	1.28189000	6.50047000
C	0.57367200	3.24140600	6.85220700
H	1.21847900	3.44978300	7.69573900
C	-0.37354400	4.16178100	6.41039500
H	-0.49050800	5.11858200	6.90489800

C	-1.16800300	3.83736900	5.31535600
H	-1.90462700	4.53918100	4.94814200
C	1.43383500	-1.54435700	6.22035600
H	0.43030900	-1.77613500	6.55083000
C	2.54601200	-2.02344300	6.90330900
H	2.41138400	-2.64644500	7.77709400
C	3.81426400	-1.68304300	6.43890900
H	4.70292500	-2.03507200	6.94770000
C	3.92697900	-0.87582200	5.31153500
H	4.90070600	-0.59537100	4.93385500

[Fe(bpy)₃]²⁺ quintet in propylene carbonate, applied by CPCM, <S²> = 6.0119

Fe	-0.01291400	-0.00000300	4.07637000
N	1.73309600	0.68168400	2.92199700
C	1.65878400	1.38335500	1.78137600
H	0.65970000	1.58935000	1.41617200
C	2.78488300	1.82986400	1.09792200
H	2.67590300	2.39232300	0.18009600
C	4.03792500	1.52829900	1.62554900
H	4.94109300	1.85465200	1.12480400
C	4.12193000	0.80390400	2.81138400
H	5.08913200	0.56851700	3.23269000
C	2.94671300	0.38867900	3.44306400
C	2.94670900	-0.38866900	4.70969600
N	1.73308900	-0.68166800	5.23075800
N	-1.48830300	1.19402200	2.93499300
C	-2.09321900	0.77179600	1.81495900
H	-1.79069900	-0.20249500	1.44734200
C	-3.05473200	1.52606200	1.14886200
H	-3.51682700	1.14477400	0.24767000
C	-3.40079800	2.76863900	1.67376100
H	-4.14773400	3.38584600	1.18984400
C	-2.77653400	3.21185200	2.83585600
H	-3.04067900	4.16953500	3.26257400
C	-1.81735300	2.40121300	3.44773800
C	-1.10937300	2.79082500	4.69365200
N	-0.28326700	1.85870400	5.22137500
N	-0.28328100	-1.85871600	2.93136900
C	0.36709100	-2.12513900	1.78838900
H	1.01294900	-1.33963900	1.41398700
C	0.23478300	-3.33345900	1.11249200
H	0.77567600	-3.49995000	0.19013600
C	-0.59617900	-4.30701000	1.66115800
H	-0.71854600	-5.26785300	1.17535100
C	-1.27630100	-4.03470200	2.84513400
H	-1.92242700	-4.78404000	3.28149900
C	-1.10939200	-2.79083400	3.45908400

C	-1.81738100	-2.40121500	4.70499100
N	-1.48833400	-1.19402000	5.21772700
C	-2.09325300	-0.77178400	6.33775500
H	-1.79073500	0.20251000	6.70536500
C	-3.05476600	-1.52604700	7.00385700
H	-3.51686300	-1.14475200	7.90504500
C	-3.40082900	-2.76862700	6.47896600
H	-4.14776700	-3.38583100	6.96288600
C	-2.77656300	-3.21184900	5.31687500
H	-3.04070600	-4.16953600	4.89016400
C	0.36709200	2.12512800	6.36436300
H	1.01294700	1.33962800	6.73877000
C	0.23477700	3.33344600	7.04026100
H	0.77566000	3.49993500	7.96262300
C	-0.59617600	4.30699900	6.49158500
H	-0.71854400	5.26784400	6.97739000
C	-1.27628300	4.03469400	5.30760100
H	-1.92240100	4.78403500	4.87122900
C	1.65877000	-1.38334600	6.37137400
H	0.65968400	-1.58933500	6.73657600
C	2.78486400	-1.82986800	7.05482800
H	2.67587800	-2.39233400	7.97264900
C	4.03790900	-1.52830500	6.52720800
H	4.94107400	-1.85466500	7.02795500
C	4.12192200	-0.80390200	5.34137900
H	5.08912700	-0.56851800	4.92007800

[Fe(bpy)₃]²⁺ singlet in methanol, applied by CPCM

Fe	0.01316100	-0.00000300	4.07636700
N	1.52857300	0.75621800	3.01825400
C	1.42502600	1.52741800	1.92351900
H	0.41972300	1.75795200	1.59818400
C	2.53574100	1.99501500	1.23140700
H	2.40084500	2.61078900	0.35360000
C	3.80435500	1.65044800	1.69077000
H	4.69099500	1.99248000	1.17336000
C	3.92067000	0.85227200	2.82369500
H	4.89448900	0.56432600	3.19432300
C	2.76325500	0.42145800	3.47263800
C	2.76325500	-0.42145600	4.68010300
N	1.52857200	-0.75622100	5.13448300
N	-1.42502200	0.93629700	3.03721400
C	-2.07612400	0.46296200	1.96165100
H	-1.75688600	-0.50271000	1.59341500
C	-3.10216100	1.16450000	1.33782400
H	-3.59583300	0.74088400	0.47404400
C	-3.47225100	2.40635900	1.84789500

H	-4.26789800	2.97938100	1.39046100
C	-2.80159300	2.90418600	2.95891700
H	-3.06683900	3.86445200	3.37844400
C	-1.78078000	2.14822200	3.53506700
C	-1.00190200	2.58857000	4.70408300
N	-0.07300800	1.69607100	5.13123200
N	-0.07301100	-1.69607900	3.02150400
C	0.70700100	-2.02245000	1.97821300
H	1.43832600	-1.28353700	1.68123200
C	0.59160200	-3.23273600	1.30559000
H	1.24688500	-3.44351900	0.47171000
C	-0.37017500	-4.14616100	1.72938000
H	-0.48809200	-5.09893600	1.22856400
C	-1.17496600	-3.82102300	2.81623000
H	-1.92057500	-4.51801400	3.17345000
C	-1.00190600	-2.58857600	3.44865500
C	-1.78078100	-2.14822500	4.61767300
N	-1.42502100	-0.93630000	5.11552400
C	-2.07612100	-0.46296200	6.19108700
H	-1.75688100	0.50271000	6.55932000
C	-3.10215800	-1.16449900	6.81491700
H	-3.59582800	-0.74088000	7.67869700
C	-3.47225000	-2.40635700	6.30484800
H	-4.26789700	-2.97937800	6.76228300
C	-2.80159500	-2.90418600	5.19382500
H	-3.06684300	-3.86445300	4.77430000
C	0.70700600	2.02243900	6.17452200
H	1.43833000	1.28352300	6.47150000
C	0.59161200	3.23272400	6.84714600
H	1.24689800	3.44350500	7.68102500
C	-0.37016300	4.14615300	6.42335900
H	-0.48807500	5.09892800	6.92417500
C	-1.17495700	3.82101700	5.33651000
H	-1.92056400	4.51801200	4.97929200
C	1.42502500	-1.52741900	6.22921900
H	0.41972100	-1.75795500	6.55455200
C	2.53573900	-1.99500600	6.92133800
H	2.40084300	-2.61077700	7.79914800
C	3.80435300	-1.65043200	6.46198100
H	4.69099300	-1.99245400	6.97939900
C	3.92066900	-0.85225900	5.32905500
H	4.89448800	-0.56430500	4.95843200

[Fe(bpy)₃]²⁺ quintet in methanol, applied by CPCM, <S²> = 6.0118

Fe	-0.02363100	0.00000800	4.07637000
N	1.71326300	0.65341600	2.90894500
C	1.63591700	1.33245900	1.75548800

H	0.63500300	1.52062200	1.38667700
C	2.76000200	1.77810400	1.06945200
H	2.64989900	2.32499100	0.14297500
C	4.01389200	1.49188600	1.60317400
H	4.91491400	1.81628900	1.09903100
C	4.10079500	0.78591600	2.79956100
H	5.06776200	0.55955600	3.22510800
C	2.92714000	0.37659900	3.43657700
C	2.92713300	-0.37663200	4.71617600
N	1.71325100	-0.65344800	5.24379800
N	-1.46571700	1.20893300	2.92237700
C	-2.05334100	0.80047600	1.78834100
H	-1.74888400	-0.17172600	1.41677200
C	-3.00132200	1.56465600	1.11503900
H	-3.45112900	1.19520500	0.20361100
C	-3.35338100	2.80176700	1.64788500
H	-4.09219100	3.42459200	1.16035800
C	-2.74542700	3.23171000	2.82270000
H	-3.01334900	4.18413700	3.25759200
C	-1.79744200	2.41310500	3.43980500
C	-1.10624000	2.78985000	4.69768400
N	-0.29480800	1.84897300	5.23112100
N	-0.29478900	-1.84895700	2.92161400
C	0.33654100	-2.10317100	1.76551000
H	0.97233000	-1.31228200	1.38657100
C	0.20040400	-3.30723100	1.08378900
H	0.72499400	-3.46253500	0.15079700
C	-0.61040600	-4.29189700	1.64195900
H	-0.73167100	-5.25108800	1.15376500
C	-1.27267800	-4.03179400	2.83819500
H	-1.90290400	-4.78879300	3.28363700
C	-1.10622200	-2.78983300	3.45505500
C	-1.79742800	-2.41308900	4.71293100
N	-1.46570700	-1.20891700	5.23036600
C	-2.05334600	-0.80046400	6.36439600
H	-1.74889100	0.17173600	6.73597200
C	-3.00133700	-1.56464300	7.03768400
H	-3.45115600	-1.19519300	7.94910700
C	-3.35338800	-2.80175400	6.50483400
H	-4.09220400	-3.42458000	6.99235200
C	-2.74542000	-3.23169600	5.33002600
H	-3.01333600	-4.18412200	4.89513100
C	0.33652800	2.10318300	6.38722200
H	0.97231500	1.31229200	6.76616000
C	0.20039500	3.30724400	7.06894400
H	0.72499000	3.46254700	8.00193400

C	-0.61041600	4.29191000	6.51077900
H	-0.73168000	5.25110100	6.99897600
C	-1.27269400	4.03181000	5.31454500
H	-1.90292300	4.78881000	4.86910700
C	1.63589400	-1.33248300	6.39726000
H	0.63497700	-1.52064500	6.76606200
C	2.75997200	-1.77812400	7.08330900
H	2.64986100	-2.32500500	8.00978900
C	4.01386700	-1.49191400	6.54959400
H	4.91488400	-1.81632000	7.05374300
C	4.10078200	-0.78595100	5.35320300
H	5.06775200	-0.55959700	4.92766200

[Fe(bpy)₃]²⁺ singlet in acetonitrile, applied by CPCM

Fe	0.01236700	0.00000000	4.07637100
N	1.53076700	0.75823800	3.01892800
C	1.42855400	1.53273400	1.92616400
H	0.42384800	1.76434200	1.59950800
C	2.53968400	2.00300100	1.23610300
H	2.40473400	2.62109100	0.35951600
C	3.80820200	1.65834300	1.69598900
H	4.69552600	2.00228100	1.18038200
C	3.92336000	0.85749400	2.82736700
H	4.89734300	0.57053000	3.19877900
C	2.76548500	0.42381300	3.47411400
C	2.76548500	-0.42381300	4.67862700
N	1.53076700	-0.75823800	5.13381300
N	-1.42634100	0.93769000	3.03603500
C	-2.07902300	0.46290800	1.96188400
H	-1.76241500	-0.50464300	1.59619900
C	-3.10332700	1.16491000	1.33554000
H	-3.59754800	0.73915100	0.47278600
C	-3.47030500	2.40936800	1.84175600
H	-4.26449600	2.98329200	1.38217400
C	-2.79874900	2.90856200	2.95194100
H	-3.06278000	3.87086300	3.36797000
C	-1.77964300	2.15177700	3.53081400
C	-1.00092500	2.59253300	4.70027500
N	-0.07583800	1.69806700	5.13226000
N	-0.07583800	-1.69806600	3.02048100
C	0.69958700	-2.02350300	1.97323500
H	1.42657700	-1.28258800	1.67026300
C	0.58488700	-3.23523900	1.30251100
H	1.23633100	-3.44490600	0.46497500
C	-0.37189000	-4.15115100	1.73246700
H	-0.48977400	-5.10516000	1.23353100
C	-1.17275200	-3.82658900	2.82255200

H	-1.91526000	-4.52536600	3.18310500
C	-1.00092500	-2.59253300	3.45246600
C	-1.77964300	-2.15177600	4.62192700
N	-1.42634100	-0.93769000	5.11670600
C	-2.07902400	-0.46290800	6.19085700
H	-1.76241600	0.50464300	6.55654200
C	-3.10332800	-1.16491000	6.81720100
H	-3.59754900	-0.73915100	7.67995500
C	-3.47030500	-2.40936800	6.31098500
H	-4.26449600	-2.98329200	6.77056700
C	-2.79874900	-2.90856200	5.20079900
H	-3.06278000	-3.87086300	4.78477000
C	0.69958700	2.02350400	6.17950600
H	1.42657700	1.28258900	6.48247900
C	0.58488700	3.23524000	6.85023000
H	1.23633000	3.44490800	7.68776700
C	-0.37189000	4.15115200	6.42027500
H	-0.48977500	5.10516100	6.91921000
C	-1.17275300	3.82659000	5.33018900
H	-1.91526100	4.52536700	4.96963600
C	1.42855400	-1.53273400	6.22657700
H	0.42384800	-1.76434200	6.55323300
C	2.53968400	-2.00300200	6.91663800
H	2.40473400	-2.62109200	7.79322500
C	3.80820200	-1.65834500	6.45675100
H	4.69552600	-2.00228400	6.97235800
C	3.92336000	-0.85749500	5.32537300
H	4.89734300	-0.57053200	4.95396100

[Fe(bpy)₃]²⁺ quintet in acetonitrile, applied by CPCM, <S²> = 6.0118

Fe	-0.02047200	0.00000900	4.07637200
N	1.71975400	0.66438100	2.91399600
C	1.64342900	1.35212500	1.76542100
H	0.64306900	1.54749300	1.39836900
C	2.76827800	1.79760500	1.08000600
H	2.65860200	2.35038600	0.15676500
C	4.02188800	1.50524000	1.61125100
H	4.92371000	1.83012600	1.10817200
C	4.10778600	0.79256100	2.80384700
H	5.07486000	0.56279200	3.22781500
C	2.93356600	0.38113000	3.43898100
C	2.93355900	-0.38116900	4.71377200
N	1.71974200	-0.66441800	5.23874700
N	-1.47485200	1.20372400	2.92699800
C	-2.07068400	0.78948000	1.79927600
H	-1.76807200	-0.18403100	1.42960000
C	-3.02362900	1.55033100	1.12888000

H	-3.47946700	1.17602600	0.22210800
C	-3.37128000	2.79058400	1.65769500
H	-4.11277300	3.41173500	1.17145700
C	-2.75567400	3.22593000	2.82685800
H	-3.02067000	4.18107100	3.25802300
C	-1.80402700	2.40971500	3.44210700
C	-1.10592100	2.79108300	4.69536000
N	-0.29005700	1.85273600	5.22707700
N	-0.29003400	-1.85271600	2.92565900
C	0.34865000	-2.11101300	1.77441800
H	0.98743700	-1.32156000	1.39694100
C	0.21490600	-3.31685700	1.09497500
H	0.74555100	-3.47590400	0.16578600
C	-0.60242500	-4.29809000	1.64994700
H	-0.72337000	-5.25803200	1.16268300
C	-1.27139400	-4.03399500	2.84180400
H	-1.90681300	-4.78872900	3.28405700
C	-1.10590000	-2.79106100	3.45737800
C	-1.80401000	-2.40969700	4.71063000
N	-1.47483800	-1.20370900	5.22574800
C	-2.07068400	-0.78947000	6.35346600
H	-1.76807400	0.18403900	6.72315000
C	-3.02364000	-1.55032100	7.02384500
H	-3.47949000	-1.17601800	7.93061200
C	-3.37128500	-2.79057200	6.49502300
H	-4.11278400	-3.41172400	6.98125000
C	-2.75566400	-3.22591400	5.32586700
H	-3.02065600	-4.18105300	4.89469600
C	0.34863400	2.11102900	6.37831400
H	0.98741700	1.32157200	6.75579000
C	0.21489600	3.31687400	7.05775700
H	0.74554500	3.47592000	7.98694400
C	-0.60243800	4.29810800	6.50279000
H	-0.72338000	5.25805000	6.99005600
C	-1.27141300	4.03401500	5.31093500
H	-1.90683400	4.78874900	4.86868600
C	1.64340600	-1.35215300	6.38732600
H	0.64304200	-1.54752100	6.75436900
C	2.76824900	-1.79762800	7.07275600
H	2.65856400	-2.35040200	7.99600000
C	4.02186300	-1.50527100	6.54151600
H	4.92368100	-1.83015800	7.04460400
C	4.10777300	-0.79260000	5.34891700
H	5.07485000	-0.56283700	4.92495500

[Fe(bpy)₃]²⁺ singlet in ethanol, applied by CPCM

Fe	0.01193400	0.00000000	4.07637100
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N	1.53162200	0.75912300	3.01920000
C	1.43006300	1.53512300	1.92733200
H	0.42560400	1.76711500	1.60005200
C	2.54140300	2.00677800	1.23837700
H	2.40653600	2.62590800	0.36234100
C	3.80987300	1.66240500	1.69877700
H	4.69750400	2.00749100	1.18420800
C	3.92445500	0.86033300	2.82944000
H	4.89846700	0.57415500	3.20157900
C	2.76634200	0.42497400	3.47486100
C	2.76634200	-0.42497400	4.67788000
N	1.53162200	-0.75912300	5.13354100
N	-1.42695200	0.93824700	3.03545600
C	-2.08029800	0.46285200	1.96188600
H	-1.76487000	-0.50558200	1.59744100
C	-3.10376500	1.16509300	1.33435900
H	-3.59826700	0.73847600	0.47204700
C	-3.46935300	2.41071300	1.83884100
H	-4.26285500	2.98503900	1.37827000
C	-2.79742300	2.91048600	2.94867300
H	-3.06088800	3.87369200	3.36314200
C	-1.77913600	2.15331900	3.52882400
C	-1.00054000	2.59428000	4.69850800
N	-0.07713600	1.69895700	5.13263900
N	-0.07713600	-1.69895700	3.02010200
C	0.69629100	-2.02406300	1.97115600
H	1.42134700	-1.28225300	1.66555500
C	0.58193400	-3.23646000	1.30132900
H	1.23169600	-3.44573600	0.46223600
C	-0.37260000	-4.15347900	1.73403600
H	-0.49037700	-5.10806600	1.23599100
C	-1.17177200	-3.82908800	2.82548500
H	-1.91287100	-4.52866600	3.18755200
C	-1.00054100	-2.59428000	3.45423300
C	-1.77913600	-2.15331800	4.62391700
N	-1.42695200	-0.93824700	5.11728500
C	-2.08029800	-0.46285200	6.19085500
H	-1.76487000	0.50558200	6.55530000
C	-3.10376500	-1.16509200	6.81838100
H	-3.59826700	-0.73847600	7.68069300
C	-3.46935400	-2.41071300	6.31390000
H	-4.26285500	-2.98503900	6.77447100
C	-2.79742300	-2.91048500	5.20406800
H	-3.06088900	-3.87369200	4.78959900
C	0.69629100	2.02406300	6.18158500
H	1.42134700	1.28225300	6.48718600

C	0.58193500	3.23646000	6.85141200
H	1.23169600	3.44573600	7.69050500
C	-0.37260000	4.15347900	6.41870500
H	-0.49037700	5.10806600	6.91675000
C	-1.17177200	3.82908800	5.32725600
H	-1.91287100	4.52866600	4.96518900
C	1.43006300	-1.53512300	6.22540900
H	0.42560400	-1.76711600	6.55268900
C	2.54140200	-2.00677900	6.91436400
H	2.40653600	-2.62590900	7.79040000
C	3.80987300	-1.66240500	6.45396400
H	4.69750400	-2.00749100	6.96853300
C	3.92445400	-0.86033300	5.32330100
H	4.89846700	-0.57415500	4.95116200

[Fe(bpy)₃]²⁺ quintet in ethanol, applied by CPCM, <S²> = 6.0118

Fe	-0.01832500	0.00000100	4.07637000
N	1.72345200	0.66997100	2.91657700
C	1.64782900	1.36217600	1.77051500
H	0.64785100	1.56138800	1.40433600
C	2.77308000	1.80768000	1.08557700
H	2.66372200	2.36358900	0.16409400
C	4.02650800	1.51208600	1.61553300
H	4.92873600	1.83723000	1.11307400
C	4.11176100	0.79583900	2.80607200
H	5.07883600	0.56412100	3.22917300
C	2.93721600	0.38343600	3.44021900
C	2.93721600	-0.38341500	4.71253400
N	1.72345100	-0.66995200	5.23617400
N	-1.47857300	1.20120400	2.92940600
C	-2.07757800	0.78486300	1.80407800
H	-1.77522200	-0.18887400	1.43478300
C	-3.03303400	1.54411600	1.13531700
H	-3.49120800	1.16806800	0.23030700
C	-3.37967500	2.78513200	1.66317900
H	-4.12270900	3.40536000	1.17785800
C	-2.76111500	3.22245300	2.83018400
H	-3.02551300	4.17831900	3.26030500
C	-1.80738200	2.40751600	3.44415500
C	-1.10646100	2.79066600	4.69553000
N	-0.28825000	1.85355900	5.22610700
N	-0.28824700	-1.85357400	2.92663900
C	0.35334600	-2.11342800	1.77730900
H	0.99368100	-1.32461900	1.40082200
C	0.22020400	-3.31973200	1.09842200
H	0.75334000	-3.48030900	0.17081400
C	-0.60022100	-4.29942700	1.65170900

H	-0.72128200	-5.25950400	1.16455600
C	-1.27199800	-4.03374500	2.84172600
H	-1.90993700	-4.78741100	3.28232300
C	-1.10646000	-2.79068100	3.45721000
C	-1.80739700	-2.40752100	4.70857400
N	-1.47859800	-1.20120500	5.22331500
C	-2.07761200	-0.78485400	6.34863300
H	-1.77526100	0.18888600	6.71792300
C	-3.03307100	-1.54410500	7.01739400
H	-3.49125200	-1.16805100	7.92239700
C	-3.37970300	-2.78512600	6.48954000
H	-4.12273800	-3.40535300	6.97486200
C	-2.76113300	-3.22245600	5.32254400
H	-3.02552200	-4.17832800	4.89243100
C	0.35332700	2.11341000	6.37544800
H	0.99366500	1.32460400	6.75193600
C	0.22016800	3.31970700	7.05434200
H	0.75329100	3.48028200	7.98195900
C	-0.60025200	4.29940300	6.50104900
H	-0.72132200	5.25947700	6.98820500
C	-1.27201000	4.03372600	5.31102100
H	-1.90994200	4.78739500	4.87041900
C	1.64782800	-1.36216900	6.38222800
H	0.64785100	-1.56138400	6.74840800
C	2.77307900	-1.80767400	7.06716600
H	2.66372000	-2.36359100	7.98864400
C	4.02650800	-1.51206800	6.53721900
H	4.92873600	-1.83720600	7.03968100
C	4.11176100	-0.79581500	5.34668300
H	5.07883600	-0.56408700	4.92358800

[Fe(bpy)₃]²⁺ singlet in propionitrile, applied by CPCM

Fe	0.01107800	0.00000000	4.07637000
N	1.53265100	0.76066700	3.01972200
C	1.43216200	1.53950600	1.92963300
H	0.42817300	1.77170400	1.60093100
C	2.54392700	2.01429100	1.24325000
H	2.40919700	2.63525800	0.36824500
C	3.81228800	1.67130100	1.70523300
H	4.70045100	2.01922000	1.19310400
C	3.92589200	0.86687800	2.83443600
H	4.89979900	0.58295000	3.20882700
C	2.76731200	0.42742000	3.47652000
C	2.76731100	-0.42742000	4.67622100
N	1.53265100	-0.76066800	5.13301900
N	-1.42793900	0.93886100	3.03441700
C	-2.08228900	0.46222800	1.96189900

H	-1.76872400	-0.50761000	1.59953300
C	-3.10443800	1.16474200	1.33241900
H	-3.59934600	0.73653700	0.47092300
C	-3.46776900	2.41229500	1.83388100
H	-4.26015600	2.98717900	1.37164000
C	-2.79522300	2.91327600	2.94298700
H	-3.05765900	3.87802400	3.35476700
C	-1.77827900	2.15558900	3.52527400
C	-0.99981800	2.59708300	4.69514300
N	-0.07924100	1.70039900	5.13289500
N	-0.07924200	-1.70039900	3.01984600
C	0.69111100	-2.02506100	1.96834900
H	1.41289600	-1.28181600	1.65830300
C	0.57748300	-3.23871200	1.30030600
H	1.22461000	-3.44741000	0.45881600
C	-0.37328800	-4.15751600	1.73763300
H	-0.49072800	-5.11316400	1.24126200
C	-1.16990600	-3.83326500	2.83108100
H	-1.90868800	-4.53405900	3.19573300
C	-0.99981900	-2.59708300	3.45759800
C	-1.77828000	-2.15558900	4.62746700
N	-1.42793900	-0.93886100	5.11832400
C	-2.08228900	-0.46222800	6.19084200
H	-1.76872400	0.50761000	6.55320800
C	-3.10443800	-1.16474200	6.82032200
H	-3.59934600	-0.73653700	7.68181800
C	-3.46776900	-2.41229500	6.31886000
H	-4.26015600	-2.98717900	6.78110100
C	-2.79522400	-2.91327600	5.20975400
H	-3.05766000	-3.87802400	4.79797400
C	0.69111100	2.02506100	6.18439200
H	1.41289600	1.28181600	6.49443800
C	0.57748300	3.23871200	6.85243500
H	1.22461000	3.44740900	7.69392500
C	-0.37328700	4.15751500	6.41510800
H	-0.49072700	5.11316400	6.91147900
C	-1.16990500	3.83326500	5.32166000
H	-1.90868800	4.53405900	4.95700800
C	1.43216200	-1.53950600	6.22310800
H	0.42817300	-1.77170400	6.55180900
C	2.54392700	-2.01429100	6.90949100
H	2.40919700	-2.63525800	7.78449700
C	3.81228800	-1.67130100	6.44750800
H	4.70045100	-2.01921900	6.95963700
C	3.92589100	-0.86687800	5.31830500
H	4.89979900	-0.58295000	4.94391400

[Fe(bpy)₃]²⁺ quintet in propionitrile, applied by CPCM, <S²> = 6.0119

Fe	-0.01523500	0.00000300	4.07637200
N	1.72887900	0.67642200	2.91951100
C	1.65410000	1.37386300	1.77643000
H	0.65466700	1.57725300	1.41088100
C	2.77986400	1.81966500	1.09222500
H	2.67079300	2.37917800	0.17274400
C	4.03305300	1.52061100	1.62087100
H	4.93582700	1.84625100	1.11930700
C	4.11751200	0.80002600	2.80891900
H	5.08462400	0.56625300	3.23108900
C	2.94255500	0.38622800	3.44173900
C	2.94255000	-0.38624400	4.71102200
N	1.72886900	-0.67643300	5.23324300
N	-1.48394400	1.19668700	2.93192100
C	-2.08661900	0.77655500	1.80991200
H	-1.78436600	-0.19772200	1.44199400
C	-3.04543500	1.53288400	1.14243700
H	-3.50614500	1.15356200	0.23988000
C	-3.39130000	2.77518100	1.66800100
H	-4.13644100	3.39363900	1.18325800
C	-2.76924300	3.21624900	2.83193000
H	-3.03319100	4.17340100	3.25973500
C	-1.81260300	2.40378800	3.44504000
C	-1.10780900	2.79082900	4.69333900
N	-0.28563100	1.85641700	5.22287600
N	-0.28562200	-1.85640600	2.92986400
C	0.36039500	-2.11993700	1.78378900
H	1.00339400	-1.33279700	1.40805000
C	0.22774700	-3.32752600	1.10686000
H	0.76475200	-3.49144000	0.18191100
C	-0.59795500	-4.30396400	1.65823400
H	-0.71966200	-5.26461700	1.17211400
C	-1.27395700	-4.03452400	2.84513000
H	-1.91606700	-4.78586500	3.28382500
C	-1.10780400	-2.79081800	3.45939700
C	-1.81260500	-2.40377700	4.70769200
N	-1.48394800	-1.19667800	5.22081600
C	-2.08663100	-0.77654800	6.34282200
H	-1.78438000	0.19772800	6.71074400
C	-3.04545400	-1.53287700	7.01028700
H	-3.50617000	-1.15355600	7.91284200
C	-3.39131400	-2.77517400	6.48472000
H	-4.13645900	-3.39363200	6.96945600
C	-2.76924900	-3.21624000	5.32079400
H	-3.03319500	-4.17339100	4.89298700

C	0.36038500	2.11994800	6.36895100
H	1.00337900	1.33280600	6.74469400
C	0.22773800	3.32753900	7.04587700
H	0.76474200	3.49145400	7.97082600
C	-0.59796100	4.30397800	6.49450000
H	-0.71966800	5.26463100	6.98061900
C	-1.27396200	4.03453700	5.30760300
H	-1.91607000	4.78587800	4.86890600
C	1.65408000	-1.37387400	6.37632300
H	0.65464400	-1.57726000	6.74186600
C	2.77983800	-1.81968300	7.06053400
H	2.67076000	-2.37919600	7.98001400
C	4.03303100	-1.52063800	6.53189200
H	4.93580100	-1.84628700	7.03345800
C	4.11750000	-0.80005300	5.34384500
H	5.08461600	-0.56628800	4.92167900

[Fe(bpy)₃]²⁺ singlet in 2-propanol, applied by CPCM

Fe	0.01062600	0.00000000	4.07637100
N	1.53315700	0.76144000	3.01997100
C	1.43323500	1.54178800	1.93082000
H	0.42944300	1.77399100	1.60141200
C	2.54520000	2.01837200	1.24587800
H	2.41061700	2.64032200	0.37142900
C	3.81351700	1.67633900	1.70884700
H	4.70193200	2.02596900	1.19814100
C	3.92660500	0.87065200	2.83726100
H	4.90046500	0.58812600	3.21298100
C	2.76779600	0.42875000	3.47741800
C	2.76779600	-0.42875000	4.67532300
N	1.53315700	-0.76144100	5.13277000
N	-1.42846300	0.93912700	3.03383400
C	-2.08328500	0.46191600	1.96178700
H	-1.77065000	-0.50867600	1.60056600
C	-3.10472600	1.16457400	1.33126000
H	-3.59987000	0.73566500	0.47014700
C	-3.46695800	2.41309600	1.83120300
H	-4.25876300	2.98824900	1.36809500
C	-2.79414000	2.91463700	2.93998800
H	-3.05609100	3.88014700	3.35042600
C	-1.77789900	2.15669600	3.52341200
C	-0.99955000	2.59850000	4.69340400
N	-0.08031500	1.70119200	5.13294000
N	-0.08031500	-1.70119200	3.01980100
C	0.68855500	-2.02577000	1.96709800
H	1.40881600	-1.28185600	1.65496200
C	0.57527400	-3.24004700	1.29996500

H	1.22113600	-3.44860600	0.45736100
C	-0.37367900	-4.15969200	1.73957500
H	-0.49090800	-5.11589200	1.24408400
C	-1.16906700	-3.83539000	2.83395600
H	-1.90669900	-4.53678400	3.19990800
C	-0.99955000	-2.59850000	3.45933700
C	-1.77790000	-2.15669600	4.62932900
N	-1.42846300	-0.93912700	5.11890700
C	-2.08328500	-0.46191600	6.19095400
H	-1.77065000	0.50867600	6.55217500
C	-3.10472700	-1.16457400	6.82148100
H	-3.59987000	-0.73566500	7.68259400
C	-3.46695800	-2.41309500	6.32153800
H	-4.25876300	-2.98824900	6.78464600
C	-2.79414000	-2.91463700	5.21275300
H	-3.05609100	-3.88014700	4.80231500
C	0.68855500	2.02577000	6.18564300
H	1.40881600	1.28185600	6.49777900
C	0.57527500	3.24004700	6.85277600
H	1.22113600	3.44860600	7.69537900
C	-0.37367800	4.15969200	6.41316600
H	-0.49090800	5.11589200	6.90865700
C	-1.16906700	3.83539000	5.31878500
H	-1.90669900	4.53678400	4.95283300
C	1.43323500	-1.54178800	6.22192100
H	0.42944300	-1.77399100	6.55132900
C	2.54520000	-2.01837200	6.90686300
H	2.41061700	-2.64032200	7.78131200
C	3.81351700	-1.67633900	6.44389500
H	4.70193200	-2.02596900	6.95460000
C	3.92660500	-0.87065200	5.31548000
H	4.90046500	-0.58812600	4.93976000

[Fe(bpy)₃]²⁺ quintet in 2-propanol, applied by CPCM, <S²> = 6.0118

Fe	-0.01413400	-0.00000300	4.07636900
N	1.73107700	0.67892900	2.92066000
C	1.65663700	1.37841200	1.77871100
H	0.65735300	1.58324600	1.41341400
C	2.78255200	1.82444900	1.09478500
H	2.67361000	2.38542500	0.17610200
C	4.03568800	1.52409700	1.62290600
H	4.93866100	1.85001200	1.12169400
C	4.11984600	0.80171800	2.80993300
H	5.08703400	0.56712300	3.23162000
C	2.94476000	0.38734700	3.44231600
C	2.94475700	-0.38733600	4.71044400
N	1.73107000	-0.67891200	5.23209500

N	-1.48573300	1.19569900	2.93303000
C	-2.08931100	0.77478300	1.81175000
H	-1.78685800	-0.19948000	1.44391700
C	-3.04932400	1.53017100	1.14484900
H	-3.51060100	1.15008400	0.24280600
C	-3.39545300	2.77251100	1.67024700
H	-4.14141800	3.39040000	1.18586800
C	-2.77255500	3.21439500	2.83351300
H	-3.03681000	4.17171700	3.26088700
C	-1.81476300	2.40276800	3.44612300
C	-1.10876500	2.79086100	4.69356200
N	-0.28488500	1.85742300	5.22237700
N	-0.28490100	-1.85743700	2.93036600
C	0.36281000	-2.12226400	1.78548900
H	1.00710100	-1.33583000	1.41034100
C	0.23019200	-3.33011900	1.10892900
H	0.76875300	-3.49522800	0.18501600
C	-0.59779900	-4.30531300	1.65918500
H	-0.71988500	-5.26602800	1.17315900
C	-1.27540200	-4.03460700	2.84493800
H	-1.91923200	-4.78512100	3.28263100
C	-1.10878700	-2.79087200	3.45917200
C	-1.81479300	-2.40277200	4.70660500
N	-1.48576500	-1.19569800	5.21968800
C	-2.08934400	-0.77477100	6.34096300
H	-1.78689400	0.19949700	6.70878600
C	-3.04935600	-1.53015500	7.00787000
H	-3.51063400	-1.15006100	7.90990900
C	-3.39548400	-2.77250000	6.48248200
H	-4.14144900	-3.39038500	6.96686500
C	-2.77258500	-3.21439400	5.31922000
H	-3.03683800	-4.17171900	4.89185300
C	0.36281300	2.12225000	6.36726200
H	1.00710200	1.33581600	6.74241400
C	0.23019000	3.33010300	7.04382200
H	0.76874200	3.49521100	7.96774200
C	-0.59779200	4.30530000	6.49355700
H	-0.71988000	5.26601600	6.97958200
C	-1.27538100	4.03459600	5.30779700
H	-1.91920300	4.78511300	4.87009700
C	1.65662300	-1.37840200	6.37403800
H	0.65733700	-1.58323100	6.73933400
C	2.78253300	-1.82445200	7.05796400
H	2.67358500	-2.38543400	7.97664300
C	4.03567300	-1.52410000	6.52985300
H	4.93864300	-1.85002000	7.03106700

C	4.11983900	-0.80171400	5.34283100
H	5.08702900	-0.56711900	4.92114900

[Fe(bpy)₃]²⁺ singlet in butyronitrile, applied by CPCM

Fe	0.01000800	0.00000000	4.07637100
N	1.53361500	0.76252300	3.02040200
C	1.43430700	1.54522600	1.93281000
H	0.43080900	1.77700400	1.60215700
C	2.54652100	2.02502500	1.25037400
H	2.41200200	2.64842500	0.37680900
C	3.81477500	1.68503200	1.71515600
H	4.70350900	2.03776900	1.20692000
C	3.92729700	0.87732700	2.84223600
H	4.90105600	0.59748300	3.22035900
C	2.76820700	0.43097100	3.47896100
C	2.76820700	-0.43097200	4.67378000
N	1.53361500	-0.76252300	5.13233900
N	-1.42909800	0.93918500	3.03300000
C	-2.08446700	0.46096700	1.96168500
H	-1.77292000	-0.51052500	1.60193500
C	-3.10511600	1.16363600	1.32982500
H	-3.60048200	0.73357000	0.46930500
C	-3.46600000	2.41341500	1.82765600
H	-4.25712500	2.98878600	1.36340400
C	-2.79282300	2.91597400	2.93586900
H	-3.05410900	3.88251300	3.34444200
C	-1.77741100	2.15786300	3.52075900
C	-0.99910000	2.60028500	4.69070400
N	-0.08162100	1.70224000	5.13263700
N	-0.08162100	-1.70224000	3.02010400
C	0.68552100	-2.02680600	1.96605700
H	1.40376700	-1.28208100	1.65110300
C	0.57281500	-3.24205200	1.30038600
H	1.21716500	-3.45048600	0.45647400
C	-0.37376300	-4.16272000	1.74303600
H	-0.49063000	-5.11973500	1.24887700
C	-1.16775900	-3.83821500	2.83841400
H	-1.90394600	-4.54027000	3.20611500
C	-0.99910100	-2.60028500	3.46203700
C	-1.77741100	-2.15786200	4.63198200
N	-1.42909900	-0.93918400	5.11974100
C	-2.08446800	-0.46096700	6.19105600
H	-1.77292000	0.51052500	6.55080600
C	-3.10511600	-1.16363600	6.82291600
H	-3.60048200	-0.73357000	7.68343600
C	-3.46600100	-2.41341500	6.32508500
H	-4.25712500	-2.98878500	6.78933600

C	-2.79282300	-2.91597300	5.21687200
H	-3.05410900	-3.88251300	4.80829900
C	0.68552100	2.02680600	6.18668400
H	1.40376700	1.28208100	6.50163800
C	0.57281600	3.24205200	6.85235500
H	1.21716500	3.45048600	7.69626700
C	-0.37376300	4.16272000	6.40970500
H	-0.49063000	5.11973500	6.90386400
C	-1.16775900	3.83821500	5.31432700
H	-1.90394500	4.54027100	4.94662600
C	1.43430600	-1.54522600	6.21993200
H	0.43080900	-1.77700400	6.55058400
C	2.54652100	-2.02502600	6.90236700
H	2.41200200	-2.64842500	7.77593200
C	3.81477500	-1.68503200	6.43758500
H	4.70350900	-2.03776900	6.94582100
C	3.92729700	-0.87732700	5.31050500
H	4.90105500	-0.59748300	4.93238200

[Fe(bpy)₃]²⁺ quintet in butyronitrile, applied by CPCM, <S²> = 6.0118

Fe	-0.01268300	0.00000100	4.07637100
N	1.73376200	0.68214200	2.92218200
C	1.65961500	1.38428200	1.78177500
H	0.66053700	1.59065400	1.41666400
C	2.78573100	1.83083900	1.09835300
H	2.67684600	2.39367400	0.18071100
C	4.03878100	1.52896100	1.62585400
H	4.94200100	1.85536900	1.12517800
C	4.12265600	0.80416600	2.81148000
H	5.08991500	0.56859500	3.23262000
C	2.94741300	0.38886000	3.44314200
C	2.94740800	-0.38887100	4.70961700
N	1.73375300	-0.68214900	5.23056900
N	-1.48853400	1.19401800	2.93495100
C	-2.09351400	0.77173900	1.81492400
H	-1.79088600	-0.20254700	1.44731800
C	-3.05525100	1.52576600	1.14886000
H	-3.51738500	1.14439200	0.24768700
C	-3.40156100	2.76828300	1.67380500
H	-4.14868500	3.38534100	1.18993100
C	-2.77728400	3.21157300	2.83590400
H	-3.04171200	4.16923900	3.26254800
C	-1.81785400	2.40115600	3.44776700
C	-1.10981700	2.79096400	4.69365800
N	-0.28335200	1.85905600	5.22131300
N	-0.28334900	-1.85905300	2.93142700
C	0.36721400	-2.12586500	1.78859700

H	1.01342400	-1.34055800	1.41430400
C	0.23479900	-3.33422100	1.11276400
H	0.77591500	-3.50108800	0.19057000
C	-0.59667100	-4.30747900	1.66126700
H	-0.71920900	-5.26833500	1.17548600
C	-1.27695700	-4.03482000	2.84509300
H	-1.92341800	-4.78399600	3.28129500
C	-1.10982000	-2.79095900	3.45907700
C	-1.81786200	-2.40114900	4.70496500
N	-1.48854300	-1.19401200	5.21778200
C	-2.09353000	-0.77173100	6.33780500
H	-1.79090200	0.20255500	6.70541300
C	-3.05527200	-1.52575600	7.00386400
H	-3.51741100	-1.14438100	7.90503300
C	-3.40158100	-2.76827300	6.47891700
H	-4.14870900	-3.38532900	6.96278700
C	-2.77729800	-3.21156400	5.31682200
H	-3.04172400	-4.16923000	4.89017700
C	0.36720800	2.12586600	6.36414500
H	1.01341300	1.34055700	6.73844200
C	0.23479300	3.33422400	7.03997700
H	0.77590600	3.50109000	7.96217300
C	-0.59667100	4.30748400	6.49146900
H	-0.71920900	5.26834100	6.97724900
C	-1.27695200	4.03482600	5.30764000
H	-1.92340900	4.78400400	4.87143500
C	1.65959700	-1.38429000	6.37097500
H	0.66051600	-1.59065800	6.73608000
C	2.78570700	-1.83085200	7.05440400
H	2.67681400	-2.39368700	7.97204500
C	4.03876100	-1.52897800	6.52691000
H	4.94197600	-1.85539000	7.02759100
C	4.12264600	-0.80418300	5.34128600
H	5.08990800	-0.56861500	4.92015100

[Fe(bpy)₃]²⁺ singlet in 1-butanol, applied by CPCM

Fe	0.00974900	0.00000000	4.07637100
N	1.53390500	0.76300700	3.02059000
C	1.43486900	1.54678200	1.93368900
H	0.43145400	1.77837300	1.60258100
C	2.54714500	2.02806900	1.25233500
H	2.41269300	2.65215400	0.37918500
C	3.81539400	1.68902200	1.71791500
H	4.70424300	2.04321200	1.21079300
C	3.92768000	0.88039600	2.84439400
H	4.90146200	0.60182700	3.22347800
C	2.76850500	0.43196400	3.47962800

C	2.76850500	-0.43196400	4.67311300
N	1.53390500	-0.76300700	5.13215100
N	-1.42941000	0.93925200	3.03260200
C	-2.08504700	0.46064100	1.96157800
H	-1.77401300	-0.51131300	1.60257600
C	-3.10529700	1.16333800	1.32907100
H	-3.60082000	0.73284200	0.46880000
C	-3.46557300	2.41369300	1.82596300
H	-4.25637400	2.98917200	1.36118600
C	-2.79223500	2.91664000	2.93395900
H	-3.05325500	3.88363500	3.34170300
C	-1.77721600	2.15844000	3.51955100
C	-0.99895600	2.60114000	4.68952400
N	-0.08222600	1.70278200	5.13252600
N	-0.08222600	-1.70278200	3.02021500
C	0.68413200	-2.02743500	1.96556300
H	1.40154300	-1.28236300	1.64942300
C	0.57166200	-3.24310300	1.30053000
H	1.21533600	-3.45158400	0.45605500
C	-0.37388700	-4.16421100	1.74453900
H	-0.49057800	-5.12159900	1.25098900
C	-1.16724300	-3.83954400	2.84036400
H	-1.90276800	-4.54191800	3.20885500
C	-0.99895600	-2.60114000	3.46321700
C	-1.77721600	-2.15844000	4.63319000
N	-1.42941000	-0.93925200	5.12013900
C	-2.08504700	-0.46064100	6.19116300
H	-1.77401300	0.51131300	6.55016500
C	-3.10529700	-1.16333800	6.82367000
H	-3.60082000	-0.73284200	7.68394100
C	-3.46557300	-2.41369300	6.32677800
H	-4.25637400	-2.98917200	6.79155500
C	-2.79223500	-2.91663900	5.21878200
H	-3.05325500	-3.88363500	4.81103800
C	0.68413200	2.02743500	6.18717800
H	1.40154300	1.28236300	6.50331800
C	0.57166200	3.24310300	6.85221100
H	1.21533700	3.45158400	7.69668600
C	-0.37388700	4.16421100	6.40820200
H	-0.49057800	5.12159900	6.90175200
C	-1.16724200	3.83954400	5.31237700
H	-1.90276800	4.54191800	4.94388600
C	1.43486900	-1.54678300	6.21905200
H	0.43145400	-1.77837300	6.55016000
C	2.54714500	-2.02806900	6.90040600
H	2.41269300	-2.65215400	7.77355600

C	3.81539400	-1.68902200	6.43482600
H	4.70424300	-2.04321200	6.94194800
C	3.92768000	-0.88039600	5.30834700
H	4.90146200	-0.60182700	4.92926300

[Fe(bpy)₃]²⁺ quintet in 1-butanol, applied by CPCM, <S²> = 6.0118

Fe	-0.01218800	0.00000300	4.07637200
N	1.73486600	0.68320700	2.92267000
C	1.66089300	1.38631200	1.78278400
H	0.66186000	1.59327700	1.41778200
C	2.78706100	1.83306200	1.09951600
H	2.67824900	2.39660900	0.18225500
C	4.04010100	1.53062100	1.62678200
H	4.94341000	1.85720700	1.12628500
C	4.12382900	0.80496000	2.81191900
H	5.09114700	0.56903800	3.23281200
C	2.94853500	0.38935300	3.44339400
C	2.94853000	-0.38937000	4.70936400
N	1.73485600	-0.68322000	5.23008000
N	-1.48935900	1.19363600	2.93538800
C	-2.09472800	0.77100700	1.81566500
H	-1.79197400	-0.20327200	1.44809900
C	-3.05705500	1.52453200	1.14984800
H	-3.51942600	1.14279700	0.24889700
C	-3.40359700	2.76703400	1.67474400
H	-4.15114800	3.38378200	1.19104100
C	-2.77897500	3.21070300	2.83656500
H	-3.04365300	4.16842800	3.26300300
C	-1.81895400	2.40073800	3.44821100
C	-1.11037800	2.79109600	4.69370800
N	-0.28301200	1.85971600	5.22101000
N	-0.28300600	-1.85970900	2.93172800
C	0.36842500	-2.12729300	1.78953000
H	1.01537200	-1.34240900	1.41553900
C	0.23599500	-3.33579900	1.11392000
H	0.77792500	-3.50337000	0.19228500
C	-0.59671400	-4.30836500	1.66184900
H	-0.71948000	-5.26926200	1.17614000
C	-1.27780100	-4.03497100	2.84507600
H	-1.92515900	-4.78369800	3.28078000
C	-1.11037600	-2.79108700	3.45902700
C	-1.81895800	-2.40072900	4.70452100
N	-1.48936300	-1.19362800	5.21734800
C	-2.09473800	-0.77100000	6.33706800
H	-1.79198500	0.20327700	6.70463800
C	-3.05707200	-1.52452400	7.00287700
H	-3.51944800	-1.14278900	7.90382500

C	-3.40361300	-2.76702400	6.47797700
H	-4.15116800	-3.38377100	6.96167500
C	-2.77898400	-3.21069300	5.31616000
H	-3.04366100	-4.16841700	4.88972000
C	0.36841600	2.12729800	6.36321000
H	1.01535800	1.34241200	6.73720400
C	0.23598900	3.33580600	7.03881800
H	0.77791800	3.50337700	7.96045400
C	-0.59671500	4.30837400	6.49088600
H	-0.71948000	5.26927200	6.97659300
C	-1.27780000	4.03498100	5.30765700
H	-1.92515400	4.78371000	4.87195000
C	1.66087300	-1.38632400	6.36996700
H	0.66183800	-1.59328600	6.73496200
C	2.78703600	-1.83307600	7.05324300
H	2.67821700	-2.39662200	7.97050400
C	4.04008000	-1.53064100	6.52598300
H	4.94338600	-1.85723000	7.02648500
C	4.12381800	-0.80498100	5.34084600
H	5.09114000	-0.56906300	4.91995800

[Fe(bpy)₃]²⁺ singlet in tetrahydrofuran, applied by CPCM

Fe	0.01024900	0.00000000	4.07637100
N	1.53387800	0.76209800	3.02010500
C	1.43459200	1.54361600	1.93158000
H	0.43084500	1.77606100	1.60192600
C	2.54665800	2.02142200	1.24753200
H	2.41242700	2.64422200	0.37351200
C	3.81498300	1.67993500	1.71114400
H	4.70358500	2.03078600	1.20143600
C	3.92752700	0.87329700	2.83902900
H	4.90147600	0.59174400	3.21546600
C	2.76855800	0.42968300	3.47798300
C	2.76855800	-0.42968300	4.67475800
N	1.53387800	-0.76209800	5.13263600
N	-1.42904900	0.93963600	3.03329800
C	-2.08439000	0.46219500	1.96151800
H	-1.77269400	-0.50924500	1.60153500
C	-3.10505300	1.16512000	1.32994900
H	-3.60060300	0.73594700	0.46909000
C	-3.46626000	2.41452500	1.82865600
H	-4.25747900	2.99000900	1.36477600
C	-2.79319200	2.91623700	2.93732500
H	-3.05480800	3.88238100	3.34667400
C	-1.77765500	2.15796300	3.52185800
C	-0.99953100	2.59993100	4.69217600
N	-0.08138300	1.70207800	5.13323100

N	-0.08138300	-1.70207800	3.01951000
C	0.68609000	-2.02678200	1.96566000
H	1.40520500	-1.28228900	1.65194800
C	0.57303300	-3.24151500	1.29916100
H	1.21774600	-3.45020200	0.45559400
C	-0.37441400	-4.16189400	1.74072400
H	-0.49144400	-5.11856400	1.24596400
C	-1.16860500	-3.83741600	2.83601200
H	-1.90516800	-4.53945900	3.20308900
C	-0.99953100	-2.59993100	3.46056500
C	-1.77765500	-2.15796300	4.63088300
N	-1.42904900	-0.93963600	5.11944300
C	-2.08439000	-0.46219500	6.19122300
H	-1.77269400	0.50924500	6.55120600
C	-3.10505300	-1.16512000	6.82279200
H	-3.60060300	-0.73594600	7.68365100
C	-3.46626000	-2.41452500	6.32408500
H	-4.25747900	-2.99000900	6.78796500
C	-2.79319200	-2.91623600	5.21541600
H	-3.05480800	-3.88238100	4.80606700
C	0.68609000	2.02678200	6.18708100
H	1.40520600	1.28228900	6.50079300
C	0.57303300	3.24151500	6.85358000
H	1.21774700	3.45020200	7.69714700
C	-0.37441400	4.16189400	6.41201700
H	-0.49144400	5.11856400	6.90677700
C	-1.16860500	3.83741600	5.31672900
H	-1.90516800	4.53945900	4.94965200
C	1.43459200	-1.54361600	6.22116100
H	0.43084500	-1.77606100	6.55081500
C	2.54665800	-2.02142200	6.90520900
H	2.41242700	-2.64422200	7.77922900
C	3.81498300	-1.67993500	6.44159700
H	4.70358500	-2.03078600	6.95130500
C	3.92752700	-0.87329700	5.31371200
H	4.90147600	-0.59174400	4.93727500

[Fe(bpy)₃]²⁺ quintet in tetrahydrofuran, applied by CPCM, <S²> = 6.0117

Fe	-0.01362600	-0.00000100	4.07636800
N	1.73277900	0.67983700	2.92098000
C	1.65881900	1.38030200	1.77941600
H	0.65953000	1.58609700	1.41437700
C	2.78476300	1.82633700	1.09547300
H	2.67611300	2.38813900	0.17716500
C	4.03793600	1.52524800	1.62330500
H	4.94103700	1.85120300	1.12219500
C	4.12172100	0.80207500	2.80994500

H	5.08906500	0.56704500	3.23121200
C	2.94656900	0.38765300	3.44241400
C	2.94656000	-0.38767600	4.71035100
N	1.73276200	-0.67986000	5.23176900
N	-1.48596400	1.19593600	2.93253600
C	-2.08951800	0.77506400	1.81108100
H	-1.78673400	-0.19917800	1.44325300
C	-3.04996400	1.52991200	1.14414300
H	-3.51122700	1.14975800	0.24202400
C	-3.39682900	2.77204600	1.66974500
H	-4.14319900	3.38959500	1.18541200
C	-2.77410500	3.21395400	2.83320000
H	-3.03920100	4.17117100	3.26046200
C	-1.81579800	2.40283000	3.44588100
C	-1.10997600	2.79126900	4.69351200
N	-0.28547100	1.85821600	5.22236600
N	-0.28546200	-1.85820400	2.93036400
C	0.36230100	-2.12389000	1.78556600
H	1.00729100	-1.33783200	1.41055700
C	0.22932600	-3.33179100	1.10910500
H	0.76809900	-3.49775800	0.18536900
C	-0.59957800	-4.30643500	1.65922700
H	-0.72210800	-5.26718300	1.17326200
C	-1.27719000	-4.03496600	2.84486900
H	-1.92158000	-4.78521400	3.28235400
C	-1.10997200	-2.79125500	3.45921600
C	-1.81578900	-2.40282200	4.70685000
N	-1.48595500	-1.19593100	5.22020200
C	-2.08951300	-0.77506500	6.34165800
H	-1.78672900	0.19917700	6.70949000
C	-3.04996100	-1.52991400	7.00859000
H	-3.51122800	-1.14976400	7.91070900
C	-3.39682400	-2.77204700	6.48298300
H	-4.14319500	-3.38959800	6.96731300
C	-2.77409700	-3.21394900	5.31952800
H	-3.03919500	-4.17116500	4.89226100
C	0.36229900	2.12390400	6.36715800
H	1.00728200	1.33784100	6.74217100
C	0.22933700	3.33181200	7.04361000
H	0.76811700	3.49778100	7.96734100
C	-0.59956500	4.30645600	6.49348800
H	-0.72209000	5.26720700	6.97944900
C	-1.27718700	4.03498300	5.30785200
H	-1.92157800	4.78523000	4.87036600
C	1.65878600	-1.38031700	6.37333700
H	0.65949100	-1.58611000	6.73836100

C	2.78472000	-1.82634800	7.05729900
H	2.67605700	-2.38814200	7.97561000
C	4.03790000	-1.52526500	6.52947900
H	4.94099400	-1.85122100	7.03060200
C	4.12170200	-0.80209900	5.34283700
H	5.08905200	-0.56707400	4.92158100

[Fe(bpy)₃]²⁺ singlet in hexanenitrile, applied by CPCM

Fe	0.00883200	0.00000000	4.07637100
N	1.53518600	0.76521600	3.02172400
C	1.43665700	1.55478400	1.93881500
H	0.43358400	1.78451900	1.60525400
C	2.54884800	2.04508700	1.26353500
H	2.41403400	2.67290600	0.39283700
C	3.81714100	1.71179400	1.73328300
H	4.70632500	2.07455400	1.23238300
C	3.92909500	0.89793100	2.85615600
H	4.90335900	0.62692000	3.23969600
C	2.76992000	0.43729900	3.48324000
C	2.76992000	-0.43729900	4.66950100
N	1.53518600	-0.76521600	5.13101700
N	-1.43059200	0.93896800	3.03069600
C	-2.08731800	0.45801400	1.96126300
H	-1.77820700	-0.51574800	1.60543700
C	-3.10625500	1.16030700	1.32606100
H	-3.60227100	0.72729300	0.46710400
C	-3.46417100	2.41313100	1.81857400
H	-4.25385700	2.98870100	1.35152500
C	-2.79005900	2.91850100	2.92522100
H	-3.04999000	3.88757200	3.32901600
C	-1.77637900	2.16040100	3.51376800
C	-0.99800900	2.60491300	4.68334000
N	-0.08454000	1.70540500	5.13126300
N	-0.08454000	-1.70540500	3.02147800
C	0.67875700	-2.03077900	1.96463800
H	1.39246400	-1.28441300	1.64291100
C	0.56754700	-3.24868500	1.30309100
H	1.20849600	-3.45755700	0.45639700
C	-0.37343400	-4.17153200	1.75335200
H	-0.48919500	-5.13082600	1.26297900
C	-1.16440400	-3.84572500	2.85066500
H	-1.89714900	-4.54922100	3.22278300
C	-0.99800900	-2.60491300	3.46940100
C	-1.77637900	-2.16040100	4.63897300
N	-1.43059200	-0.93896800	5.12204500
C	-2.08731800	-0.45801400	6.19147800
H	-1.77820700	0.51574800	6.54730400

C	-3.10625500	-1.16030700	6.82668000
H	-3.60227100	-0.72729300	7.68563700
C	-3.46417200	-2.41313100	6.33416700
H	-4.25385700	-2.98870100	6.80121600
C	-2.79005900	-2.91850000	5.22752000
H	-3.04999000	-3.88757200	4.82372500
C	0.67875800	2.03077900	6.18810300
H	1.39246400	1.28441300	6.50983000
C	0.56754700	3.24868500	6.84965000
H	1.20849600	3.45755700	7.69634400
C	-0.37343400	4.17153200	6.39938900
H	-0.48919500	5.13082600	6.88976200
C	-1.16440400	3.84572600	5.30207600
H	-1.89714900	4.54922100	4.92995800
C	1.43665700	-1.55478400	6.21392600
H	0.43358400	-1.78451900	6.54748700
C	2.54884800	-2.04508700	6.88920600
H	2.41403400	-2.67290600	7.75990500
C	3.81714100	-1.71179400	6.41945800
H	4.70632500	-2.07455400	6.92035800
C	3.92909500	-0.89793100	5.29658500
H	4.90335900	-0.62692000	4.91304500

[Fe(bpy)₃]²⁺ quintet in hexanenitrile, applied by CPCM, <S²> = 6.0117

Fe	-0.00941100	-0.00000600	4.07636600
N	1.74012900	0.68862700	2.92528600
C	1.66661000	1.39657200	1.78820000
H	0.66782400	1.60578600	1.42349500
C	2.79303100	1.84481200	1.10601500
H	2.68427400	2.41185000	0.19070400
C	4.04599600	1.53993400	1.63221600
H	4.94970200	1.86777000	1.13280100
C	4.12930400	0.80970600	2.81470200
H	5.09685000	0.57222200	3.23453200
C	2.95380400	0.39210800	3.44486600
C	2.95380200	-0.39208000	4.70789400
N	1.74012400	-0.68859300	5.22747000
N	-1.49449900	1.19094300	2.93926700
C	-2.10251100	0.76607100	1.82176100
H	-1.79910000	-0.20797700	1.45411200
C	-3.06855100	1.51681400	1.15798800
H	-3.53250500	1.13285800	0.25857200
C	-3.41605000	2.75920000	1.68270100
H	-4.16620300	3.37420500	1.20037300
C	-2.78886100	3.20524600	2.84244300
H	-3.05437200	4.16329800	3.26793600
C	-1.82520800	2.39780300	3.45216900

C	-1.11265700	2.79134300	4.69469100
N	-0.27963600	1.86317400	5.21916000
N	-0.27965100	-1.86319600	2.93358300
C	0.37794800	-2.13499700	1.79582300
H	1.02927000	-1.35262100	1.42400700
C	0.24584500	-3.34437200	1.12146100
H	0.79334100	-3.51567200	0.20361800
C	-0.59456700	-4.31276400	1.66517800
H	-0.71837900	-5.27380800	1.17972600
C	-1.28141200	-4.03530600	2.84424200
H	-1.93446000	-4.78119200	3.27652600
C	-1.11267700	-2.79136400	3.45804300
C	-1.82523800	-2.39781600	4.70055700
N	-1.49453800	-1.19094700	5.21344300
C	-2.10255100	-0.76606200	6.33094200
H	-1.79914600	0.20799400	6.69857600
C	-3.06858400	-1.51680300	6.99472600
H	-3.53254000	-1.13283800	7.89413800
C	-3.41607600	-2.75919800	6.47002900
H	-4.16622600	-3.37420100	6.95236600
C	-2.78888600	-3.20525600	5.31029100
H	-3.05439100	-4.16331500	4.88481100
C	0.37794400	2.13497500	6.35693200
H	1.02926600	1.35260100	6.72875300
C	0.24582900	3.34434600	7.03129700
H	0.79331100	3.51564400	7.94914900
C	-0.59457400	4.31274000	6.48756900
H	-0.71839400	5.27378400	6.97302000
C	-1.28140100	4.03528400	5.30849400
H	-1.93444100	4.78117200	4.87620200
C	1.66659800	-1.39654700	6.36454900
H	0.66781000	-1.60575400	6.72925400
C	2.79301500	-1.84480000	7.04673300
H	2.68425300	-2.41184400	7.96204000
C	4.04598400	-1.53991800	6.52054200
H	4.94968700	-1.86775800	7.01996000
C	4.12929800	-0.80968200	5.33806100
H	5.09684700	-0.57219400	4.91823900

[Fe(bpy)₃]²⁺ singlet in diethyl ether, applied by CPCM

Fe	0.00900600	0.00000000	4.07637100
N	1.53546600	0.76462000	3.02116000
C	1.43742900	1.55196900	1.93643600
H	0.43401400	1.78302100	1.60438700
C	2.54966400	2.03820800	1.25831900
H	2.41570600	2.66465700	0.38653900
C	3.81801200	1.70239800	1.72645900

H	4.70713000	2.06154900	1.22296100
C	3.92952100	0.89075100	2.85104400
H	4.90373400	0.61683100	3.23279300
C	2.77024300	0.43521200	3.48169300
C	2.77024300	-0.43521200	4.67104800
N	1.53546500	-0.76462000	5.13158100
N	-1.43066600	0.93982400	3.03117000
C	-2.08743600	0.46027100	1.96095000
H	-1.77830600	-0.51355600	1.60491000
C	-3.10616200	1.16320300	1.32607600
H	-3.60260500	0.73178500	0.46656900
C	-3.46432300	2.41556500	1.81991500
H	-4.25397400	2.99149800	1.35337600
C	-2.79036100	2.91936600	2.92737700
H	-3.05064600	3.88784400	3.33245800
C	-1.77673500	2.16077400	3.51550800
C	-0.99880300	2.60437700	4.68585200
N	-0.08437300	1.70506000	5.13239800
N	-0.08437300	-1.70506000	3.02034300
C	0.67926800	-2.03052900	1.96362800
H	1.39428800	-1.28438600	1.64394500
C	0.56745800	-3.24752300	1.30058700
H	1.20887600	-3.45671900	0.45433600
C	-0.37486000	-4.17000900	1.74909400
H	-0.49093000	-5.12868300	1.25762700
C	-1.16593700	-3.84439200	2.84646800
H	-1.89919600	-4.54796600	3.21762400
C	-0.99880300	-2.60437700	3.46688900
C	-1.77673500	-2.16077400	4.63723300
N	-1.43066600	-0.93982400	5.12157100
C	-2.08743600	-0.46027100	6.19179100
H	-1.77830600	0.51355600	6.54783100
C	-3.10616200	-1.16320300	6.82666500
H	-3.60260500	-0.73178500	7.68617200
C	-3.46432400	-2.41556500	6.33282600
H	-4.25397400	-2.99149800	6.79936500
C	-2.79036100	-2.91936600	5.22536400
H	-3.05064700	-3.88784400	4.82028300
C	0.67926800	2.03052900	6.18911300
H	1.39428800	1.28438600	6.50879600
C	0.56745800	3.24752300	6.85215400
H	1.20887600	3.45671900	7.69840500
C	-0.37486000	4.17000900	6.40364700
H	-0.49093000	5.12868300	6.89511400
C	-1.16593700	3.84439200	5.30627300
H	-1.89919500	4.54796600	4.93511700

C	1.43742900	-1.55196900	6.21630500
H	0.43401400	-1.78302100	6.54835400
C	2.54966400	-2.03820900	6.89442200
H	2.41570600	-2.66465800	7.76620200
C	3.81801200	-1.70239900	6.42628200
H	4.70713000	-2.06154900	6.92978000
C	3.92952100	-0.89075100	5.30169700
H	4.90373400	-0.61683100	4.91994800

[Fe(bpy)₃]²⁺ quintet in diethyl ether, applied by CPCM, <S²> = 6.0115

Fe	-0.01148300	-0.00000200	4.07636900
N	1.73806200	0.68485600	2.92324900
C	1.66502500	1.38990800	1.78412100
H	0.66593400	1.59861200	1.41965600
C	2.79120400	1.83684700	1.10087400
H	2.68295700	2.40205300	0.18437100
C	4.04434800	1.53307300	1.62758900
H	4.94788600	1.85986900	1.12732600
C	4.12735800	0.80581100	2.81194300
H	5.09500100	0.56912400	3.23203600
C	2.95196800	0.38998400	3.44357600
C	2.95196400	-0.38998000	4.70918400
N	1.73805400	-0.68484800	5.22950400
N	-1.48987800	1.19461700	2.93449400
C	-2.09549800	0.77227700	1.81448900
H	-1.79225000	-0.20196200	1.44677000
C	-3.05879500	1.52482400	1.14888200
H	-3.52136900	1.14310200	0.24783300
C	-3.40665500	2.76686100	1.67441200
H	-4.15509500	3.38301500	1.19102900
C	-2.78212600	3.21036600	2.83655500
H	-3.04839800	4.16781900	3.26296800
C	-1.82098100	2.40130600	3.44806800
C	-1.11259100	2.79218800	4.69391200
N	-0.28407200	1.86142900	5.22119700
N	-0.28407600	-1.86143400	2.93154400
C	0.36780100	-2.13079000	1.78970800
H	1.01616200	-1.34663200	1.41610100
C	0.23501100	-3.33945100	1.11433600
H	0.77764200	-3.50872800	0.19322200
C	-0.59952300	-4.31099900	1.66182600
H	-0.72293200	-5.27200600	1.17624600
C	-1.28091800	-4.03608300	2.84466700
H	-1.92934300	-4.78436600	3.27988100
C	-1.11259900	-2.79219200	3.45882300
C	-1.82099700	-2.40130700	4.70466300
N	-1.48989700	-1.19461500	5.21823200

C	-2.09552200	-0.77227000	6.33823200
H	-1.79227700	0.20197100	6.70594700
C	-3.05882000	-1.52481500	7.00384000
H	-3.52139800	-1.14309000	7.90488500
C	-3.40667700	-2.76685500	6.47831400
H	-4.15511700	-3.38300700	6.96169700
C	-2.78214300	-3.21036500	5.31617500
H	-3.04841200	-4.16782000	4.88976500
C	0.36779700	2.13078400	6.36303900
H	1.01615500	1.34662600	6.73665100
C	0.23500200	3.33944600	7.03841000
H	0.77762700	3.50872200	7.95952800
C	-0.59952500	4.31099500	6.49091300
H	-0.72293600	5.27200200	6.97649100
C	-1.28091100	4.03607900	5.30806700
H	-1.92933000	4.78436400	4.87284700
C	1.66501000	-1.38990300	6.36863000
H	0.66591600	-1.59860200	6.73309100
C	2.79118400	-1.83685000	7.05188000
H	2.68293000	-2.40205900	7.96838000
C	4.04433100	-1.53307900	6.52517100
H	4.94786600	-1.85988000	7.02543800
C	4.12734900	-0.80581300	5.34082100
H	5.09499600	-0.56912800	4.92073300

[Fe(bpy)₃]²⁺ singlet in dichloromethane, applied by CPCM

Fe	0.01148100	0.00000000	4.07637000
N	1.53259700	0.75994900	3.01937100
C	1.43182100	1.53729000	1.92821100
H	0.42750000	1.76979800	1.60059000
C	2.54332700	2.01009900	1.24014000
H	2.40877500	2.63023000	0.36459100
C	3.81178400	1.66592500	1.70101000
H	4.69969100	2.01204600	1.18737200
C	3.92568900	0.86278000	2.83110000
H	4.89980000	0.57730900	3.20378900
C	2.76735300	0.42595700	3.47544500
C	2.76735300	-0.42595700	4.67729600
N	1.53259700	-0.75995000	5.13337000
N	-1.42765900	0.93898400	3.03485200
C	-2.08169800	0.46323700	1.96169600
H	-1.76751300	-0.50621900	1.59867400
C	-3.10419600	1.16583600	1.33289300
H	-3.59913000	0.73871900	0.47092500
C	-3.46840200	2.41260900	1.83576900
H	-4.26115300	2.98740000	1.37421100
C	-2.79612700	2.91266400	2.94541300

H	-3.05911500	3.87671900	3.35844400
C	-1.77873200	2.15503000	3.52692200
C	-1.00037900	2.59611300	4.69701000
N	-0.07851900	1.69997300	5.13316600
N	-0.07851900	-1.69997400	3.01957500
C	0.69294200	-2.02495700	1.96895800
H	1.41628900	-1.28228700	1.66105800
C	0.57887300	-3.23792700	1.29988900
H	1.22701000	-3.44707300	0.45934700
C	-0.37357500	-4.15600400	1.73519900
H	-0.49119500	-5.11115000	1.23800100
C	-1.17106100	-3.83163800	2.82799400
H	-1.91074200	-4.53208900	3.19151700
C	-1.00038000	-2.59611300	3.45573100
C	-1.77873200	-2.15503000	4.62581800
N	-1.42765900	-0.93898400	5.11788900
C	-2.08169800	-0.46323700	6.19104500
H	-1.76751300	0.50621900	6.55406700
C	-3.10419600	-1.16583600	6.81984800
H	-3.59912900	-0.73871900	7.68181600
C	-3.46840200	-2.41260800	6.31697200
H	-4.26115400	-2.98740000	6.77853000
C	-2.79612700	-2.91266400	5.20732800
H	-3.05911500	-3.87671900	4.79429700
C	0.69294300	2.02495600	6.18378200
H	1.41628900	1.28228600	6.49168300
C	0.57887400	3.23792600	6.85285200
H	1.22701100	3.44707300	7.69339400
C	-0.37357400	4.15600400	6.41754200
H	-0.49119400	5.11114900	6.91474000
C	-1.17106000	3.83163800	5.32474700
H	-1.91074100	4.53208900	4.96122400
C	1.43182100	-1.53729000	6.22453000
H	0.42749900	-1.76979900	6.55215100
C	2.54332700	-2.01009900	6.91260100
H	2.40877500	-2.63022900	7.78815000
C	3.81178400	-1.66592400	6.45173100
H	4.69969100	-2.01204500	6.96537000
C	3.92568900	-0.86277900	5.32164200
H	4.89980000	-0.57730900	4.94895300

[Fe(bpy)₃]²⁺ quintet in dichloromethane, applied by CPCM, <S²> = 6.0117

Fe	-0.01682900	-0.00001000	4.07636700
N	1.72658200	0.67275500	2.91774400
C	1.65165100	1.36734900	1.77288100
H	0.65184900	1.56892100	1.40721700
C	2.77709300	1.81273600	1.08804300

H	2.66809700	2.37041700	0.16747100
C	4.03047800	1.51533100	1.61729200
H	4.93298100	1.84051600	1.11511300
C	4.11515000	0.79720600	2.80681500
H	5.08236500	0.56440900	3.22923400
C	2.94041600	0.38450300	3.44072300
C	2.94041300	-0.38446600	4.71204400
N	1.72657700	-0.67271300	5.23501800
N	-1.48034500	1.19966800	2.92957100
C	-2.08069700	0.78194600	1.80532600
H	-1.77818600	-0.19204200	1.43665100
C	-3.03757600	1.53978300	1.13689000
H	-3.49675400	1.16251000	0.23275900
C	-3.38433400	2.78122900	1.66391300
H	-4.12834000	3.40058800	1.17874100
C	-2.76463000	3.21994700	2.82993000
H	-3.02940800	4.17625700	3.25905600
C	-1.80962000	2.40621500	3.44380100
C	-1.10767100	2.79094800	4.69437700
N	-0.28794500	1.85492000	5.22491100
N	-0.28796700	-1.85494400	2.92783400
C	0.35476500	-2.11655700	1.77939400
H	0.99627300	-1.32843500	1.40309900
C	0.22148600	-3.32333800	1.10127100
H	0.75573100	-3.48562400	0.17447000
C	-0.60099300	-4.30170200	1.65415700
H	-0.72257200	-5.26203400	1.16746500
C	-1.27385000	-4.03427700	2.84326900
H	-1.91333500	-4.78707500	3.28330000
C	-1.10770000	-2.79097100	3.45835500
C	-1.80965800	-2.40623000	4.70892400
N	-1.48038900	-1.19967600	5.22314000
C	-2.08073800	-0.78194000	6.34737900
H	-1.77823200	0.19205300	6.71604100
C	-3.03761100	-1.53977600	7.01582700
H	-3.49678800	-1.16249400	7.91995600
C	-3.38436700	-2.78122800	6.48881900
H	-4.12837000	-3.40058300	6.97399800
C	-2.76466400	-3.21995800	5.32280400
H	-3.02943900	-4.17627200	4.89368700
C	0.35476900	2.11653700	6.37336100
H	0.99627500	1.32841900	6.74966500
C	0.22147800	3.32331700	7.05148400
H	0.75570800	3.48560300	7.97829300
C	-0.60099000	4.30168200	6.49858400
H	-0.72257600	5.26201500	6.98527200

C	-1.27382700	4.03425500	5.30946100
H	-1.91330200	4.78705600	4.86942000
C	1.65163900	-1.36732200	6.37987100
H	0.65183600	-1.56888800	6.74553500
C	2.77707800	-1.81272700	7.06470500
H	2.66807600	-2.37041900	7.98527000
C	4.03046500	-1.51531900	6.53546500
H	4.93296600	-1.84051100	7.03764500
C	4.11514500	-0.79717900	5.34595200
H	5.08236200	-0.56438200	4.92353800

[Fe(bpy)₃]²⁺ singlet in water, applied by SMD

Fe	-0.00820400	0.00000000	4.07637100
N	1.52530500	0.76664900	3.01929300
C	1.43083700	1.55142600	1.93139200
H	0.43158000	1.79059100	1.59014000
C	2.54500800	2.03735800	1.25489500
H	2.40980100	2.66430400	0.38102200
C	3.81267000	1.70062700	1.72428900
H	4.70510900	2.06079600	1.22344500
C	3.92105600	0.89070700	2.85086100
H	4.89720500	0.61951300	3.23267600
C	2.75986800	0.43450200	3.48037000
C	2.75986800	-0.43450200	4.67237100
N	1.52530500	-0.76664900	5.13344800
N	-1.43432200	0.94912100	3.01911000
C	-2.07563100	0.47409500	1.93689100
H	-1.79617400	-0.51728300	1.60279300
C	-3.04693200	1.20278100	1.25797200
H	-3.53245100	0.77078300	0.39044900
C	-3.36850800	2.47913000	1.71512500
H	-4.11884500	3.07865200	1.21057700
C	-2.71071000	2.97893300	2.83517400
H	-2.94287100	3.96889100	3.20747800
C	-1.74809400	2.19138400	3.47175500
C	-0.99713400	2.62116600	4.66618300
N	-0.10966000	1.70714200	5.13881100
N	-0.10966100	-1.70714200	3.01393000
C	0.60799700	-2.00971100	1.91791200
H	1.29876600	-1.25384400	1.56623400
C	0.48328000	-3.22261400	1.24810600
H	1.08740400	-3.41305100	0.36845800
C	-0.42279500	-4.16428700	1.73090500
H	-0.54767600	-5.12104300	1.23492600
C	-1.17294600	-3.85895100	2.86266400
H	-1.88703600	-4.57388200	3.25198500
C	-0.99713400	-2.62116600	3.48655800

C	-1.74809400	-2.19138400	4.68098600
N	-1.43432200	-0.94912100	5.13363100
C	-2.07563100	-0.47409500	6.21585000
H	-1.79617400	0.51728300	6.54994800
C	-3.04693200	-1.20278100	6.89476900
H	-3.53245100	-0.77078300	7.76229200
C	-3.36850800	-2.47913000	6.43761600
H	-4.11884500	-3.07865200	6.94216400
C	-2.71071000	-2.97893300	5.31756700
H	-2.94287100	-3.96889000	4.94526300
C	0.60799700	2.00971100	6.23482900
H	1.29876600	1.25384400	6.58650700
C	0.48328000	3.22261400	6.90463500
H	1.08740400	3.41305100	7.78428300
C	-0.42279500	4.16428700	6.42183600
H	-0.54767600	5.12104400	6.91781500
C	-1.17294600	3.85895100	5.29007700
H	-1.88703600	4.57388200	4.90075600
C	1.43083700	-1.55142600	6.22134900
H	0.43158000	-1.79059100	6.56260100
C	2.54500800	-2.03735800	6.89784600
H	2.40980100	-2.66430400	7.77171900
C	3.81267000	-1.70062800	6.42845200
H	4.70510900	-2.06079600	6.92929600
C	3.92105600	-0.89070700	5.30188000
H	4.89720500	-0.61951300	4.92006500

[Fe(bpy)₃]²⁺ quintet in water, applied by SMD, <S²> = 6.0182

Fe	0.05600200	0.00005400	4.07634300
N	1.82721700	0.68611300	2.91959800
C	1.75479600	1.37894000	1.77215600
H	0.75710200	1.57503500	1.39273700
C	2.88235200	1.82754800	1.09090400
H	2.77351200	2.38363500	0.16683200
C	4.13447000	1.54177100	1.63070100
H	5.04045600	1.87632700	1.13596000
C	4.21672700	0.81756100	2.81780400
H	5.18604300	0.59519300	3.24529900
C	3.04032400	0.39220200	3.44394400
C	3.04028900	-0.39243500	4.70881700
N	1.82715400	-0.68625400	5.23315100
N	-1.50837900	1.13570700	2.95394800
C	-2.07669800	0.71608800	1.81261100
H	-1.75491100	-0.25084300	1.44086400
C	-3.03008800	1.45998700	1.12340900
H	-3.45842400	1.07461000	0.20516000
C	-3.40897600	2.69441600	1.64614600

H	-4.15044000	3.30720300	1.14406100
C	-2.82171100	3.13909500	2.82761800
H	-3.10607300	4.09826200	3.24108900
C	-1.86625400	2.33781500	3.46285500
C	-1.18365100	2.74221400	4.71832100
N	-0.26511600	1.87457900	5.20649400
N	-0.26510000	-1.87448600	2.94620500
C	0.38546200	-2.17420000	1.80931300
H	1.10431200	-1.44135900	1.45928000
C	0.16669100	-3.35241600	1.10377400
H	0.71886600	-3.54878300	0.19192300
C	-0.77172500	-4.25370800	1.60190200
H	-0.97486100	-5.18587300	1.08490900
C	-1.45345000	-3.94680800	2.77642600
H	-2.18558400	-4.64065700	3.16867800
C	-1.18363700	-2.74211000	3.43439600
C	-1.86621100	-2.33770900	4.68987500
N	-1.50836200	-1.13557900	5.19875200
C	-2.07666600	-0.71596100	6.34009900
H	-1.75490000	0.25098500	6.71182300
C	-3.03001200	-1.45987800	7.02934000
H	-3.45833500	-1.07449800	7.94759300
C	-3.40887100	-2.69433000	6.50663600
H	-4.15029900	-3.30713600	7.00875400
C	-2.82162300	-3.13900900	5.32515700
H	-3.10596300	-4.09819600	4.91171500
C	0.38548600	2.17428300	6.34336500
H	1.10432600	1.44142400	6.69338200
C	0.16675700	3.35250900	7.04890100
H	0.71896200	3.54887400	7.96073500
C	-0.77166200	4.25381100	6.55079500
H	-0.97476800	5.18598200	7.06779100
C	-1.45342900	3.94691800	5.37629400
H	-2.18556400	4.64077500	4.98406000
C	1.75467700	-1.37904500	6.38060900
H	0.75696700	-1.57507200	6.76002200
C	2.88219700	-1.82770500	7.06189000
H	2.77330900	-2.38375600	7.98597800
C	4.13434100	-1.54203500	6.52209600
H	5.04029900	-1.87664200	7.01685400
C	4.21665800	-0.81786200	5.33497400
H	5.18599300	-0.59557300	4.90748200

[Fe(bpy)₃]²⁺ singlet in dimethyl sulfoxide, applied by SMD

Fe	-0.00890700	0.00000000	4.07637100
N	1.52744300	0.77556500	3.02562700
C	1.43371900	1.58850200	1.95902700

H	0.43372000	1.82243800	1.61631300
C	2.54806500	2.10762100	1.30742200
H	2.41317600	2.75664100	0.44942400
C	3.81545700	1.77550300	1.78076600
H	4.70802100	2.16195600	1.29954500
C	3.92319700	0.93677500	2.88618000
H	4.89883200	0.66722600	3.27108000
C	2.76168400	0.44883600	3.49095700
C	2.76168300	-0.44883600	4.66178400
N	1.52744300	-0.77556500	5.12711400
N	-1.44340000	0.94847100	3.02557400
C	-2.10307100	0.46204300	1.95991600
H	-1.81010900	-0.52277000	1.61854100
C	-3.10712400	1.17090700	1.30786300
H	-3.60510400	0.73008300	0.45152100
C	-3.44675000	2.43714200	1.77908000
H	-4.22606900	3.01938600	1.29823500
C	-2.77023200	2.94927400	2.88238700
H	-3.02143600	3.93023900	3.26629600
C	-1.77017700	2.18382800	3.48827600
C	-0.98885000	2.63035900	4.65786200
N	-0.10466700	1.71419700	5.13308300
N	-0.10466700	-1.71419700	3.01965800
C	0.64227500	-2.03193800	1.94805600
H	1.32903800	-1.27285100	1.59540800
C	0.55024100	-3.26195900	1.30426500
H	1.17613800	-3.46418000	0.44226700
C	-0.34999300	-4.20675600	1.79143400
H	-0.44726000	-5.17832400	1.31793900
C	-1.12910200	-3.88684600	2.89940800
H	-1.83320800	-4.60871800	3.29448900
C	-0.98885000	-2.63035900	3.49487900
C	-1.77017700	-2.18382800	4.66446500
N	-1.44340000	-0.94847100	5.12716700
C	-2.10307100	-0.46204300	6.19282500
H	-1.81010900	0.52277000	6.53420000
C	-3.10712500	-1.17090700	6.84487800
H	-3.60510500	-0.73008300	7.70122000
C	-3.44675000	-2.43714200	6.37366100
H	-4.22606900	-3.01938500	6.85450600
C	-2.77023200	-2.94927300	5.27035400
H	-3.02143600	-3.93023900	4.88644500
C	0.64227500	2.03193800	6.20468500
H	1.32903800	1.27285100	6.55733300
C	0.55024100	3.26195900	6.84847600
H	1.17613800	3.46418000	7.71047400

C	-0.34999300	4.20675600	6.36130700
H	-0.44726000	5.17832400	6.83480200
C	-1.12910200	3.88684600	5.25333300
H	-1.83320800	4.60871800	4.85825200
C	1.43371900	-1.58850200	6.19371400
H	0.43371900	-1.82243800	6.53642800
C	2.54806500	-2.10762100	6.84532000
H	2.41317600	-2.75664100	7.70331700
C	3.81545700	-1.77550300	6.37197500
H	4.70802100	-2.16195600	6.85319600
C	3.92319700	-0.93677500	5.26656100
H	4.89883200	-0.66722700	4.88166100

[Fe(bpy)₃]²⁺ quintet in dimethyl sulfoxide, applied by SMD, <S²> = 6.0181

Fe	0.03672100	0.00005700	4.07629400
N	1.80554700	0.73142000	2.94441700
C	1.73486100	1.52924000	1.86792300
H	0.74092700	1.71686100	1.47494600
C	2.86026900	2.09067300	1.27135300
H	2.75309000	2.72580900	0.39915300
C	4.10734100	1.81845300	1.82965200
H	5.01005900	2.24517100	1.40412000
C	4.18775000	0.99290500	2.94883000
H	5.15049300	0.78731900	3.40001700
C	3.01469200	0.45050200	3.48416300
C	3.01463200	-0.45064900	4.66869200
N	1.80543400	-0.73152400	5.20834100
N	-1.54852300	1.12364500	2.97898300
C	-2.19638200	0.65780800	1.90017000
H	-1.87256700	-0.30750400	1.52531900
C	-3.22856300	1.35514400	1.27856400
H	-3.71914400	0.93512700	0.40746000
C	-3.60667400	2.58700000	1.80817300
H	-4.41216000	3.16041700	1.36061000
C	-2.93785400	3.07850900	2.92627400
H	-3.22803900	4.03114200	3.35116100
C	-1.90157700	2.32566400	3.49009800
C	-1.12689100	2.78101100	4.67309300
N	-0.23800500	1.89438900	5.18098600
N	-0.23795100	-1.89429200	2.97163000
C	0.49280400	-2.23391900	1.89736700
H	1.18436500	-1.48280600	1.53032500
C	0.38291700	-3.47303700	1.27440100
H	0.99386200	-3.70115600	0.40820700
C	-0.52124300	-4.39570200	1.79636300
H	-0.63390100	-5.37692100	1.34625400
C	-1.28358300	-4.04850600	2.90869800

H	-1.98279400	-4.76243400	3.32547000
C	-1.12682300	-2.78092100	3.47953600
C	-1.90142800	-2.32562000	4.66260000
N	-1.54846400	-1.12354100	5.17363900
C	-2.19626800	-0.65774600	6.25250500
H	-1.87253000	0.30761700	6.62729000
C	-3.22829600	-1.35518600	6.87424600
H	-3.71883600	-0.93519700	7.74538600
C	-3.60630300	-2.58711400	6.34473000
H	-4.41166000	-3.16062200	6.79240800
C	-2.93754300	-3.07857800	5.22657500
H	-3.22764200	-4.03127200	4.80176600
C	0.49282400	2.23404600	6.25518700
H	1.18438400	1.48292900	6.62222300
C	0.38300300	3.47319600	6.87810100
H	0.99400300	3.70134300	7.74424900
C	-0.52117000	4.39585500	6.35615100
H	-0.63377700	5.37709900	6.80622000
C	-1.28358700	4.04862600	5.24387800
H	-1.98280400	4.76255200	4.82711000
C	1.73464500	-1.52930800	6.28485300
H	0.74067600	-1.71690100	6.67775300
C	2.85999400	-2.09074400	6.88153500
H	2.75272900	-2.72584500	7.75375000
C	4.10711700	-1.81858100	6.32332400
H	5.00978900	-2.24530900	6.74894100
C	4.18763500	-0.99307100	5.20412600
H	5.15041900	-0.78752300	4.75300800

[Fe(bpy)₃]²⁺ singlet in ethylene glycol, applied by SMD

Fe	-0.00905800	0.00000000	4.07637100
N	1.52362800	0.77153700	3.02371000
C	1.42791700	1.56701800	1.94415400
H	0.42807200	1.80690300	1.60434900
C	2.54133800	2.06056900	1.27211000
H	2.40526100	2.69506100	0.40339800
C	3.80921400	1.72170600	1.73860600
H	4.70137200	2.08749600	1.24054900
C	3.91898400	0.90307800	2.85860700
H	4.89626800	0.63101400	3.23764200
C	2.75853300	0.43954000	3.48394200
C	2.75853300	-0.43954000	4.66879900
N	1.52362800	-0.77153700	5.12903100
N	-1.43960900	0.94953900	3.02764000
C	-2.09648400	0.46740100	1.95830800
H	-1.81233900	-0.52093000	1.61826500
C	-3.08799800	1.18554700	1.29792800

H	-3.58530400	0.74852400	0.43914200
C	-3.41637700	2.45692900	1.76299600
H	-4.18497200	3.04722700	1.27456000
C	-2.74303900	2.96400700	2.87031300
H	-2.98515000	3.94928500	3.24935200
C	-1.75727700	2.18871900	3.48624200
C	-0.98523200	2.62654300	4.66465500
N	-0.10460600	1.70696600	5.13963800
N	-0.10460600	-1.70696600	3.01310300
C	0.62812900	-2.01339100	1.92851000
H	1.31244500	-1.25279700	1.57374100
C	0.52609600	-3.23576500	1.27251500
H	1.14101300	-3.42885400	0.40046700
C	-0.36911600	-4.18465400	1.76028700
H	-0.47387600	-5.15049600	1.27657900
C	-1.13481900	-3.87584200	2.88044600
H	-1.83754400	-4.60019000	3.27369500
C	-0.98523200	-2.62654300	3.48808600
C	-1.75727700	-2.18871900	4.66649900
N	-1.43960900	-0.94953900	5.12510100
C	-2.09648400	-0.46740100	6.19443300
H	-1.81233900	0.52093000	6.53447600
C	-3.08799800	-1.18554700	6.85481300
H	-3.58530400	-0.74852400	7.71359900
C	-3.41637700	-2.45692900	6.38974500
H	-4.18497300	-3.04722600	6.87818100
C	-2.74303900	-2.96400700	5.28242800
H	-2.98515100	-3.94928500	4.90338900
C	0.62812900	2.01339100	6.22423100
H	1.31244500	1.25279700	6.57900000
C	0.52609600	3.23576600	6.88022600
H	1.14101300	3.42885400	7.75227400
C	-0.36911600	4.18465400	6.39245400
H	-0.47387600	5.15049700	6.87616200
C	-1.13481800	3.87584200	5.27229500
H	-1.83754300	4.60019000	4.87904600
C	1.42791700	-1.56701800	6.20858800
H	0.42807200	-1.80690300	6.54839200
C	2.54133800	-2.06057000	6.88063100
H	2.40526100	-2.69506200	7.74934300
C	3.80921400	-1.72170600	6.41413500
H	4.70137100	-2.08749600	6.91219200
C	3.91898400	-0.90307800	5.29413400
H	4.89626800	-0.63101400	4.91509900

[Fe(bpy)₃]²⁺ quintet in ethylene glycol, applied by SMD, <S²> = 6.0193

Fe	0.01788100	0.03826900	4.05902900
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N	1.80000600	0.69191900	2.94551500
C	1.73411300	1.43602200	1.82990000
H	0.73843400	1.66169600	1.46109900
C	2.86662900	1.89539900	1.16563800
H	2.76462800	2.49116500	0.26546800
C	4.11498800	1.56663200	1.68941900
H	5.02514100	1.90570700	1.20475900
C	4.18914100	0.79611500	2.84714800
H	5.15647600	0.54367200	3.26254800
C	3.00854200	0.36402200	3.46018600
C	2.99362100	-0.46201900	4.69691100
N	1.77309100	-0.74595600	5.20791000
N	-1.55342700	1.16949300	2.96335300
C	-2.16187000	0.73122800	1.85081900
H	-1.84745400	-0.23916400	1.47999000
C	-3.14256300	1.46402400	1.18859000
H	-3.60500800	1.06699300	0.29165900
C	-3.50505800	2.70348600	1.71064000
H	-4.26779800	3.30732500	1.22917100
C	-2.87706400	3.16528000	2.86466300
H	-3.15248200	4.12719900	3.27834600
C	-1.89641100	2.37510000	3.47337500
C	-1.17155000	2.79433000	4.70188200
N	-0.27819200	1.90693900	5.19970100
N	-0.22760400	-1.85553100	2.93882000
C	0.44014100	-2.16063200	1.81455900
H	1.13647600	-1.41296700	1.44966300
C	0.26746400	-3.36215500	1.13528200
H	0.83301400	-3.55993800	0.23137400
C	-0.64111000	-4.28503300	1.64814500
H	-0.80723400	-5.23581500	1.15145700
C	-1.34035200	-3.97458200	2.81083300
H	-2.05136300	-4.68465400	3.21380700
C	-1.11610600	-2.74558300	3.44168800
C	-1.82336900	-2.33700600	4.68179800
N	-1.51690400	-1.11087500	5.16801900
C	-2.11711500	-0.68178800	6.28996700
H	-1.83249600	0.30426300	6.64210800
C	-3.05338600	-1.44140500	6.98380900
H	-3.51053000	-1.04865500	7.88530800
C	-3.37665200	-2.70290600	6.48889400
H	-4.10163200	-3.33050900	6.99753700
C	-2.75619400	-3.15622300	5.32830200
H	-2.99868300	-4.13688800	4.93888400
C	0.41523200	2.21770400	6.30632800
H	1.11180200	1.46639700	6.66455200

C	0.26202100	3.42802600	6.97476200
H	0.84580800	3.63460400	7.86488100
C	-0.65393600	4.34775700	6.46943300
H	-0.80578600	5.30451800	6.95922600
C	-1.37898900	4.02978400	5.32376400
H	-2.09252600	4.74053300	4.92616100
C	1.68461700	-1.47438500	6.33057100
H	0.68294600	-1.66834100	6.70092300
C	2.80199700	-1.95934100	7.00454500
H	2.67913800	-2.54002400	7.91210100
C	4.06148000	-1.68097600	6.47892800
H	4.95947300	-2.04513200	6.96801900
C	4.16077000	-0.92640000	5.31257000
H	5.13577400	-0.71071900	4.89386400

[Fe(bpy)₃]²⁺ singlet in methanol, applied by SMD

Fe	-0.00965300	0.00000000	4.07637100
N	1.52558600	0.77361600	3.02451700
C	1.43125400	1.57705700	1.95061800
H	0.43139600	1.81437300	1.60927500
C	2.54521200	2.08283700	1.28813900
H	2.40965700	2.72426000	0.42438700
C	3.81296800	1.74694500	1.75788800
H	4.70555700	2.12265800	1.26797600
C	3.92134300	0.91816900	2.87082800
H	4.89790100	0.64670200	3.25223100
C	2.76022900	0.44359900	3.48692300
C	2.76022900	-0.44359900	4.66581800
N	1.52558600	-0.77361600	5.12822400
N	-1.44215400	0.94955600	3.02634600
C	-2.10046800	0.46537100	1.95866800
H	-1.81384800	-0.52237700	1.61949000
C	-3.09589600	1.18011500	1.30007700
H	-3.59323500	0.74087000	0.44236900
C	-3.42737000	2.45056300	1.76597400
H	-4.19920100	3.03809500	1.27922200
C	-2.75269100	2.96001100	2.87170700
H	-2.99761800	3.94443300	3.25122200
C	-1.76238700	2.18808300	3.48529700
C	-0.98701300	2.62930900	4.66076800
N	-0.10557500	1.71076800	5.13669600
N	-0.10557500	-1.71076800	3.01604500
C	0.63219900	-2.02174400	1.93596400
H	1.31698500	-1.26140800	1.58151400
C	0.53427400	-3.24738500	1.28493400
H	1.15272900	-3.44412900	0.41613200
C	-0.36245600	-4.19499900	1.77325600

H	-0.46446200	-5.16326700	1.29371900
C	-1.13270500	-3.88174500	2.88935800
H	-1.83538300	-4.60531700	3.28413600
C	-0.98701300	-2.62930900	3.49197300
C	-1.76238700	-2.18808300	4.66744400
N	-1.44215400	-0.94955600	5.12639500
C	-2.10046800	-0.46537100	6.19407300
H	-1.81384800	0.52237700	6.53325100
C	-3.09589600	-1.18011500	6.85266400
H	-3.59323500	-0.74087000	7.71037200
C	-3.42737000	-2.45056200	6.38676700
H	-4.19920200	-3.03809500	6.87351900
C	-2.75269200	-2.96001100	5.28103400
H	-2.99761800	-3.94443300	4.90151900
C	0.63219900	2.02174400	6.21677700
H	1.31698500	1.26140800	6.57122700
C	0.53427400	3.24738500	6.86780700
H	1.15272900	3.44412900	7.73660900
C	-0.36245600	4.19499900	6.37948500
H	-0.46446200	5.16326700	6.85902200
C	-1.13270500	3.88174500	5.26338300
H	-1.83538300	4.60531700	4.86860500
C	1.43125400	-1.57705700	6.20212300
H	0.43139600	-1.81437300	6.54346600
C	2.54521100	-2.08283700	6.86460200
H	2.40965700	-2.72426000	7.72835400
C	3.81296700	-1.74694500	6.39485300
H	4.70555700	-2.12265800	6.88476500
C	3.92134300	-0.91816900	5.28191300
H	4.89790100	-0.64670300	4.90051000

[Fe(bpy)₃]²⁺ quintet in methanol, applied by SMD, <S²> = 6.0182

Fe	0.02936600	0.00007000	4.07627500
N	1.79898200	0.72057800	2.93644200
C	1.72980700	1.50436200	1.84935600
H	0.73650500	1.68713800	1.45189600
C	2.85557800	2.05812500	1.24676500
H	2.74915600	2.68138600	0.36579100
C	4.10184900	1.79467400	1.81117300
H	5.00505800	2.21735600	1.38232800
C	4.18091800	0.98287400	2.94055500
H	5.14316000	0.78506500	3.39654200
C	3.00773700	0.44475100	3.47991400
C	3.00768700	-0.44493500	4.67287700
N	1.79888200	-0.72079000	5.21622000
N	-1.53662000	1.12356300	2.95202900
C	-2.14338200	0.67304800	1.84292100

H	-1.84022400	-0.30832600	1.49287500
C	-3.10888500	1.40539500	1.15802600
H	-3.56882500	0.99511300	0.26565600
C	-3.45737400	2.66137000	1.64985100
H	-4.20584000	3.26679200	1.14833800
C	-2.83202400	3.13653600	2.79967100
H	-3.09431000	4.11166700	3.19048700
C	-1.86946500	2.34342500	3.43463800
C	-1.15239700	2.77529100	4.66223600
N	-0.25896300	1.89461300	5.17286100
N	-0.25885200	-1.89452900	2.97977000
C	0.42723700	-2.21711000	1.87109100
H	1.12607400	-1.47224100	1.50427400
C	0.26448400	-3.43130100	1.21222500
H	0.84195500	-3.64659800	0.31998900
C	-0.65227200	-4.34401300	1.72984300
H	-0.81186400	-5.30329700	1.24741300
C	-1.36807000	-4.01445800	2.87788300
H	-2.08342200	-4.71797400	3.28487600
C	-1.15226100	-2.77520600	3.49044400
C	-1.86925600	-2.34335300	4.71808400
N	-1.53648000	-1.12344400	5.20063300
C	-2.14319900	-0.67295400	6.30977900
H	-1.84010100	0.30845300	6.65977900
C	-3.10858800	-1.40536100	6.99476700
H	-3.56849600	-0.99508900	7.88715800
C	-3.45700300	-2.66138300	6.50300900
H	-4.20537300	-3.26686000	7.00460000
C	-2.83169500	-3.13652800	5.35316000
H	-3.09392000	-4.11170000	4.96240400
C	0.42721600	2.21719300	6.28148200
H	1.12605700	1.47231100	6.64826300
C	0.26452700	3.43139800	6.94034100
H	0.84206300	3.64670400	7.83253200
C	-0.65226400	4.34410800	6.42278000
H	-0.81181300	5.30339800	6.90521300
C	-1.36815400	4.01454900	5.27479600
H	-2.08352900	4.71806700	4.86784500
C	1.72962600	-1.50454100	6.30332100
H	0.73629000	-1.68735800	6.70067700
C	2.85535700	-2.05822700	6.90606100
H	2.74886500	-2.68145600	7.78705100
C	4.10167900	-1.79476100	6.34177300
H	5.00485800	-2.21739500	6.77072800
C	4.18083400	-0.98300400	5.21236600
H	5.14311500	-0.78518000	4.75646800

[Fe(bpy)₃]²⁺ singlet in acetonitrile, applied by SMD

Fe	-0.00957700	0.00000000	4.07637100
N	1.52817700	0.77664600	3.02588100
C	1.43528600	1.59402400	1.96241200
H	0.43544600	1.82596800	1.61793900
C	2.54983400	2.12152700	1.31765400
H	2.41527900	2.77498900	0.46298100
C	3.81711700	1.79137400	1.79323100
H	4.70982900	2.18432100	1.31759600
C	3.92403100	0.94580000	2.89369300
H	4.89922500	0.67583400	3.27940500
C	2.76221500	0.45104300	3.49260900
C	2.76221500	-0.45104300	4.66013200
N	1.52817700	-0.77664600	5.12686000
N	-1.44420200	0.94783200	3.02362000
C	-2.10297100	0.46034500	1.95774700
H	-1.80985500	-0.52510800	1.61856600
C	-3.10603600	1.16855300	1.30325400
H	-3.60272900	0.72642500	0.44683400
C	-3.44559400	2.43578800	1.77230100
H	-4.22389800	3.01769300	1.28941700
C	-2.77006100	2.94914700	2.87588200
H	-3.02100000	3.93092300	3.25791600
C	-1.77107600	2.18399300	3.48433900
C	-0.99051200	2.63176400	4.65421900
N	-0.10617700	1.71631100	5.13079500
N	-0.10617700	-1.71631100	3.02194600
C	0.64079700	-2.03575900	1.95070200
H	1.32771600	-1.27696800	1.59760700
C	0.54861400	-3.26667600	1.30833400
H	1.17423800	-3.47032600	0.44647000
C	-0.35226700	-4.21067700	1.79658500
H	-0.45001400	-5.18280000	1.32434300
C	-1.13114300	-3.88900200	2.90444700
H	-1.83547900	-4.60988400	3.30089600
C	-0.99051300	-2.63176400	3.49852200
C	-1.77107600	-2.18399300	4.66840200
N	-1.44420300	-0.94783200	5.12912100
C	-2.10297100	-0.46034500	6.19499400
H	-1.80985500	0.52510800	6.53417500
C	-3.10603600	-1.16855200	6.84948700
H	-3.60272900	-0.72642500	7.70590700
C	-3.44559500	-2.43578800	6.38044000
H	-4.22389900	-3.01769300	6.86332400
C	-2.77006200	-2.94914700	5.27685900
H	-3.02100100	-3.93092200	4.89482500

C	0.64079700	2.03575900	6.20203900
H	1.32771600	1.27696800	6.55513400
C	0.54861400	3.26667600	6.84440700
H	1.17423800	3.47032600	7.70627100
C	-0.35226700	4.21067700	6.35615600
H	-0.45001400	5.18280000	6.82839800
C	-1.13114200	3.88900200	5.24829400
H	-1.83547900	4.60988400	4.85184500
C	1.43528600	-1.59402400	6.19032900
H	0.43544600	-1.82596800	6.53480200
C	2.54983400	-2.12152700	6.83508700
H	2.41527900	-2.77498900	7.68976000
C	3.81711700	-1.79137400	6.35951000
H	4.70982900	-2.18432200	6.83514500
C	3.92403100	-0.94580000	5.25904800
H	4.89922500	-0.67583400	4.87333600

[Fe(bpy)₃]²⁺ quintet in acetonitrile, applied by SMD, <S²> = 6.0179

Fe	0.03732100	0.00000100	4.07636700
N	1.80918500	0.73199400	2.94371900
C	1.73985000	1.53184200	1.86835400
H	0.74656800	1.71899800	1.47370700
C	2.86550000	2.09685100	1.27526600
H	2.75872000	2.73406500	0.40453000
C	4.11215900	1.82533500	1.83520900
H	5.01501500	2.25461900	1.41258300
C	4.19141200	0.99646300	2.95218300
H	5.15346600	0.79088400	3.40478500
C	3.01805100	0.45154400	3.48475500
C	3.01804400	-0.45155700	4.66800800
N	1.80917200	-0.73199900	5.20903400
N	-1.54665000	1.12451200	2.97326300
C	-2.18871700	0.65958700	1.89044400
H	-1.86620500	-0.30773900	1.51990500
C	-3.21335200	1.35988600	1.25952900
H	-3.69878200	0.93966500	0.38564000
C	-3.58965400	2.59490400	1.78337500
H	-4.38852500	3.17136100	1.32794700
C	-2.92731600	3.08533800	2.90601400
H	-3.21567400	4.04052700	3.32629900
C	-1.89929400	2.32859900	3.48010900
C	-1.13291900	2.78234900	4.66942100
N	-0.24349200	1.89711300	5.17915200
N	-0.24349300	-1.89710900	2.97358100
C	0.48056200	-2.23623900	1.89438300
H	1.17337200	-1.48666700	1.52658400
C	0.36268500	-3.47269600	1.26739800

H	0.96819500	-3.70016800	0.39722500
C	-0.54320200	-4.39345900	1.79030400
H	-0.66282300	-5.37224200	1.33670900
C	-1.29813400	-4.04709800	2.90815800
H	-1.99850300	-4.75934800	3.32579600
C	-1.13292300	-2.78234200	3.48330900
C	-1.89930100	-2.32859100	4.67261900
N	-1.54665800	-1.12450400	5.17946500
C	-2.18872600	-0.65957800	6.26228200
H	-1.86621500	0.30774800	6.63282000
C	-3.21336200	-1.35987700	6.89319600
H	-3.69879300	-0.93965700	7.76708500
C	-3.58966200	-2.59489700	6.36935200
H	-4.38853400	-3.17135400	6.82477900
C	-2.92732300	-3.08533100	5.24671300
H	-3.21568000	-4.04052000	4.82642900
C	0.48056100	2.23624200	6.25835200
H	1.17336800	1.48666800	6.62615300
C	0.36268500	3.47270000	6.88533600
H	0.96819300	3.70017000	7.75551000
C	-0.54319800	4.39346400	6.36242700
H	-0.66281900	5.37224700	6.81602100
C	-1.29812800	4.04710500	5.24457100
H	-1.99849500	4.75935500	4.82693000
C	1.73982300	-1.53184700	6.28439900
H	0.74653700	-1.71899700	6.67903800
C	2.86546600	-2.09686100	6.87749700
H	2.75867500	-2.73407300	7.74823200
C	4.11213100	-1.82535200	6.31756300
H	5.01498000	-2.25464100	6.74019800
C	4.19139700	-0.99648200	5.20059000
H	5.15345700	-0.79090900	4.74799600

[Fe(bpy)₃]²⁺ singlet in ethanol, applied by SMD

Fe	-0.01045000	0.00000000	4.07637100
N	1.52525500	0.77446200	3.02503300
C	1.43118700	1.58031600	1.95293700
H	0.43126100	1.81698400	1.61139300
C	2.54520800	2.08935300	1.29302900
H	2.40985800	2.73277600	0.43075300
C	3.81290000	1.75399200	1.76336600
H	4.70550500	2.13223700	1.27547400
C	3.92103000	0.92244600	2.87426900
H	4.89745600	0.65105000	3.25604200
C	2.75982700	0.44483400	3.48785200
C	2.75982700	-0.44483400	4.66488900
N	1.52525500	-0.77446200	5.12770800

N	-1.44335000	0.94994800	3.02670700
C	-2.10332300	0.46487600	1.96047500
H	-1.81643300	-0.52289600	1.62168500
C	-3.10049400	1.17852900	1.30333600
H	-3.59906600	0.73851100	0.44675200
C	-3.43226800	2.44878300	1.76952200
H	-4.20569100	3.03531200	1.28413100
C	-2.75591700	2.95920500	2.87381100
H	-3.00155400	3.94331100	3.25365400
C	-1.76356400	2.18848300	3.48570900
C	-0.98595600	2.63073100	4.65944100
N	-0.10589900	1.71138600	5.13647100
N	-0.10589900	-1.71138600	3.01627000
C	0.63345100	-2.02310800	1.93747700
H	1.31698200	-1.26194300	1.58238000
C	0.53873400	-3.25034200	1.28893800
H	1.15825800	-3.44775000	0.42106500
C	-0.35610600	-4.19898400	1.77876400
H	-0.45527600	-5.16867400	1.30156000
C	-1.12801100	-3.88496600	2.89351800
H	-1.82877900	-4.60958400	3.28976600
C	-0.98595600	-2.63073000	3.49330000
C	-1.76356400	-2.18848300	4.66703200
N	-1.44335000	-0.94994800	5.12603400
C	-2.10332300	-0.46487500	6.19226600
H	-1.81643200	0.52289600	6.53105600
C	-3.10049500	-1.17852900	6.84940500
H	-3.59906600	-0.73851100	7.70598900
C	-3.43226800	-2.44878300	6.38321900
H	-4.20569200	-3.03531200	6.86861000
C	-2.75591700	-2.95920500	5.27893000
H	-3.00155400	-3.94331100	4.89908700
C	0.63345100	2.02310800	6.21526400
H	1.31698200	1.26194300	6.57036200
C	0.53873400	3.25034200	6.86380300
H	1.15825800	3.44775000	7.73167600
C	-0.35610600	4.19898400	6.37397700
H	-0.45527600	5.16867400	6.85118100
C	-1.12801100	3.88496600	5.25922300
H	-1.82877800	4.60958400	4.86297500
C	1.43118700	-1.58031600	6.19980400
H	0.43126100	-1.81698400	6.54134800
C	2.54520800	-2.08935300	6.85971200
H	2.40985800	-2.73277600	7.72198800
C	3.81290000	-1.75399200	6.38937500
H	4.70550500	-2.13223700	6.87726700

C	3.92103000	-0.92244700	5.27847200
H	4.89745600	-0.65105000	4.89669900

[Fe(bpy)₃]²⁺ quintet in ethanol, applied by SMD, <S²> = 6.0186

Fe	0.03105600	-0.03917000	4.10786600
N	1.77133100	0.76866900	2.93984500
C	1.66911600	1.55978100	1.86135800
H	0.66471000	1.74403100	1.49386700
C	2.77543600	2.12206400	1.23021500
H	2.64075100	2.75025600	0.35657400
C	4.03882800	1.86260700	1.75699700
H	4.92732100	2.29280000	1.30556600
C	4.15281700	1.04379600	2.87810000
H	5.12799700	0.84628800	3.30585800
C	2.99698400	0.49578800	3.44445200
C	3.03218400	-0.40763000	4.62481000
N	1.83649300	-0.70856000	5.18409200
N	-1.52233500	1.09593600	3.00290300
C	-2.13816700	0.65011700	1.89607400
H	-1.85066900	-0.33782800	1.55136500
C	-3.09234700	1.39510600	1.21017200
H	-3.56106000	0.98918700	0.32045800
C	-3.41736700	2.65936900	1.69747000
H	-4.15523200	3.27604300	1.19395000
C	-2.78233900	3.12903200	2.84394600
H	-3.02623200	4.11129800	3.22849200
C	-1.83275000	2.32336600	3.48334200
C	-1.10876500	2.74909200	4.70865100
N	-0.21001400	1.86727000	5.20766400
N	-0.26343000	-1.93334200	3.00133500
C	0.47860300	-2.29576100	1.94257700
H	1.17226800	-1.55156700	1.56442800
C	0.37742600	-3.54905400	1.34658600
H	0.99704200	-3.79542600	0.49145200
C	-0.52961500	-4.46193100	1.88068400
H	-0.63459900	-5.45398300	1.45270200
C	-1.30368900	-4.09164300	2.97789200
H	-2.00189600	-4.79919000	3.40763200
C	-1.15556100	-2.81055800	3.51951300
C	-1.94273600	-2.33251700	4.68635400
N	-1.56075100	-1.14681200	5.21454400
C	-2.21599900	-0.66475200	6.28166000
H	-1.86723600	0.28620400	6.67108000
C	-3.28649400	-1.32894900	6.87392000
H	-3.78188900	-0.89836400	7.73723500
C	-3.69817400	-2.54046200	6.32282100
H	-4.53707700	-3.08531700	6.74428300

C	-3.02121200	-3.04865700	5.21667300
H	-3.33910800	-3.98381000	4.77287700
C	0.47814500	2.18775100	6.31535300
H	1.18345000	1.44531700	6.67456400
C	0.31336900	3.39687000	6.98355500
H	0.89429600	3.60808800	7.87462700
C	-0.60857700	4.31024800	6.47660700
H	-0.76982400	5.26563200	6.96610200
C	-1.32727100	3.98436200	5.32970300
H	-2.04814400	4.68684800	4.93075000
C	1.79308800	-1.51488900	6.25697800
H	0.80817100	-1.71752100	6.66575900
C	2.93474600	-2.06759800	6.82870100
H	2.85030100	-2.71137900	7.69712500
C	4.16865400	-1.77471800	6.25123700
H	5.08376200	-2.19358600	6.65788700
C	4.21990700	-0.93927600	5.13778400
H	5.17230600	-0.71896700	4.67153600

[Fe(bpy)₃]²⁺ singlet in propionitrile, applied by SMD

Fe	-0.01001900	0.00000000	4.07637100
N	1.52807300	0.77731000	3.02626500
C	1.43533700	1.59639900	1.96409900
H	0.43544400	1.82811400	1.61963600
C	2.54990000	2.12595900	1.32102600
H	2.41545800	2.78093200	0.46748900
C	3.81714100	1.79565500	1.79661800
H	4.70985700	2.19000400	1.32215100
C	3.92392200	0.94809500	2.89556200
H	4.89908000	0.67757500	3.28098800
C	2.76206200	0.45173800	3.49312700
C	2.76206200	-0.45173800	4.65961400
N	1.52807300	-0.77731000	5.12647600
N	-1.44503700	0.94816200	3.02394300
C	-2.10486500	0.46017500	1.95897200
H	-1.81129700	-0.52510200	1.61973500
C	-3.10939300	1.16750400	1.30575400
H	-3.60683000	0.72492300	0.44999100
C	-3.44952400	2.43435800	1.77539900
H	-4.22914500	3.01546400	1.29368000
C	-2.77288300	2.94830900	2.87805000
H	-3.02454000	3.92971000	3.26057100
C	-1.77219300	2.18413400	3.48501300
C	-0.98995900	2.63266500	4.65356600
N	-0.10626900	1.71681500	5.13064500
N	-0.10626900	-1.71681500	3.02209600
C	0.64215900	-2.03697200	1.95208200

H	1.32848800	-1.27776100	1.59874300
C	0.55219300	-3.26897900	1.31145100
H	1.17885600	-3.47322100	0.45047600
C	-0.34779500	-4.21348200	1.80040200
H	-0.44361600	-5.18656500	1.32974500
C	-1.12813800	-3.89111300	2.90704000
H	-1.83147800	-4.61256000	3.30426100
C	-0.98995900	-2.63266500	3.49917500
C	-1.77219300	-2.18413400	4.66772800
N	-1.44503700	-0.94816200	5.12879800
C	-2.10486500	-0.46017500	6.19376900
H	-1.81129700	0.52510200	6.53300600
C	-3.10939300	-1.16750400	6.84698700
H	-3.60683000	-0.72492300	7.70275000
C	-3.44952400	-2.43435800	6.37734200
H	-4.22914600	-3.01546400	6.85906100
C	-2.77288300	-2.94830800	5.27469100
H	-3.02454000	-3.92971000	4.89217000
C	0.64215900	2.03697100	6.20065900
H	1.32848800	1.27776100	6.55399800
C	0.55219300	3.26897900	6.84129000
H	1.17885600	3.47322100	7.70226500
C	-0.34779500	4.21348200	6.35233900
H	-0.44361600	5.18656500	6.82299600
C	-1.12813800	3.89111300	5.24570100
H	-1.83147800	4.61256000	4.84848000
C	1.43533600	-1.59639900	6.18864200
H	0.43544400	-1.82811400	6.53310500
C	2.54990000	-2.12595900	6.83171500
H	2.41545800	-2.78093200	7.68525200
C	3.81714100	-1.79565500	6.35612400
H	4.70985700	-2.19000400	6.83059000
C	3.92392200	-0.94809500	5.25717900
H	4.89908000	-0.67757500	4.87175300

[Fe(bpy)₃]²⁺ quintet in propionitrile, applied by SMD, <S²> = 6.0177

Fe	0.03787100	0.00014700	4.07622800
N	1.81041700	0.73273400	2.94407000
C	1.74154200	1.53449500	1.87007000
H	0.74846400	1.72213400	1.47522700
C	2.86730900	2.10090400	1.27849400
H	2.76074800	2.73961400	0.40882600
C	4.11379200	1.82882300	1.83852300
H	5.01672000	2.25906500	1.41702900
C	4.19263400	0.99816500	2.95418200
H	5.15449400	0.79231900	3.40709100
C	3.01915900	0.45212200	3.48541100

C	3.01903400	-0.45248400	4.66754800
N	1.81018800	-0.73297600	5.20871300
N	-1.54764500	1.12492100	2.97393300
C	-2.19230300	0.65877000	1.89321300
H	-1.86893000	-0.30784700	1.52163800
C	-3.22064800	1.35679300	1.26578300
H	-3.70797400	0.93553800	0.39344000
C	-3.59813900	2.59079300	1.79114200
H	-4.39994900	3.16537700	1.33852200
C	-2.93317500	3.08255300	2.91167000
H	-3.22258900	4.03687700	3.33322100
C	-1.90140300	2.32811100	3.48212800
C	-1.13205800	2.78330400	4.66906500
N	-0.24255000	1.89805300	5.17871700
N	-0.24238800	-1.89780000	2.97377800
C	0.48385900	-2.23819000	1.89643300
H	1.17669100	-1.48864900	1.52865500
C	0.36824300	-3.47581100	1.27129400
H	0.97541400	-3.70419900	0.40251400
C	-0.53756300	-4.39661900	1.79425400
H	-0.65532900	-5.37635000	1.34222300
C	-1.29470000	-4.04903900	2.91024000
H	-1.99488900	-4.76132600	3.32814700
C	-1.13186700	-2.78307500	3.48344100
C	-1.90103500	-2.32800600	4.67053400
N	-1.54747600	-1.12469300	5.17858800
C	-2.19201300	-0.65865600	6.25943400
H	-1.86881300	0.30806800	6.63088200
C	-3.22002000	-1.35691900	6.88714500
H	-3.70725800	-0.93574300	7.75957600
C	-3.59728100	-2.59106600	6.36196300
H	-4.39880800	-3.16585800	6.81482300
C	-2.93245000	-3.08270300	5.24130700
H	-3.22167800	-4.03714900	4.81990400
C	0.48385600	2.23852400	6.25592600
H	1.17668200	1.48897900	6.62371000
C	0.36838000	3.47622800	6.88093200
H	0.97566900	3.70469100	7.74961000
C	-0.53745000	4.39701500	6.35797800
H	-0.65510700	5.37680600	6.80990400
C	-1.29475400	4.04934200	5.24213100
H	-1.99496100	4.76161100	4.82422000
C	1.74110400	-1.53465100	6.28275900
H	0.74795400	-1.72220200	6.67746500
C	2.86674600	-2.10109200	6.87454900
H	2.76001000	-2.73971900	7.74425700

C	4.11333100	-1.82916300	6.31467400
H	5.01616400	-2.25944900	6.73632500
C	4.19239500	-0.99859300	5.19896500
H	5.15433500	-0.79285000	4.74617900

[Fe(bpy)₃]²⁺ singlet in 2-propanol, applied by SMD

Fe	-0.01125400	0.00000000	4.07637100
N	1.52459600	0.77504800	3.02545800
C	1.43058700	1.58189500	1.95412500
H	0.43056200	1.81857700	1.61285100
C	2.54457800	2.09175700	1.29481600
H	2.40932100	2.73595000	0.43309700
C	3.81225700	1.75606900	1.76491400
H	4.70483800	2.13482400	1.27736900
C	3.92035100	0.92355600	2.87508700
H	4.89683300	0.65191200	3.25656200
C	2.75916400	0.44524300	3.48815100
C	2.75916400	-0.44524300	4.66459000
N	1.52459600	-0.77504800	5.12728400
N	-1.44441100	0.95056200	3.02752500
C	-2.10627400	0.46490800	1.96275300
H	-1.81986900	-0.52314800	1.62433900
C	-3.10460600	1.17811000	1.30692400
H	-3.60474100	0.73761100	0.45148700
C	-3.43577800	2.44847700	1.77317200
H	-4.21030100	3.03454100	1.28897800
C	-2.75757200	2.95948400	2.87605700
H	-3.00328700	3.94351300	3.25607300
C	-1.76386200	2.18932100	3.48649400
C	-0.98432000	2.63192500	4.65888900
N	-0.10600100	1.71140000	5.13692300
N	-0.10600100	-1.71140000	3.01581800
C	0.63418000	-2.02300500	1.93756300
H	1.31623000	-1.26082300	1.58173700
C	0.54231600	-3.25135200	1.29073300
H	1.16233300	-3.44873400	0.42319800
C	-0.35014300	-4.20144900	1.78204000
H	-0.44670100	-5.17221900	1.30650500
C	-1.12300900	-3.88753300	2.89614600
H	-1.82164400	-4.61354200	3.29365800
C	-0.98432000	-2.63192500	3.49385200
C	-1.76386200	-2.18932100	4.66624700
N	-1.44441100	-0.95056200	5.12521600
C	-2.10627400	-0.46490800	6.18998800
H	-1.81986900	0.52314800	6.52840200
C	-3.10460600	-1.17811000	6.84581700
H	-3.60474100	-0.73761100	7.70125400

C	-3.43577800	-2.44847600	6.37956800
H	-4.21030100	-3.03454100	6.86376300
C	-2.75757200	-2.95948400	5.27668400
H	-3.00328700	-3.94351200	4.89666800
C	0.63418000	2.02300500	6.21517800
H	1.31623000	1.26082200	6.57100400
C	0.54231600	3.25135200	6.86200800
H	1.16233300	3.44873400	7.72954300
C	-0.35014300	4.20144900	6.37070100
H	-0.44670000	5.17221900	6.84623600
C	-1.12300900	3.88753300	5.25659500
H	-1.82164400	4.61354300	4.85908300
C	1.43058700	-1.58189500	6.19861600
H	0.43056200	-1.81857700	6.53989000
C	2.54457800	-2.09175700	6.85792500
H	2.40932100	-2.73595000	7.71964400
C	3.81225700	-1.75606900	6.38782700
H	4.70483700	-2.13482400	6.87537200
C	3.92035100	-0.92355600	5.27765400
H	4.89683300	-0.65191200	4.89617900

[Fe(bpy)₃]²⁺ quintet in 2-propanol, applied by SMD, <S²> = 6.0179

Fe	0.02939200	0.00000000	4.07637000
N	1.79901400	0.72140000	2.93629600
C	1.73047400	1.50959900	1.85233700
H	0.73751900	1.69190200	1.45385400
C	2.85606400	2.06873800	1.25438000
H	2.74998200	2.69553200	0.37589000
C	4.10187200	1.80583300	1.82001300
H	5.00485900	2.23243700	1.39465900
C	4.18044500	0.98961700	2.94620200
H	5.14218500	0.79235500	3.40356300
C	3.00744100	0.44684400	3.48133500
C	3.00743800	-0.44685000	4.67141100
N	1.79901100	-0.72140300	5.21644800
N	-1.53718300	1.12368600	2.95170000
C	-2.14765800	0.67103500	1.84554400
H	-1.84435100	-0.31043200	1.49584300
C	-3.11682000	1.40110300	1.16339100
H	-3.57967400	0.98906200	0.27334700
C	-3.46512100	2.65722200	1.65488400
H	-4.21618300	3.26095900	1.15526900
C	-2.83634800	3.13440500	2.80198000
H	-3.09851900	4.10963100	3.19260900
C	-1.87065200	2.34323000	3.43462300
C	-1.15058600	2.77716700	4.65994400
N	-0.25668500	1.89694400	5.17080100

N	-0.25668700	-1.89694300	2.98193900
C	0.43267400	-2.22217400	1.87606500
H	1.13239700	-1.47796400	1.50958200
C	0.27218300	-3.43800700	1.21966600
H	0.85210300	-3.65548000	0.32955900
C	-0.64564400	-4.34979600	1.73694500
H	-0.80357400	-5.31020200	1.25623000
C	-1.36441500	-4.01785600	2.88241600
H	-2.08045700	-4.72079500	3.28922300
C	-1.15059000	-2.77716400	3.49279500
C	-1.87065600	-2.34322700	4.71811500
N	-1.53718500	-1.12368300	5.20103900
C	-2.14766000	-0.67103200	6.30719500
H	-1.84435200	0.31043500	6.65689600
C	-3.11682300	-1.40109800	6.98934700
H	-3.57967700	-0.98905700	7.87939100
C	-3.46512500	-2.65721700	6.49785400
H	-4.21618800	-3.26095300	6.99746900
C	-2.83635200	-3.13440000	5.35075800
H	-3.09852500	-4.10962600	4.96012900
C	0.43267600	2.22217400	6.27667500
H	1.13239800	1.47796400	6.64315800
C	0.27218700	3.43800900	6.93307300
H	0.85210600	3.65548000	7.82318000
C	-0.64563900	4.34979900	6.41579400
H	-0.80356700	5.31020600	6.89650700
C	-1.36440900	4.01786000	5.27032200
H	-2.08045000	4.72079900	4.86351400
C	1.73046700	-1.50960100	6.30040700
H	0.73751000	-1.69190100	6.69888900
C	2.85605400	-2.06874400	6.89836600
H	2.74997000	-2.69553700	7.77685500
C	4.10186300	-1.80584200	6.33273500
H	5.00484900	-2.23244800	6.75808900
C	4.18044000	-0.98962600	5.20654500
H	5.14218200	-0.79236700	4.74918500

[Fe(bpy)₃]²⁺ singlet in butyronitrile, applied by SMD

Fe	-0.01053400	0.00000000	4.07637100
N	1.52768600	0.77773500	3.02654600
C	1.43501400	1.59762500	1.96499600
H	0.43505600	1.82932300	1.62070900
C	2.54956700	2.12794800	1.32253500
H	2.41520600	2.78362100	0.46953200
C	3.81680200	1.79733000	1.79792700
H	4.70950000	2.19211100	1.32381200
C	3.92352700	0.94888100	2.89618700

H	4.89867900	0.67788600	3.28129300
C	2.76166000	0.45201200	3.49332800
C	2.76166000	-0.45201200	4.65941300
N	1.52768600	-0.77773500	5.12619500
N	-1.44570600	0.94856400	3.02440800
C	-2.10653600	0.46025200	1.96022400
H	-1.81301000	-0.52508700	1.62113800
C	-3.11187700	1.16719500	1.30785200
H	-3.61010900	0.72433400	0.45270200
C	-3.45191400	2.43398700	1.77772100
H	-4.23229500	3.01470700	1.29679100
C	-2.77425600	2.94829300	2.87959500
H	-3.02610400	3.92954700	3.26235800
C	-1.77259900	2.18457800	3.48557500
C	-0.98912900	2.63340600	4.65323700
N	-0.10639800	1.71690600	5.13088800
N	-0.10639800	-1.71690600	3.02185300
C	0.64273600	-2.03714100	1.95235600
H	1.32822500	-1.27734200	1.59863700
C	0.55460900	-3.26989900	1.31290900
H	1.18172700	-3.47424100	0.45229800
C	-0.34406800	-4.21521500	1.80271200
H	-0.43822100	-5.18900400	1.33321100
C	-1.12518400	-3.89275500	2.90878000
H	-1.82732200	-4.61494100	3.30680000
C	-0.98912900	-2.63340600	3.49950400
C	-1.77259900	-2.18457800	4.66716600
N	-1.44570600	-0.94856400	5.12833300
C	-2.10653600	-0.46025200	6.19251700
H	-1.81301000	0.52508700	6.53160300
C	-3.11187700	-1.16719400	6.84488900
H	-3.61010900	-0.72433400	7.70003900
C	-3.45191500	-2.43398700	6.37502000
H	-4.23229500	-3.01470700	6.85595000
C	-2.77425600	-2.94829300	5.27314600
H	-3.02610400	-3.92954700	4.89038300
C	0.64273600	2.03714100	6.20038500
H	1.32822500	1.27734200	6.55410400
C	0.55460900	3.26989900	6.83983200
H	1.18172800	3.47424100	7.70044300
C	-0.34406700	4.21521500	6.35002900
H	-0.43822100	5.18900400	6.81953000
C	-1.12518300	3.89275500	5.24396100
H	-1.82732200	4.61494100	4.84594100
C	1.43501400	-1.59762500	6.18774500
H	0.43505500	-1.82932300	6.53203200

C	2.54956700	-2.12794800	6.83020600
H	2.41520500	-2.78362100	7.68320900
C	3.81680200	-1.79733000	6.35481400
H	4.70950000	-2.19211100	6.82892900
C	3.92352700	-0.94888100	5.25655400
H	4.89867900	-0.67788700	4.87144800

[Fe(bpy)₃]²⁺ quintet in butyronitrile, applied by SMD, <S²> = 6.0176

Fe	0.03788600	-0.00000200	4.07637100
N	1.81046100	0.73318400	2.94410000
C	1.74177300	1.53588200	1.87076700
H	0.74876400	1.72375400	1.47590400
C	2.86751400	2.10302800	1.27985500
H	2.76100600	2.74242900	0.41070000
C	4.11394500	1.83082000	1.83991200
H	5.01684200	2.26160500	1.41894200
C	4.19265300	0.99937300	2.95497500
H	5.15443300	0.79356600	3.40808500
C	3.01919900	0.45266300	3.48558200
C	3.01919500	-0.45267000	4.66717500
N	1.81045300	-0.73318600	5.20865200
N	-1.54782300	1.12510600	2.97394900
C	-2.19352800	0.65858700	1.89402300
H	-1.87009400	-0.30790900	1.52221100
C	-3.22300700	1.35596500	1.26774600
H	-3.71111600	0.93437400	0.39601000
C	-3.60061600	2.58974600	1.79350000
H	-4.40329400	3.16380800	1.34178300
C	-2.93465300	3.08188400	2.91327100
H	-3.22427000	4.03599700	3.33516400
C	-1.90177200	2.32806600	3.48258100
C	-1.13141400	2.78363000	4.66878200
N	-0.24226000	1.89813700	5.17872300
N	-0.24226300	-1.89813800	2.97401700
C	0.48481400	-2.23901000	1.89737000
H	1.17742500	-1.48934200	1.52943500
C	0.37039500	-3.47721200	1.27317700
H	0.97814500	-3.70595400	0.40490400
C	-0.53497300	-4.39824600	1.79648400
H	-0.65171400	-5.37847800	1.34530400
C	-1.29291600	-4.05022700	2.91178200
H	-1.99266400	-4.76272500	3.33006900
C	-1.13142200	-2.78362900	3.48395400
C	-1.90178700	-2.32806100	4.67014900
N	-1.54783100	-1.12510500	5.17878700
C	-2.19354100	-0.65858300	6.25870800
H	-1.87010200	0.30791000	6.63052500

C	-3.22303100	-1.35595300	6.88497600
H	-3.71114400	-0.93436000	7.75670900
C	-3.60064700	-2.58973000	6.35921600
H	-4.40333400	-3.16378600	6.81092500
C	-2.93467900	-3.08187100	5.23944900
H	-3.22430000	-4.03598100	4.81755100
C	0.48481100	2.23900600	6.25537500
H	1.17741800	1.48933600	6.62331300
C	0.37039000	3.47720700	6.87957000
H	0.97813400	3.70594600	7.74784700
C	-0.53497300	4.39824300	6.35626000
H	-0.65171600	5.37847500	6.80744000
C	-1.29291000	4.05022700	5.24095600
H	-1.99265500	4.76272700	4.82266600
C	1.74175700	-1.53588400	6.28198400
H	0.74874600	-1.72375200	6.67684200
C	2.86749300	-2.10303500	6.87290000
H	2.76097900	-2.74243600	7.74205500
C	4.11392800	-1.83083000	6.31285000
H	5.01682100	-2.26161900	6.73382300
C	4.19264500	-0.99938400	5.19778700
H	5.15442700	-0.79358000	4.74468200

[Fe(bpy)₃]²⁺ singlet in 1-butanol, applied by SMD

Fe	-0.01149300	0.00000000	4.07637100
N	1.52414900	0.77493000	3.02545600
C	1.43004200	1.58097800	1.95353500
H	0.42997500	1.81795200	1.61256900
C	2.54396000	2.08952700	1.29314500
H	2.40868300	2.73300700	0.43092700
C	3.81167200	1.75346400	1.76285300
H	4.70418900	2.13116600	1.27443400
C	3.91986700	0.92194200	2.87374400
H	4.89640500	0.65028900	3.25503000
C	2.75875500	0.44480900	3.48782800
C	2.75875500	-0.44480900	4.66491300
N	1.52414900	-0.77493100	5.12728500
N	-1.44439600	0.95082800	3.02786900
C	-2.10660600	0.46526200	1.96327800
H	-1.82079300	-0.52308100	1.62514600
C	-3.10452400	1.17886100	1.30731500
H	-3.60505500	0.73846000	0.45209200
C	-3.43491000	2.44954500	1.77324800
H	-4.20913600	3.03589300	1.28898200
C	-2.75637600	2.96042300	2.87597400
H	-3.00160400	3.94460900	3.25586700
C	-1.76308500	2.18987600	3.48656600

C	-0.98356100	2.63204900	4.65911900
N	-0.10609100	1.71091300	5.13754000
N	-0.10609100	-1.71091300	3.01520100
C	0.63331000	-2.02175400	1.93619000
H	1.31468300	-1.25912800	1.57999300
C	0.54168600	-3.24998000	1.28915100
H	1.16104300	-3.44677400	0.42104400
C	-0.34956300	-4.20085500	1.78111900
H	-0.44574700	-5.17161900	1.30556600
C	-1.12174600	-3.88767400	2.89588500
H	-1.81948100	-4.61425200	3.29391300
C	-0.98356100	-2.63204900	3.49362200
C	-1.76308500	-2.18987600	4.66617500
N	-1.44439600	-0.95082800	5.12487200
C	-2.10660600	-0.46526200	6.18946300
H	-1.82079300	0.52308100	6.52759500
C	-3.10452400	-1.17886100	6.84542600
H	-3.60505500	-0.73846000	7.70064900
C	-3.43491000	-2.44954500	6.37949300
H	-4.20913600	-3.03589300	6.86375900
C	-2.75637600	-2.96042300	5.27676700
H	-3.00160400	-3.94460900	4.89687400
C	0.63331000	2.02175400	6.21655100
H	1.31468300	1.25912800	6.57274800
C	0.54168600	3.24998000	6.86359000
H	1.16104300	3.44677400	7.73169700
C	-0.34956300	4.20085500	6.37162200
H	-0.44574600	5.17161900	6.84717500
C	-1.12174600	3.88767400	5.25685600
H	-1.81948100	4.61425200	4.85882800
C	1.43004200	-1.58097800	6.19920600
H	0.42997500	-1.81795200	6.54017200
C	2.54396000	-2.08952700	6.85959700
H	2.40868300	-2.73300700	7.72181400
C	3.81167200	-1.75346400	6.38988800
H	4.70418900	-2.13116600	6.87830700
C	3.91986700	-0.92194200	5.27899700
H	4.89640500	-0.65028900	4.89771100

[Fe(bpy)₃]²⁺ quintet in 1-butanol, applied by SMD, <S²> = 6.0179

Fe	0.02901400	0.00001700	4.07635200
N	1.79800800	0.72068600	2.93587600
C	1.72944700	1.50814900	1.85138900
H	0.73642400	1.69023900	1.45293100
C	2.85498600	2.06679300	1.25297400
H	2.74896200	2.69294200	0.37405100
C	4.10078400	1.80432500	1.81883000

H	5.00372200	2.23065900	1.39318100
C	4.17937800	0.98896100	2.94562300
H	5.14109200	0.79210800	3.40321700
C	3.00643600	0.44645700	3.48108800
C	3.00642100	-0.44650900	4.67167100
N	1.79798000	-0.72073400	5.21685400
N	-1.53636800	1.12384800	2.95087000
C	-2.14612100	0.67171600	1.84410200
H	-1.84336300	-0.31004500	1.49471200
C	-3.11396200	1.40257600	1.16098900
H	-3.57636700	0.99094000	0.27055800
C	-3.46163600	2.65901400	1.65208700
H	-4.21165800	3.26338000	1.15173100
C	-2.83358900	3.13566400	2.79978400
H	-3.09521900	4.11114100	3.19009900
C	-1.86928700	2.34367500	3.43347100
C	-1.15040900	2.77686700	4.65972100
N	-0.25717700	1.89627700	5.17114500
N	-0.25714800	-1.89625500	2.98157500
C	0.43086300	-2.22077700	1.87465300
H	1.13014800	-1.47631700	1.50780900
C	0.26974300	-3.43621500	1.21775900
H	0.84859300	-3.65314900	0.32685700
C	-0.64729900	-4.34841900	1.73567700
H	-0.80565800	-5.30857300	1.25466300
C	-1.36471700	-4.01719900	2.88218300
H	-2.08025400	-4.72038600	3.28941800
C	-1.15037800	-2.77684300	3.49300500
C	-1.86924600	-2.34365300	4.71926000
N	-1.53633600	-1.12382000	5.20185600
C	-2.14608500	-0.67169400	6.30863000
H	-1.84333500	0.31007100	6.65801600
C	-3.11391400	-1.40256200	6.99175100
H	-3.57631600	-0.99092800	7.88218500
C	-3.46157700	-2.65900500	6.50065900
H	-4.21158900	-3.26337800	7.00102300
C	-2.83353400	-3.13565100	5.35296000
H	-3.09515600	-4.11113200	4.96265100
C	0.43084700	2.22079700	6.27805800
H	1.13013000	1.47633300	6.64489800
C	0.26973800	3.43623900	6.93495000
H	0.84859800	3.65317300	7.82584700
C	-0.64730600	4.34844300	6.41704000
H	-0.80565900	5.30859800	6.89805500
C	-1.36473900	4.01722400	5.27054200
H	-2.08027800	4.72041200	4.86331200

C	1.72939500	-1.50818800	6.30134600
H	0.73636100	-1.69027900	6.69977900
C	2.85492000	-2.06682300	6.89979500
H	2.74887400	-2.69296300	7.77872200
C	4.10073100	-1.80436200	6.33396500
H	5.00365900	-2.23069300	6.75963900
C	4.17935100	-0.98901000	5.20716600
H	5.14107600	-0.79216300	4.74959200

[Fe(bpy)₃]²⁺ singlet in tetrahydrofuran, applied by SMD

Fe	-0.01548300	0.00000000	4.07637100
N	1.52231400	0.77930800	3.02798000
C	1.42948800	1.59846600	1.96593200
H	0.42882400	1.83163700	1.62429100
C	2.54368200	2.12452400	1.31959200
H	2.40971800	2.77921600	0.46580900
C	3.81112300	1.79009700	1.79162100
H	4.70355300	2.18052700	1.31352800
C	3.91804700	0.94343800	2.89120800
H	4.89377500	0.66996800	3.27320400
C	2.75649400	0.45099000	3.49248500
C	2.75649400	-0.45099000	4.66025600
N	1.52231400	-0.77930800	5.12476100
N	-1.45052900	0.95256300	3.02931700
C	-2.12081200	0.46276600	1.97180500
H	-1.83449300	-0.52644000	1.63717100
C	-3.12640400	1.17155200	1.32217000
H	-3.63304000	0.72746400	0.47260600
C	-3.45733700	2.44192800	1.78871300
H	-4.23829200	3.02387700	1.31032800
C	-2.77091400	2.95720800	2.88469400
H	-3.01817600	3.94033400	3.26578400
C	-1.76894900	2.19177500	3.48797200
C	-0.97929700	2.63884300	4.65240000
N	-0.10724200	1.71483500	5.13555100
N	-0.10724200	-1.71483500	3.01719000
C	0.64116700	-2.03047800	1.94575400
H	1.31789800	-1.26461500	1.58774200
C	0.56447900	-3.26627800	1.31093600
H	1.19010600	-3.46739100	0.44848900
C	-0.32023000	-4.22051500	1.80866900
H	-0.40356500	-5.19764800	1.34426400
C	-1.10131300	-3.90256200	2.91599500
H	-1.79233500	-4.63230600	3.31991000
C	-0.97929700	-2.63884300	3.50034100
C	-1.76894900	-2.19177500	4.66476900
N	-1.45052900	-0.95256300	5.12342400

C	-2.12081200	-0.46276600	6.18093600
H	-1.83449300	0.52644000	6.51557000
C	-3.12640400	-1.17155200	6.83057100
H	-3.63304000	-0.72746400	7.68013500
C	-3.45733800	-2.44192800	6.36402800
H	-4.23829200	-3.02387700	6.84241300
C	-2.77091400	-2.95720800	5.26804700
H	-3.01817700	-3.94033400	4.88695700
C	0.64116700	2.03047800	6.20698700
H	1.31789800	1.26461500	6.56499900
C	0.56447900	3.26627800	6.84180500
H	1.19010600	3.46739100	7.70425200
C	-0.32022900	4.22051500	6.34407200
H	-0.40356500	5.19764800	6.80847700
C	-1.10131300	3.90256200	5.23674600
H	-1.79233500	4.63230600	4.83283100
C	1.42948800	-1.59846600	6.18680900
H	0.42882400	-1.83163700	6.52845000
C	2.54368200	-2.12452400	6.83315000
H	2.40971800	-2.77921600	7.68693200
C	3.81112300	-1.79009700	6.36112000
H	4.70355300	-2.18052700	6.83921300
C	3.91804700	-0.94343800	5.26153300
H	4.89377500	-0.66996900	4.87953700

[Fe(bpy)₃]²⁺ quintet in tetrahydrofuran, applied by SMD, <S²> = 6.0181

Fe	0.02962700	-0.04295900	4.09716900
N	1.76476100	0.77897100	2.93648700
C	1.65882800	1.58491900	1.86916000
H	0.65325500	1.76591500	1.50344400
C	2.76155200	2.16629500	1.24908200
H	2.62393200	2.80614500	0.38460300
C	4.02608700	1.90951300	1.77445100
H	4.91162600	2.35325300	1.33092100
C	4.14407100	1.07585600	2.88407200
H	5.12019400	0.88030300	3.31059700
C	2.99165300	0.51113000	3.44135800
C	3.03262400	-0.40707700	4.61063200
N	1.83951000	-0.71985200	5.17022600
N	-1.52468900	1.09944200	3.00225100
C	-2.15175400	0.65563600	1.90095100
H	-1.86651500	-0.33163100	1.55278200
C	-3.11462100	1.40043100	1.22691800
H	-3.59212000	0.99625200	0.34127400
C	-3.43721100	2.66262300	1.72120800
H	-4.18104000	3.27913900	1.22673100
C	-2.79237100	3.12913300	2.86344700

H	-3.03443100	4.10928100	3.25413400
C	-1.83518800	2.32342800	3.49148800
C	-1.10213600	2.74675900	4.71280100
N	-0.20265800	1.86239700	5.20648100
N	-0.25861200	-1.94843300	3.00280900
C	0.49869000	-2.33256200	1.96233100
H	1.19115900	-1.59308500	1.57363900
C	0.41623700	-3.60180500	1.39778700
H	1.04710500	-3.86413300	0.55594500
C	-0.48599900	-4.51064100	1.94674600
H	-0.57470500	-5.51508500	1.54530100
C	-1.27443100	-4.11929000	3.02628500
H	-1.96628100	-4.82325300	3.47152600
C	-1.14733400	-2.82211900	3.53360900
C	-1.95390700	-2.32598000	4.67971200
N	-1.56688200	-1.14354900	5.21171700
C	-2.23959200	-0.64987500	6.26268900
H	-1.88804500	0.29891600	6.65423800
C	-3.33021000	-1.29870800	6.83494000
H	-3.83749100	-0.85903400	7.68652300
C	-3.74820200	-2.50513300	6.27720300
H	-4.60465900	-3.03557800	6.68098800
C	-3.05516600	-3.02465700	5.18633000
H	-3.37938300	-3.95289000	4.73205200
C	0.49793800	2.18517400	6.30573000
H	1.20570400	1.44213700	6.65831600
C	0.34245400	3.39605300	6.97317100
H	0.93273400	3.60899200	7.85748500
C	-0.58342900	4.30985000	6.47426400
H	-0.73842100	5.26591600	6.96405000
C	-1.31311400	3.98316400	5.33455400
H	-2.03642200	4.68611900	4.94099900
C	1.80440000	-1.54717200	6.22754300
H	0.82207800	-1.76304900	6.63517600
C	2.95030300	-2.10542300	6.78554800
H	2.87178000	-2.76660600	7.64119500
C	4.18135100	-1.79602000	6.21075000
H	5.09929400	-2.21776400	6.60730700
C	4.22436700	-0.94113300	5.11196100
H	5.17370700	-0.70864500	4.64551500

[Fe(bpy)₃]²⁺ singlet in diethyl ether, applied by SMD

Fe	-0.01769600	0.00000000	4.07637100
N	1.52096400	0.78038800	3.02854100
C	1.42862200	1.60127400	1.96767300
H	0.42757700	1.83401000	1.62654200
C	2.54266000	2.12897400	1.32240300

H	2.40922100	2.78517800	0.46968600
C	3.81015500	1.79335500	1.79361700
H	4.70250500	2.18429100	1.31581500
C	3.91667300	0.94460300	2.89170200
H	4.89266600	0.66970100	3.27213200
C	2.75521600	0.45139400	3.49269100
C	2.75521600	-0.45139400	4.66005000
N	1.52096400	-0.78038800	5.12420000
N	-1.45311900	0.95454200	3.03025200
C	-2.12774900	0.46404900	1.97573500
H	-1.84560100	-0.52762200	1.64459400
C	-3.13252600	1.17377900	1.32593000
H	-3.64279600	0.72877400	0.47898400
C	-3.45856100	2.44651100	1.78959000
H	-4.23890700	3.02925800	1.31120400
C	-2.76836900	2.96229100	2.88305700
H	-3.01294600	3.94690000	3.26224600
C	-1.76738400	2.19573400	3.48674600
C	-0.97587100	2.64237500	4.65034700
N	-0.10805800	1.71570000	5.13647700
N	-0.10805800	-1.71570000	3.01626400
C	0.63980000	-2.03062700	1.94406100
H	1.31326700	-1.26259900	1.58413400
C	0.56719000	-3.26779300	1.31141300
H	1.19169100	-3.46846100	0.44800800
C	-0.31248300	-4.22496400	1.81266100
H	-0.39220000	-5.20342900	1.35047800
C	-1.09289800	-3.90790100	2.92077800
H	-1.77989300	-4.64014200	3.32721100
C	-0.97587100	-2.64237500	3.50239400
C	-1.76738400	-2.19573400	4.66599500
N	-1.45311900	-0.95454200	5.12248900
C	-2.12774900	-0.46404900	6.17700600
H	-1.84560100	0.52762200	6.50814700
C	-3.13252600	-1.17377900	6.82681100
H	-3.64279600	-0.72877400	7.67375700
C	-3.45856100	-2.44651100	6.36315100
H	-4.23890700	-3.02925800	6.84153700
C	-2.76836900	-2.96229100	5.26968400
H	-3.01294600	-3.94689900	4.89049500
C	0.63980000	2.03062700	6.20868000
H	1.31326700	1.26259900	6.56860700
C	0.56719000	3.26779300	6.84132800
H	1.19169100	3.46846100	7.70473300
C	-0.31248300	4.22496400	6.34008000
H	-0.39220000	5.20342900	6.80226300

C	-1.09289700	3.90790100	5.23196300
H	-1.77989300	4.64014200	4.82553000
C	1.42862200	-1.60127400	6.18506800
H	0.42757700	-1.83401000	6.52619900
C	2.54266000	-2.12897400	6.83033800
H	2.40922100	-2.78517800	7.68305500
C	3.81015500	-1.79335500	6.35912400
H	4.70250500	-2.18429100	6.83692600
C	3.91667300	-0.94460300	5.26103900
H	4.89266600	-0.66970100	4.88060900

[Fe(bpy)₃]²⁺ quintet in diethyl ether, applied by SMD, <S²> = 6.0121

Fe	0.01718000	0.00001800	4.07635700
N	1.79191700	0.71817400	2.93530900
C	1.72514900	1.51103600	1.85420100
H	0.73253900	1.69075400	1.45409400
C	2.84964200	2.07980800	1.26277300
H	2.74372400	2.71117000	0.38772100
C	4.09526800	1.81994100	1.83026400
H	4.99703700	2.25331200	1.40979800
C	4.17314800	0.99750400	2.95203500
H	5.13407700	0.80242200	3.41234900
C	3.00088800	0.44873900	3.48270800
C	3.00087100	-0.44880400	4.67005200
N	1.79188500	-0.71822700	5.21742700
N	-1.53595000	1.15955800	2.96196300
C	-2.18074000	0.69418200	1.88120900
H	-1.86067600	-0.27495300	1.51276100
C	-3.20458100	1.39563900	1.25037600
H	-3.69378600	0.97540700	0.37862800
C	-3.57465200	2.63367200	1.77091700
H	-4.37112700	3.21191100	1.31376600
C	-2.90998900	3.12385800	2.89274100
H	-3.19597900	4.08097100	3.31061800
C	-1.88636300	2.36396500	3.46940000
C	-1.12191500	2.81005100	4.66471100
N	-0.24777200	1.91264100	5.18008700
N	-0.24774300	-1.91260700	2.97262900
C	0.47020300	-2.24167600	1.88648700
H	1.15369100	-1.48432200	1.51663400
C	0.35970400	-3.47701600	1.25582600
H	0.95855000	-3.69627300	0.37892900
C	-0.52952500	-4.40984000	1.78524900
H	-0.64147100	-5.38877300	1.33015000
C	-1.27683800	-4.07531500	2.91215300
H	-1.96272200	-4.79842600	3.33546500
C	-1.12188600	-2.81001600	3.48800800

C	-1.88632400	-2.36393900	4.68332800
N	-1.53591700	-1.15953300	5.19077000
C	-2.18070300	-0.69417100	6.27153200
H	-1.86064600	0.27496400	6.63998500
C	-3.20453500	-1.39564000	6.90236800
H	-3.69373800	-0.97541700	7.77412200
C	-3.57459700	-2.63367500	6.38182500
H	-4.37106100	-3.21192500	6.83897900
C	-2.90993700	-3.12384700	5.25999400
H	-3.19592000	-4.08096100	4.84211400
C	0.47018800	2.24171100	6.26621900
H	1.15367100	1.48435100	6.63607200
C	0.35970200	3.47705600	6.89687200
H	0.95855900	3.69631600	7.77376200
C	-0.52952800	4.40988100	6.36745300
H	-0.64146400	5.38881600	6.82254800
C	-1.27685600	4.07535300	5.24055900
H	-1.96274300	4.79846300	4.81725100
C	1.72508900	-1.51106900	6.29854800
H	0.73246900	-1.69077900	6.69863200
C	2.84956700	-2.07983400	6.89001200
H	2.74362600	-2.71117700	7.76507500
C	4.09520600	-1.81999000	6.32254000
H	4.99696200	-2.25336100	6.74303100
C	4.17311500	-0.99757300	5.20075600
H	5.13405600	-0.80250700	4.74045800

[Fe(bpy)₃]²⁺ singlet in dichloromethane, applied by SMD

Fe	-0.01465600	0.00000000	4.07637100
N	1.52393600	0.77925300	3.02764400
C	1.43153300	1.59988700	1.96658000
H	0.43115300	1.83200900	1.62350600
C	2.54587800	2.12996000	1.32364900
H	2.41191900	2.78643700	0.47123400
C	3.81324700	1.79706900	1.79724200
H	4.70581400	2.19079400	1.32211400
C	3.91976500	0.94744800	2.89466900
H	4.89516600	0.67382900	3.27734000
C	2.75801600	0.45181100	3.49310700
C	2.75801600	-0.45181200	4.65963400
N	1.52393600	-0.77925300	5.12509700
N	-1.44949600	0.95149900	3.02709900
C	-2.11635300	0.46194800	1.96722400
H	-1.82800600	-0.52646600	1.63223100
C	-3.12088700	1.17022100	1.31527100
H	-3.62426600	0.72608000	0.46380700
C	-3.45416600	2.44010300	1.78173000

H	-4.23413200	3.02179200	1.30140600
C	-2.77095200	2.95543000	2.87980400
H	-3.01933300	3.93844800	3.26040600
C	-1.77000900	2.19033800	3.48542400
C	-0.98266400	2.63809400	4.65120000
N	-0.10814100	1.71604600	5.13370600
N	-0.10814100	-1.71604600	3.01903500
C	0.63966000	-2.03307800	1.94751500
H	1.31833100	-1.26869600	1.59007600
C	0.55974300	-3.26825200	1.31172800
H	1.18495800	-3.47034800	0.44921200
C	-0.32824400	-4.22025900	1.80825900
H	-0.41466100	-5.19666400	1.34286200
C	-1.10849600	-3.90090200	2.91588900
H	-1.80198400	-4.62857100	3.31922900
C	-0.98266400	-2.63809400	3.50154100
C	-1.77000900	-2.19033800	4.66731700
N	-1.44949600	-0.95149900	5.12564200
C	-2.11635300	-0.46194800	6.18551700
H	-1.82800600	0.52646600	6.52051000
C	-3.12088700	-1.17022100	6.83747000
H	-3.62426600	-0.72608000	7.68893400
C	-3.45416600	-2.44010200	6.37101100
H	-4.23413200	-3.02179200	6.85133500
C	-2.77095300	-2.95543000	5.27293700
H	-3.01933400	-3.93844800	4.89233500
C	0.63966100	2.03307800	6.20522600
H	1.31833100	1.26869600	6.56266600
C	0.55974300	3.26825200	6.84101300
H	1.18495800	3.47034800	7.70352900
C	-0.32824400	4.22025900	6.34448200
H	-0.41466000	5.19666400	6.80987900
C	-1.10849600	3.90090200	5.23685200
H	-1.80198400	4.62857100	4.83351200
C	1.43153300	-1.59988700	6.18616100
H	0.43115200	-1.83200900	6.52923500
C	2.54587800	-2.12996000	6.82909200
H	2.41191900	-2.78643700	7.68150700
C	3.81324700	-1.79706900	6.35549900
H	4.70581400	-2.19079500	6.83062700
C	3.91976500	-0.94744800	5.25807200
H	4.89516600	-0.67383000	4.87540100

[Fe(bpy)₃]²⁺ quintet in dichloromethane, applied by SMD, <S²> = 6.0181

Fe	0.03105400	0.04193400	4.05673000
N	1.83922500	0.71882400	2.97756500
C	1.80051100	1.54274600	1.91763500

H	0.81713800	1.75561500	1.51118300
C	2.94424700	2.10140200	1.35539900
H	2.86239300	2.75979100	0.49791600
C	4.17715400	1.79605100	1.92857600
H	5.09353700	2.21826900	1.52889200
C	4.22398200	0.94372100	3.02934200
H	5.17468500	0.71376900	3.49416600
C	3.03416100	0.40902700	3.53484900
C	2.99748500	-0.50761800	4.70553500
N	1.77236700	-0.77629600	5.21452400
N	-1.56411200	1.14325400	2.94106200
C	-2.22756000	0.65193300	1.88310200
H	-1.87864200	-0.30065500	1.49863100
C	-3.30562800	1.30768000	1.29502400
H	-3.80586800	0.86880100	0.43888700
C	-3.71848700	2.52085700	1.84184600
H	-4.56342300	3.05872300	1.42389900
C	-3.03451900	3.03814200	2.93960700
H	-3.35284200	3.97371100	3.38211800
C	-1.94790700	2.33038400	3.46510500
C	-1.15377400	2.82115600	4.62250000
N	-0.26416800	1.94756600	5.15215600
N	-0.20690200	-1.86755500	2.95220500
C	0.48894300	-2.19188900	1.85025600
H	1.19814600	-1.45111400	1.49582500
C	0.32667600	-3.40157600	1.18214200
H	0.91305200	-3.61565300	0.29550500
C	-0.60112900	-4.31242700	1.68324600
H	-0.76173600	-5.26723500	1.19279900
C	-1.32572300	-3.98415400	2.82586500
H	-2.05039600	-4.68451200	3.22142300
C	-1.10809600	-2.74899600	3.44796300
C	-1.83580500	-2.32371100	4.67184200
N	-1.52143500	-1.09976200	5.15880400
C	-2.14291700	-0.65478000	6.26287900
H	-1.85477000	0.33209800	6.60952100
C	-3.10366000	-1.39791600	6.94186700
H	-3.57593100	-0.99232200	7.82966800
C	-3.43049600	-2.65984100	6.44954800
H	-4.17284600	-3.27511900	6.94778700
C	-2.79157400	-3.12773000	5.30442700
H	-3.03690300	-4.10762900	4.91514400
C	0.48242000	2.32547000	6.20264800
H	1.17608300	1.58608800	6.58936600
C	0.38767700	3.58831500	6.77959200
H	1.01022000	3.84575500	7.62911400

C	-0.51660400	4.49686600	6.23319400
H	-0.61555600	5.49620900	6.64485500
C	-1.29399700	4.11194700	5.14325200
H	-1.98705500	4.81629700	4.70030900
C	1.67082900	-1.58222500	6.28240400
H	0.66680200	-1.76365000	6.65203400
C	2.77610600	-2.16345700	6.89831300
H	2.64165900	-2.80382000	7.76291300
C	4.03877900	-1.90569800	6.36870400
H	4.92620000	-2.34913000	6.80879500
C	4.15230400	-1.07125800	5.25910900
H	5.12662900	-0.87467200	4.82903200

[Fe(dmb)₃]²⁺ singlet in gas phase

Fe	3.18172900	23.20219400	10.42254000
C	5.28476200	21.09311600	9.87225800
H	5.66724100	21.38892000	10.84156200
C	5.90215800	20.08474000	9.14531700
H	6.77566700	19.58978000	9.55747500
C	5.39262300	19.71635500	7.89168800
C	4.26683300	20.41398000	7.44215300
H	3.83946400	20.16087600	6.47906600
C	3.69292600	21.42249300	8.22016900
C	2.50702900	22.20373800	7.80959500
C	1.86569300	22.05332800	6.57761500
H	2.23683400	21.33537600	5.85577500
C	0.74368900	22.82395400	6.25600700
C	0.30818500	23.73727100	7.22710400
H	-0.55805600	24.36650600	7.04943800
C	0.99048300	23.84248500	8.43122600
H	0.66538600	24.54287500	9.19092000
C	6.02199800	18.61767300	7.08029600
H	7.10255100	18.76639000	6.99102900
H	5.59760100	18.56005700	6.07598500
H	5.87093400	17.64767100	7.56750800
C	0.04303900	22.69172800	4.93193400
H	0.19489400	23.59306300	4.32721200
H	-1.03648800	22.57645000	5.06957100
H	0.41129500	21.83706100	4.36094500
C	1.11704200	24.67067800	12.08273300
H	0.77535000	23.67256700	12.32841500
C	0.49449500	25.78572600	12.62635600
H	-0.34153300	25.65058500	13.30508900
C	0.95079400	27.07001700	12.29571300
C	2.03061700	27.14360600	11.40990200
H	2.41622100	28.11632800	11.12818700
C	2.61223500	25.98299100	10.89367000

C	0.31433200	28.30290000	12.87579100
H	-0.77251100	28.27883700	12.74934200
H	0.69542700	29.21419100	12.41064100
H	0.51060200	28.36471300	13.95220500
N	4.20146100	21.76132900	9.43342200
N	2.15598100	24.74842500	11.22993100
N	2.06993600	23.09732200	8.73478100
C	1.07869700	21.09311700	10.97282900
H	0.69622200	21.38891500	10.00352000
C	0.46129600	20.08474900	11.69977600
H	-0.41221400	19.58979000	11.28762000
C	0.97082500	19.71637400	12.95341000
C	2.09661700	20.41399800	13.40294200
H	2.52398200	20.16090200	14.36603300
C	2.67053000	21.42250200	12.62491800
C	3.85642900	22.20374600	13.03548900
C	4.49776700	22.05333700	14.26746800
H	4.12662700	21.33538600	14.98931000
C	5.61977400	22.82396100	14.58907200
C	6.05527800	23.73727400	13.61797200
H	6.92152200	24.36650600	13.79563500
C	5.37297900	23.84248700	12.41385200
H	5.69807600	24.54287400	11.65415500
C	0.34144400	18.61770200	13.76481000
H	-0.73911100	18.76641700	13.85406200
H	0.76582900	18.56010200	14.76912700
H	0.49251700	17.64769400	13.27761400
C	6.32042400	22.69173800	15.91314500
H	6.16852100	23.59305200	16.51788700
H	7.39995700	22.57651500	15.77551300
H	5.95220500	21.83704000	16.48411300
C	5.24641100	24.67067900	8.76234400
H	5.58809800	23.67256800	8.51665600
C	5.86896000	25.78572700	8.21872600
H	6.70498600	25.65058600	7.53998900
C	5.41266800	27.07001800	8.54937700
C	4.33284700	27.14360700	9.43519100
H	3.94724600	28.11632900	9.71691000
C	3.75122500	25.98299100	9.95141700
C	6.04914000	28.30290100	7.96931000
H	7.13597400	28.27887000	8.09584400
H	5.66798700	29.21419500	8.43440600
H	5.85295200	28.36467700	6.89287900
N	2.16200000	21.76133000	11.41166200
N	4.20747400	24.74842500	9.61515000
N	4.29352300	23.09732700	12.11030000

[Fe(dmb)₃]²⁺ quintet in gas phase, <S²> = 6.0106

Fe	3.18217500	23.20168700	10.42242500
C	5.32849400	20.98623800	9.63708400
H	5.73516200	21.29629900	10.59446200
C	5.91187300	19.95165200	8.91801900
H	6.78719000	19.44750500	9.31474300
C	5.35548900	19.56703800	7.68985300
C	4.22382900	20.26965200	7.25829800
H	3.75715800	19.98717000	6.32219600
C	3.69320100	21.30905400	8.02667900
C	2.49553600	22.09266200	7.61470300
C	1.89769400	21.96463300	6.35829800
H	2.30901800	21.28358500	5.62286200
C	0.76900100	22.72233500	6.02296300
C	0.28559800	23.60719200	6.99724300
H	-0.58321200	24.22792800	6.80334600
C	0.93365300	23.69356200	8.22212700
H	0.58409900	24.37756100	8.98897700
C	5.95526300	18.45795300	6.87034100
H	6.88732100	18.79383000	6.40081900
H	5.28082800	18.12870500	6.07717600
H	6.20354600	17.59572500	7.49599700
C	0.09743700	22.58707700	4.68426500
H	-0.14294500	23.56763800	4.26324100
H	-0.84743800	22.04053900	4.78670700
H	0.72122100	22.04592700	3.96981900
C	1.02890000	24.91323700	12.03166200
H	0.65650800	23.91850900	12.25448800
C	0.43349600	26.03690800	12.58803700
H	-0.41836700	25.92256400	13.25062600
C	0.95010900	27.30669300	12.29296600
C	2.05346800	27.35876500	11.43282300
H	2.48981600	28.32252300	11.19937900
C	2.59674200	26.18878300	10.89468900
C	0.33881700	28.55426100	12.86838900
H	-0.62658500	28.75951800	12.39117200
H	0.97866600	29.42641300	12.71931100
H	0.14920600	28.44124600	13.93986900
N	4.24510200	21.65853900	9.21203200
N	2.08508200	24.97269600	11.20153600
N	2.01361400	22.95806900	8.53695800
C	0.99590700	21.03236500	11.23756100
H	0.56979400	21.35399400	10.29226100
C	0.42256500	19.99265600	11.95762600
H	-0.46325600	19.49660600	11.57410500
C	1.00197900	19.59359200	13.17030900

C	2.14519600	20.28714900	13.58506600
H	2.62988000	19.99230700	14.50810500
C	2.66579800	21.33140200	12.81536700
C	3.87686700	22.10167700	13.21443300
C	4.47913000	21.96827200	14.46865100
H	4.05847500	21.29876500	15.20928700
C	5.62280500	22.70624300	14.79633800
C	6.11809000	23.57933200	13.81720600
H	6.99894400	24.18474200	14.00520000
C	5.46409900	23.67543700	12.59664500
H	5.81938200	24.35329800	11.82717000
C	0.41396500	18.47920100	13.99142200
H	-0.50698500	18.81419200	14.48293800
H	1.10288900	18.13974700	14.76769500
H	0.14958300	17.62380200	13.36299000
C	6.29702900	22.56445100	16.13295500
H	6.53924100	23.54329400	16.55718900
H	7.24139000	22.01794000	16.02624300
H	5.67423400	22.02135600	16.84672300
C	5.34207800	24.92836500	8.83917300
H	5.72970400	23.93702200	8.62558200
C	5.91990300	26.05466300	8.26834300
H	6.77042400	25.94487200	7.60321600
C	5.39035100	27.32061200	8.55546500
C	4.29019900	27.36618700	9.42011800
H	3.84378200	28.32658000	9.64864200
C	3.76285300	26.19316000	9.96766500
C	5.98579500	28.57135000	7.96985600
H	6.93605000	28.80701800	8.46330100
H	5.32390100	29.43138700	8.09117700
H	6.19981900	28.44481700	6.90466300
N	2.09195100	21.69531600	11.64462400
N	4.28782500	24.98119500	9.67116500
N	4.36919700	22.95846700	12.28794400

[Fe(dmb)₃]²⁺ singlet in methanol, applied by CPCM

Fe	3.18172500	23.23896300	10.42249200
C	5.27860700	21.15105500	9.86721300
H	5.69592500	21.47412300	10.81119600
C	5.86360300	20.12068600	9.14623100
H	6.74978800	19.63184800	9.53106500
C	5.30361800	19.71737500	7.92914900
C	4.17007600	20.40437800	7.49144300
H	3.70534500	20.12943200	6.55322700
C	3.63331200	21.43631200	8.25968400
C	2.44588800	22.21423000	7.86520000
C	1.76819000	22.03472300	6.66115100

H	2.10400700	21.28783900	5.95308400
C	0.65236700	22.81682700	6.35592100
C	0.25903800	23.76515200	7.30581200
H	-0.60222200	24.39777900	7.13227300
C	0.97659900	23.89672800	8.48628600
H	0.68791400	24.61892600	9.23829000
C	5.89029700	18.58451900	7.13982200
H	6.97940100	18.61233200	7.17449400
H	5.56451600	18.61237800	6.10074100
H	5.57627700	17.62724800	7.56546800
C	-0.06923800	22.65924900	5.05092500
H	0.08054900	21.66114200	4.63826400
H	0.31260400	23.38155100	4.32340700
H	-1.13804800	22.84517000	5.16749400
C	1.09001500	24.66186400	12.03161400
H	0.76605700	23.65836000	12.27435500
C	0.41922600	25.77384600	12.51763100
H	-0.44254600	25.64051800	13.15777300
C	0.86091400	27.05679200	12.17379700
C	1.96858200	27.14646900	11.32889400
H	2.33438400	28.11962600	11.02810500
C	2.59901800	25.98997400	10.87384200
C	0.16714100	28.28462300	12.68333800
H	-0.91361400	28.19256500	12.55950100
H	0.51103800	29.17577500	12.15837700
H	0.36139000	28.42097000	13.75188100
N	4.18225700	21.80339000	9.44454600
N	2.15884000	24.75535600	11.22240300
N	2.05073000	23.14177500	8.77352600
C	1.08523800	21.15068100	10.97783200
H	0.66789800	21.47360900	10.03381300
C	0.50039300	20.12027500	11.69888200
H	-0.38569800	19.63125700	11.31406400
C	1.06039600	19.71717300	12.91602600
C	2.19380600	20.40440600	13.35370900
H	2.65854400	20.12964300	14.29197400
C	2.73043100	21.43635500	12.58538800
C	3.91772800	22.21448400	12.97983600
C	4.59544900	22.03513300	14.18389500
H	4.25974700	21.28822800	14.89199400
C	5.71115800	22.81741300	14.48908500
C	6.10435400	23.76574000	13.53914300
H	6.96552900	24.39849000	13.71265200
C	5.38677100	23.89716500	12.35866600
H	5.67536100	24.61937200	11.60663300
C	0.47386500	18.58429400	13.70543500

H	-0.61524300	18.61198600	13.67078200
H	0.79966000	18.61224700	14.74450900
H	0.78798000	17.62703500	13.27983300
C	6.43280000	22.65999900	15.79408000
H	6.28312100	21.66190600	16.20681800
H	6.05090500	23.38231400	16.52155600
H	7.50159100	22.84601400	15.67747700
C	5.27319200	24.66226500	8.81342500
H	5.59732800	23.65881900	8.57068600
C	5.94383700	25.77437000	8.32749100
H	6.80567700	25.64119700	7.68740800
C	5.50190800	27.05723200	8.67133600
C	4.39417000	27.14669900	9.51617000
H	4.02818700	28.11978400	9.81696500
C	3.76390400	25.99008600	9.97115900
C	6.19551000	28.28519700	8.16188200
H	7.27627800	28.19327500	8.28570800
H	5.85149300	29.17626600	8.68690300
H	6.00124100	28.42159100	7.09334900
N	2.18146400	21.80323700	11.40047800
N	4.20431000	24.75555500	9.62258300
N	4.31274700	23.14204300	12.07146300

[Fe(dmb)₃]²⁺ quintet in methanol, applied by CPCM, <S²> = 6.0120

Fe	3.18220500	23.18984000	10.42467100
C	5.45476300	21.18894100	9.53641000
H	5.87835800	21.51524000	10.48011900
C	6.07464000	20.21159900	8.77052100
H	6.99606600	19.75785200	9.11156700
C	5.48876700	19.81053000	7.56535700
C	4.29408900	20.43211600	7.19363100
H	3.80725700	20.13469300	6.27413700
C	3.72617800	21.41073100	8.00917600
C	2.45160300	22.09528200	7.67291600
C	1.79405500	21.91227100	6.45712700
H	2.22098300	21.27492700	5.69304600
C	0.58037900	22.56092500	6.20703900
C	0.07020600	23.38482500	7.21452800
H	-0.86557200	23.91281600	7.07897900
C	0.78730200	23.53890100	8.39318900
H	0.43058900	24.18873000	9.18340700
C	6.12419600	18.76205600	6.70099300
H	6.89977900	19.21076500	6.07466300
H	5.39158900	18.29565200	6.04134900
H	6.60073000	17.99236100	7.30931700
C	-0.15719000	22.35423200	4.91660600
H	-0.86036400	23.16552800	4.72945400

H	-0.72427800	21.41975800	4.95544600
H	0.53565000	22.27911500	4.07780000
C	0.88220500	24.86798900	11.79037000
H	0.51039300	23.87100900	11.99467600
C	0.20890100	25.99547600	12.23662600
H	-0.70912800	25.89167100	12.80027600
C	0.73124400	27.26269600	11.95140500
C	1.92185300	27.31891900	11.22516700
H	2.35702700	28.28230500	10.99617100
C	2.54557500	26.14387200	10.80438500
C	0.04333400	28.50931100	12.41925100
H	-0.92017900	28.62913700	11.91685000
H	0.64928700	29.39314100	12.21955200
H	-0.15706100	28.45510500	13.49176200
N	4.30490400	21.77852900	9.17449900
N	2.02743300	24.93067200	11.09259300
N	1.95292200	22.91712100	8.62531500
C	0.92319200	21.17899600	11.30725200
H	0.50582200	21.50651200	10.36139700
C	0.29176100	20.21034200	12.07441800
H	-0.63333800	19.76533300	11.73204600
C	0.87141700	19.80473300	13.28115000
C	2.07068600	20.41586000	13.65639700
H	2.55268600	20.11618500	14.57777400
C	2.64762000	21.38971100	12.84269000
C	3.92088600	22.07467700	13.18206800
C	4.58071300	21.89270300	14.39610300
H	4.15945300	21.24944100	15.15852000
C	5.78910600	22.55193700	14.64570800
C	6.28926900	23.38323200	13.63946300
H	7.22032300	23.91952300	13.77476200
C	5.57078700	23.53210500	12.46041600
H	5.92201300	24.18493400	11.66998700
C	0.22413300	18.76220300	14.14323600
H	-0.55852100	19.21540600	14.75721400
H	0.94795200	18.29840100	14.81410900
H	-0.24621000	17.99020000	13.53306300
C	6.53035900	22.34890700	15.93463700
H	7.22864700	23.16453300	16.12108800
H	7.10282000	21.41789700	15.89444000
H	5.83938900	22.26921400	16.77459300
C	5.47854100	24.86485700	9.04789700
H	5.84863400	23.86749300	8.84390400
C	6.15521600	25.99178600	8.60650700
H	7.07660300	25.88761300	8.04837700
C	5.62952900	27.25900700	8.88603800

C	4.43524800	27.31610100	9.60647300
H	3.99877900	28.27978900	9.83148400
C	3.80941700	26.14244300	10.02698900
C	6.31711900	28.50517600	8.41730600
H	7.28034600	28.62559300	8.92003200
H	5.71061700	29.38898200	8.61512500
H	6.51817000	28.44921600	7.34500400
N	2.07688200	21.75802600	11.67378900
N	4.32884200	24.92868900	9.73898000
N	4.41099900	22.90030500	12.23021200

[Fe(dmb)₃]²⁺ singlet in ethanol, applied by CPCM

Fe	3.18172900	23.23459000	10.42254500
C	5.27340500	21.13513500	9.88443200
H	5.67771300	21.45004600	10.83709800
C	5.86549200	20.10579300	9.16592900
H	6.74258800	19.61030700	9.56397700
C	5.32611700	19.71774700	7.93510400
C	4.20379200	20.41578000	7.48332600
H	3.75932900	20.15194200	6.53195600
C	3.65559000	21.44044900	8.25240900
C	2.47110000	22.22016300	7.85038000
C	1.80350600	22.04551900	6.63954900
H	2.14872000	21.30468500	5.92940000
C	0.68484500	22.82295800	6.33101700
C	0.27972200	23.76339900	7.28418500
H	-0.58385400	24.39301600	7.10902300
C	0.98726700	23.88988000	8.47146400
H	0.68783600	24.60536400	9.22593100
C	5.91031700	18.58669400	7.14032100
H	6.98707900	18.50832800	7.29899500
H	5.71463200	18.71235400	6.07401500
H	5.46018300	17.63876300	7.45027600
C	-0.02971100	22.66796600	5.02088200
H	0.12189100	21.67050900	4.60633100
H	0.35548900	23.39186800	4.29612800
H	-1.09957200	22.85274800	5.13178700
C	1.09397600	24.66193900	12.03714100
H	0.76514700	23.65910600	12.27604600
C	0.43198400	25.77325000	12.53706600
H	-0.42655000	25.63816400	13.18200900
C	0.88196200	27.05671200	12.20586400
C	1.98527100	27.14687500	11.35468300
H	2.35983800	28.12132200	11.06922400
C	2.60296200	25.99062900	10.87941400
C	0.20207600	28.28394400	12.73868000
H	-0.88095700	28.20116700	12.62643300

H	0.54517200	29.18041000	12.22158900
H	0.40897300	28.40493600	13.80677700
N	4.18791800	21.79659900	9.44919400
N	2.15769400	24.75532900	11.22088500
N	2.06271100	23.13826800	8.76273100
C	1.09005000	21.13513900	10.96066100
H	0.68574100	21.45005000	10.00799600
C	0.49796200	20.10579900	11.67916500
H	-0.37913500	19.61031300	11.28111700
C	1.03733700	19.71775300	12.90999000
C	2.15966300	20.41578400	13.36176700
H	2.60412600	20.15194600	14.31313700
C	2.70786600	21.44045200	12.59268300
C	3.89235600	22.22016500	12.99471100
C	4.55995100	22.04552200	14.20554200
H	4.21473600	21.30468900	14.91569300
C	5.67861200	22.82295900	14.51407300
C	6.08373700	23.76339900	13.56090400
H	6.94731400	24.39301500	13.73606500
C	5.37619200	23.88987900	12.37362500
H	5.67562300	24.60536200	11.61915700
C	0.45313600	18.58670000	13.70477300
H	-0.62362600	18.50833400	13.54610000
H	0.64882100	18.71236000	14.77108000
H	0.90326900	17.63876800	13.39481900
C	6.39316800	22.66796800	15.82420800
H	6.24156700	21.67051100	16.23875900
H	6.00796900	23.39187000	16.54896200
H	7.46303000	22.85275000	15.71330400
C	5.26948400	24.66193200	8.80794600
H	5.59831100	23.65909900	8.56904200
C	5.93147700	25.77324200	8.30801800
H	6.79001100	25.63815300	7.66307400
C	5.48150200	27.05670400	8.63921700
C	4.37819400	27.14687100	9.49040000
H	4.00362900	28.12132000	9.77585600
C	3.76050100	25.99062700	9.96567100
C	6.16138900	28.28393500	8.10639800
H	7.24442200	28.20115600	8.21864300
H	5.81829500	29.18040200	8.62348700
H	5.95449100	28.40492400	7.03830000
N	2.17553700	21.79660200	11.39589800
N	4.20576600	24.75532600	9.62420200
N	4.30074700	23.13826800	12.08235900

[Fe(dmb)₃]²⁺ quintet in ethanol, applied by CPCM, <S²> = 6.0119

Fe	3.18207100	23.20018400	10.42489500
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C	5.43754600	21.16812600	9.55476100
H	5.86263700	21.49636800	10.49723700
C	6.04935700	20.17844200	8.79770800
H	6.96531700	19.71796000	9.14582800
C	5.46367700	19.77594600	7.59260500
C	4.27651700	20.40813400	7.21300500
H	3.79011200	20.10983000	6.29335500
C	3.71602700	21.39844400	8.02010800
C	2.44889800	22.09447700	7.67573800
C	1.78912900	21.90765300	6.46145100
H	2.20658100	21.25509300	5.70486200
C	0.58427100	22.57037700	6.20306700
C	0.08636800	23.41434900	7.20023300
H	-0.84141900	23.95499400	7.05816800
C	0.80325600	23.56870600	8.37935700
H	0.45462300	24.23064600	9.16347400
C	6.09201700	18.71672800	6.73465700
H	6.86947900	19.15713400	6.10368500
H	5.35611900	18.24946500	6.07870500
H	6.56534900	17.94769000	7.34704400
C	-0.15395800	22.36065100	4.91272300
H	-0.85068500	23.17651700	4.71908900
H	-0.72855200	21.43063200	4.95694700
H	0.53878700	22.27494100	4.07421300
C	0.89832300	24.88154600	11.82102000
H	0.53094900	23.88540600	12.03845200
C	0.22469000	26.00952400	12.26643100
H	-0.68707700	25.90461100	12.84056300
C	0.73877100	27.27712500	11.96758400
C	1.92217700	27.33291500	11.22894000
H	2.35095900	28.29693900	10.98996000
C	2.54599400	26.15754500	10.80757200
C	0.04641300	28.52481200	12.42950900
H	-0.91695800	28.63841500	11.92426500
H	0.64861000	29.41061900	12.22545500
H	-0.15605200	28.47600100	13.50215400
N	4.29579500	21.76845000	9.18448300
N	2.03446900	24.94388100	11.10795300
N	1.95857100	22.93122800	8.61988700
C	0.95022300	21.14337400	11.28560000
H	0.53399700	21.46642800	10.33772100
C	0.32796200	20.16332100	12.04651700
H	-0.58810100	19.70537800	11.69557400
C	0.90423700	19.76526500	13.25764600
C	2.09198000	20.39415300	13.64190700
H	2.57138100	20.10014400	14.56666000

C	2.66064300	21.37777500	12.83370200
C	3.92317200	22.07976500	13.18190000
C	4.58568300	21.89720400	14.39467900
H	4.17684400	21.23720900	15.14968000
C	5.78276600	22.57475300	14.65241300
C	6.26726600	23.42776000	13.65652600
H	7.18815100	23.98002800	13.79845100
C	5.54883500	23.57352800	12.47674900
H	5.88976400	24.23880400	11.69183700
C	0.26537000	18.71409600	14.11709400
H	-0.51713600	19.16100900	14.73697500
H	0.99385600	18.25025600	14.78355000
H	-0.20391000	17.94189200	13.50572000
C	6.52518700	22.37161400	15.94136700
H	7.21546400	23.19329200	16.13332600
H	7.10685600	21.44615500	15.89682900
H	5.83459200	22.28102400	16.78118400
C	5.45982400	24.87940300	9.01494300
H	5.82695200	23.88272400	8.80108200
C	6.13623700	26.00685800	8.57365800
H	7.05267400	25.90184400	8.00696900
C	5.61650400	27.27429300	8.86390800
C	4.42791500	27.33066400	9.59449200
H	3.99632000	28.29489000	9.82730600
C	3.80289000	26.15653000	10.01657100
C	6.30730200	28.52163700	8.39959000
H	7.27069400	28.63710100	8.90423800
H	5.70396400	29.40713700	8.60124600
H	6.50962000	28.47018400	7.32701100
N	2.09147100	21.74065900	11.66198900
N	4.31783100	24.94266000	9.71917100
N	4.40216400	22.92138300	12.23806800

[Fe(dmb)₃]²⁺ singlet in 2-propanol, applied by CPCM

Fe	3.18172900	23.23291100	10.42254500
C	5.27480900	21.13283000	9.88386600
H	5.67779300	21.44692400	10.83747900
C	5.86920100	20.10485800	9.16503400
H	6.74633300	19.61026800	9.56465300
C	5.33198800	19.71766400	7.93277800
C	4.20919400	20.41524700	7.48075700
H	3.76622100	20.15193700	6.52845800
C	3.65882500	21.43885900	8.25014900
C	2.47427200	22.21868400	7.84702700
C	1.80828500	22.04487000	6.63488700
H	2.15492900	21.30476300	5.92455400
C	0.68945600	22.82193300	6.32507700

C	0.28257700	23.76140300	7.27872100
H	-0.58106500	24.39123500	7.10327500
C	0.98846600	23.88695200	8.46721500
H	0.68692600	24.60185300	9.22149200
C	5.91869800	18.58786000	7.13723700
H	6.99588500	18.51193800	7.29533200
H	5.72252700	18.71273900	6.07078100
H	5.47115700	17.63845500	7.44747100
C	-0.02424800	22.66760900	5.01380800
H	0.12776800	21.67055700	4.59785600
H	0.36068200	23.39266800	4.28968700
H	-1.09457500	22.85126900	5.12402700
C	1.09540400	24.66365500	12.04023400
H	0.76527600	23.66136500	12.27983500
C	0.43637300	25.77523300	12.54389700
H	-0.42038700	25.63967200	13.19163800
C	0.88710500	27.05874500	12.21325100
C	1.98870200	27.14790700	11.35942000
H	2.36413600	28.12235000	11.07463300
C	2.60354500	25.99128400	10.88042700
C	0.21136700	28.28650500	12.75170800
H	-0.87251700	28.20695500	12.64341200
H	0.55416300	29.18434800	12.23639700
H	0.42245000	28.40361100	13.81952800
N	4.18935200	21.79431800	9.44812800
N	2.15728300	24.75595600	11.22118700
N	2.06387000	23.13562200	8.75989100
C	1.08864400	21.13283600	10.96122800
H	0.68566000	21.44693000	10.00761500
C	0.49425000	20.10486600	11.68006100
H	-0.38288300	19.61027700	11.28044300
C	1.03146300	19.71767200	12.91231700
C	2.15425800	20.41525400	13.36433800
H	2.59723100	20.15194400	14.31663700
C	2.70462900	21.43886400	12.59494400
C	3.88918400	22.21868700	12.99806500
C	4.55517100	22.04487300	14.21020500
H	4.20852500	21.30476800	14.92054000
C	5.67400200	22.82193400	14.52001400
C	6.08088300	23.76140200	13.56636800
H	6.94452500	24.39123200	13.74181300
C	5.37499400	23.88695100	12.37787300
H	5.67653500	24.60184900	11.62359600
C	0.44475200	18.58787000	13.70786000
H	-0.63243600	18.51195000	13.54976500
H	0.64092300	18.71274900	14.77431500

H	0.89229000	17.63846400	13.39762600
C	6.38770500	22.66761100	15.83128300
H	6.23568900	21.67055800	16.24723500
H	6.00277500	23.39267000	16.55540400
H	7.45803200	22.85127100	15.72106400
C	5.26805700	24.66364600	8.80485200
H	5.59818200	23.66135500	8.56525300
C	5.92709000	25.77522200	8.30118600
H	6.78384900	25.63965700	7.65344400
C	5.47636200	27.05873500	8.63182900
C	4.37476600	27.14790100	9.48566100
H	3.99933500	28.12234600	9.77044600
C	3.75992000	25.99128200	9.96465800
C	6.15210200	28.28649200	8.09336800
H	7.23598600	28.20694000	8.20166300
H	5.80930800	29.18433700	8.60867600
H	5.94101900	28.40359600	7.02554800
N	2.17410200	21.79432300	11.39696500
N	4.20617900	24.75595200	9.62390000
N	4.29958800	23.13562200	12.08519900

[Fe(dmb)₃]²⁺ quintet in 2-propanol, applied by CPCM, <S²> = 6.0119

Fe	3.18290800	23.21205200	10.41845900
C	5.40138400	21.12700000	9.58314700
H	5.81671200	21.45498300	10.52974200
C	6.01809400	20.13403600	8.83424800
H	6.92952400	19.67258900	9.19349800
C	5.44331000	19.72937400	7.62442200
C	4.26178700	20.36441200	7.22996100
H	3.78409600	20.06597100	6.30558700
C	3.69866000	21.36118600	8.02632500
C	2.44501600	22.07381000	7.66563400
C	1.78029600	21.88237300	6.45443900
H	2.17589600	21.19983000	5.71243200
C	0.59838600	22.57978200	6.18148500
C	0.13227400	23.46497700	7.15881400
H	-0.77265300	24.03878200	7.00070100
C	0.84649100	23.61156600	8.34039500
H	0.51546200	24.29397000	9.11506200
C	6.07848400	18.66655400	6.77569200
H	6.86887200	19.10333800	6.15788300
H	5.35062300	18.20416900	6.10724000
H	6.53780300	17.89376300	7.39441600
C	-0.14823900	22.37233100	4.89546200
H	-0.71362700	23.26484200	4.62258200
H	-0.86163400	21.54901500	5.00453700
H	0.53158400	22.11683600	4.08099000

C	0.91210700	24.88816900	11.84795200
H	0.55039100	23.89105900	12.06950900
C	0.23214300	26.01409900	12.28829800
H	-0.68090600	25.90604100	12.86032100
C	0.74364000	27.28312900	11.99021900
C	1.92868300	27.34241000	11.25354700
H	2.35396800	28.30815600	11.01490600
C	2.55720600	26.16964200	10.83188300
C	0.04513400	28.52913800	12.44891900
H	-0.91641900	28.63843600	11.93865400
H	0.64464000	29.41752200	12.24741300
H	-0.16266700	28.48001700	13.52067500
N	4.26729300	21.73104700	9.19624000
N	2.04915000	24.95423200	11.13600400
N	1.97752100	22.93746700	8.59470500
C	0.94533400	21.15024000	11.26705900
H	0.52084600	21.48000800	10.32484500
C	0.34120100	20.14811100	12.01410100
H	-0.56803700	19.68006500	11.65764900
C	0.92476900	19.74473400	13.22014000
C	2.10296500	20.38803300	13.60997800
H	2.58712400	20.08977200	14.53097700
C	2.65678700	21.38981200	12.81203700
C	3.91496200	22.09791200	13.16677900
C	4.57370900	21.90906300	14.38146700
H	4.16436700	21.24209200	15.12996800
C	5.76821100	22.58682800	14.65066900
C	6.25635400	23.44856000	13.66383600
H	7.17529500	24.00208400	13.81437700
C	5.54268900	23.60167600	12.48235900
H	5.88540200	24.27433400	11.70449900
C	0.30254400	18.67436100	14.06960600
H	-0.48191000	19.10451400	14.69970500
H	1.03957000	18.20993000	14.72664500
H	-0.16131600	17.90375100	13.45146300
C	6.50310200	22.37691300	15.94335500
H	7.19508000	23.19590300	16.14216700
H	7.08232000	21.44952500	15.89930900
H	5.80776200	22.28599300	16.77964000
C	5.45256700	24.89948100	9.00737400
H	5.81892200	23.90407600	8.78400000
C	6.12441100	26.02867400	8.56168300
H	7.03312700	25.92431300	7.98218600
C	5.61261000	27.29577000	8.86727100
C	4.43277500	27.34958900	9.61234400
H	4.00602900	28.31338400	9.85642300

C	3.81059900	26.17316600	10.03402400
C	6.30511700	28.54529100	8.40835700
H	7.26842900	28.65721800	8.91469500
H	5.70353200	29.43114200	8.61504200
H	6.50832100	28.50000300	7.33552100
N	2.07816800	21.76122500	11.64740600
N	4.32118700	24.96016600	9.72821400
N	4.39827800	22.94888200	12.23142700

[Fe(dmb)₃]²⁺ singlet in 1-butanol, applied by CPCM

Fe	3.18173100	23.23032100	10.42254500
C	5.28237600	21.13716000	9.88009700
H	5.68463100	21.45174300	10.83386600
C	5.88284200	20.11567700	9.15830700
H	6.76402000	19.62677200	9.55607400
C	5.34547700	19.72527000	7.92623000
C	4.21508300	20.41316100	7.47954000
H	3.76761000	20.14649300	6.53027500
C	3.66106400	21.43496500	8.25038000
C	2.47446100	22.21214000	7.84727400
C	1.80810600	22.03647000	6.63541000
H	2.15465300	21.29534900	5.92604000
C	0.68950100	22.81344900	6.32400600
C	0.28314600	23.75491900	7.27606000
H	-0.58005500	24.38531200	7.09967000
C	0.98933800	23.88228300	8.46426800
H	0.68787300	24.59887700	9.21701300
C	5.95011600	18.60467100	7.13030100
H	7.03990100	18.64456600	7.16781300
H	5.62883200	18.63628400	6.08895200
H	5.64611000	17.63932900	7.54705100
C	-0.02453000	22.65739500	5.01279100
H	0.12835600	21.66031300	4.59696400
H	0.35905000	23.38281800	4.28810100
H	-1.09520900	22.83957200	5.12319700
C	1.09493000	24.66334800	12.04054600
H	0.76379800	23.66141400	12.28032100
C	0.43714100	25.77517200	12.54551100
H	-0.41921000	25.63947600	13.19406100
C	0.88839400	27.05865300	12.21505500
C	1.98975900	27.14702000	11.36069600
H	2.36573400	28.12136600	11.07604500
C	2.60352800	25.99009300	10.88058700
C	0.21436400	28.28686800	12.75539700
H	-0.86991000	28.20881400	12.64870200
H	0.55714900	29.18518600	12.24068000
H	0.42714900	28.40261100	13.82310300

N	4.19168200	21.79298900	9.44695200
N	2.15655000	24.75479800	11.22087700
N	2.06440000	23.13098700	8.75858400
C	1.08107100	21.13714300	10.96487000
H	0.67881700	21.45178600	10.01112000
C	0.48059700	20.11562300	11.68660100
H	-0.40058600	19.62674900	11.28880500
C	1.01795900	19.72514100	12.91865500
C	2.14836000	20.41299600	13.36538500
H	2.59583000	20.14626700	14.31463500
C	2.70238600	21.43484100	12.59460500
C	3.88899100	22.21198800	12.99775800
C	4.55534100	22.03625200	14.20961600
H	4.20878900	21.29509300	14.91894300
C	5.67394400	22.81321400	14.52106800
C	6.08030500	23.75473600	13.56906700
H	6.94350500	24.38512000	13.74549300
C	5.37411800	23.88216500	12.38086300
H	5.67558500	24.59879900	11.62815700
C	0.41330900	18.60450400	13.71452400
H	-0.67647500	18.64439900	13.67699600
H	0.73457700	18.63607300	14.75588000
H	0.71732500	17.63918200	13.29773700
C	6.38796500	22.65709200	15.83228000
H	6.23505000	21.66000000	16.24807000
H	6.00440100	23.38250100	16.55699400
H	7.45865000	22.83924500	15.72188600
C	5.26855600	24.66342100	8.80463600
H	5.59969200	23.66149700	8.56482300
C	5.92635100	25.77526800	8.29972800
H	6.78271300	25.63959900	7.65118600
C	5.47509700	27.05873400	8.63024000
C	4.37371800	27.14706100	9.48458500
H	3.99774200	28.12139600	9.76927800
C	3.75994400	25.99011300	9.96463700
C	6.14914100	28.28697500	8.08997900
H	7.23341200	28.20891600	8.19670400
H	5.80634100	29.18526700	8.60473300
H	5.93638800	28.40277500	7.02227300
N	2.17176900	21.79293800	11.39805300
N	4.20692500	24.75483300	9.62429500
N	4.29905600	23.13088600	12.08650100

[Fe(dmb)₃]²⁺ quintet in 1-butanol, applied by CPCM, <S²> = 6.0118

Fe	3.17628300	23.21974100	10.42136000
C	5.37821700	21.11104400	9.60224500
H	5.79019000	21.43721900	10.55098800

C	5.99045600	20.11083800	8.85914600
H	6.89589000	19.64240200	9.22494000
C	5.41937100	19.70896300	7.64651800
C	4.24516300	20.35309700	7.24440700
H	3.77021900	20.05695000	6.31779300
C	3.68582100	21.35608900	8.03583600
C	2.43884800	22.07726500	7.66831800
C	1.77682300	21.88733500	6.45536100
H	2.16884400	21.19840500	5.71732100
C	0.60164100	22.59352700	6.17542800
C	0.13957600	23.48628900	7.14793800
H	-0.75976500	24.06753200	6.98454900
C	0.85022500	23.63024300	8.33212200
H	0.52127100	24.31691200	9.10402500
C	6.05091900	18.63996800	6.80230900
H	6.84536000	19.07093800	6.18521100
H	5.32243300	18.17958400	6.13294600
H	6.50452900	17.86597000	7.42397600
C	-0.14123600	22.38750500	4.88678300
H	-0.69695900	23.28403300	4.60695300
H	-0.86292000	21.57113600	4.99580100
H	0.53992600	22.12192100	4.07646100
C	0.91346400	24.90035400	11.85816300
H	0.55289800	23.90376600	12.08460800
C	0.23406000	26.02741400	12.29692600
H	-0.67726800	25.92026500	12.87210100
C	0.74394900	27.29587500	11.99331400
C	1.92689000	27.35337600	11.25276200
H	2.35065200	28.31874800	11.00957000
C	2.55473600	26.17958400	10.83259200
C	0.04503500	28.54334900	12.44863700
H	-0.91613000	28.65119300	11.93699400
H	0.64432200	29.43156000	12.24514500
H	-0.16391400	28.49726800	13.52039600
N	4.25183900	21.72426500	9.20749900
N	2.04793000	24.96479100	11.14202600
N	1.97428400	22.94709000	8.59329300
C	0.94937900	21.14632300	11.26977500
H	0.51753000	21.48243200	10.33318900
C	0.35407400	20.13467800	12.01127400
H	-0.55608700	19.66701900	11.65620200
C	0.94658000	19.72290300	13.21017100
C	2.12518800	20.36712400	13.59797600
H	2.61606800	20.06278500	14.51346200
C	2.66967400	21.37884300	12.80597900
C	3.92472000	22.09258300	13.16156800

C	4.59222800	21.89556900	14.37110100
H	4.19664400	21.21217800	15.11219000
C	5.77646400	22.58789700	14.64579500
C	6.24489500	23.47529800	13.67134800
H	7.15186400	24.04585500	13.83039000
C	5.52812100	23.62962800	12.49266900
H	5.85895300	24.31598100	11.72162700
C	0.33234200	18.64414400	14.05542700
H	-0.44853900	19.06807100	14.69461000
H	1.07466900	18.17563800	14.70370300
H	-0.13461000	17.87739500	13.43450800
C	6.52249000	22.37376100	15.93131400
H	7.08333400	23.26672900	16.21233200
H	7.24015500	21.55472100	15.81661600
H	5.84278800	22.10818700	16.74280800
C	5.44117100	24.90224800	8.99841500
H	5.80414200	23.90563100	8.77434000
C	6.11515700	26.02955500	8.55095700
H	7.02201900	25.92231500	7.96881000
C	5.60828800	27.29822500	8.85872700
C	4.43069200	27.35542700	9.60750700
H	4.00810200	28.32062800	9.85362600
C	3.80594900	26.18068800	10.03060300
C	6.30526900	28.54589300	8.40025400
H	7.26842200	28.65447400	8.90800800
H	5.70672700	29.43404600	8.60646700
H	6.50979100	28.50028200	7.32759400
N	2.08188700	21.75875800	11.64860400
N	4.31232600	24.96634300	9.72285700
N	4.39386100	22.96064100	12.23542700

[Fe(5,5'-dmb)₃]²⁺ singlet in gas phase

Fe	-0.14295900	2.67303300	4.87127000
N	0.93371500	2.77029500	6.58466500
N	1.17525300	4.12010200	4.34962500
N	-1.31070500	1.12847600	5.46743000
C	0.76110200	2.01383600	7.68386000
H	-0.06687900	1.31530100	7.65212200
C	1.56929000	2.09032600	8.82169400
C	2.61812800	3.01960500	8.78653600
H	3.28278800	3.12437700	9.63923400
C	2.81004700	3.80739300	7.65879400
H	3.62431200	4.52144800	7.63399300
C	1.95206100	3.66752100	6.56265100
C	2.06346300	4.45295700	5.32064300
C	3.00116900	5.47122500	5.11808900
H	3.70446100	5.73620600	5.89826700

C	3.02648300	6.15111500	3.90716600
H	3.75222200	6.94314100	3.74640700
C	2.11527100	5.81560500	2.89623900
C	1.21180000	4.78816900	3.18230700
H	0.48416500	4.48272900	2.43948100
C	1.32143000	1.21223500	10.01893200
H	2.18567900	0.56941000	10.21682800
H	0.44928700	0.56996200	9.87582500
H	1.15560100	1.81352600	10.91880800
C	2.10110500	6.52385800	1.56807800
H	1.89662900	7.59189000	1.69770600
H	1.34086600	6.11378100	0.89912500
H	3.07212700	6.44096500	1.06899600
C	-2.52037200	1.21656100	6.04981500
H	-2.87542900	2.22008600	6.25335100
C	-3.30585100	0.11274500	6.39381900
C	-2.77653100	-1.15153300	6.10009900
H	-3.34035800	-2.04819800	6.34080000
C	-1.52936800	-1.25920100	5.49821700
H	-1.12572800	-2.23800400	5.26900900
C	-0.80793800	-0.10120300	5.18873500
C	-4.65329100	0.28212800	7.04309700
H	-5.44425200	-0.14467000	6.41738200
H	-4.89012200	1.33480700	7.21457400
H	-4.69198300	-0.23540900	8.00720700
N	-1.21963400	2.77029600	3.15787400
N	-1.46117100	4.12010200	5.39291600
N	1.02478600	1.12847600	4.27510800
C	-1.04702100	2.01383900	2.05867900
H	-0.21904000	1.31530300	2.09041600
C	-1.85520900	2.09032900	0.92084500
C	-2.90404700	3.01960800	0.95600400
H	-3.56870700	3.12438100	0.10330500
C	-3.09596600	3.80739500	2.08374700
H	-3.91023100	4.52145000	2.10854800
C	-2.23798000	3.66752300	3.17988900
C	-2.34938200	4.45295800	4.42189800
C	-3.28708700	5.47122600	4.62445300
H	-3.99037900	5.73620700	3.84427500
C	-3.31240200	6.15111500	5.83537600
H	-4.03814100	6.94314100	5.99613600
C	-2.40118900	5.81560400	6.84630300
C	-1.49771800	4.78816800	6.56023300
H	-0.77008400	4.48272700	7.30305900
C	-1.60735000	1.21223900	-0.27639300
H	-2.47159800	0.56941500	-0.47429100

H	-0.73520700	0.56996600	-0.13328700
H	-1.44152000	1.81353100	-1.17626900
C	-2.38702300	6.52385600	8.17446400
H	-2.18254800	7.59188800	8.04483700
H	-1.62678500	6.11377800	8.84341600
H	-3.35804500	6.44096300	8.67354600
C	2.23445300	1.21656200	3.69272300
H	2.58951000	2.22008700	3.48918800
C	3.01993100	0.11274600	3.34871900
C	2.49061100	-1.15153300	3.64243700
H	3.05443900	-2.04819700	3.40173500
C	1.24344800	-1.25920100	4.24431900
H	0.83980800	-2.23800400	4.47352700
C	0.52201900	-0.10120300	4.55380200
C	4.36737200	0.28212900	2.69944100
H	5.15833300	-0.14466900	3.32515500
H	4.60420300	1.33480800	2.52796400
H	4.40606400	-0.23540700	1.73533000

[Fe(5,5'-dmb)₃]²⁺ quintet in gas phase, <S²> = 6.0108

Fe	-0.14294900	2.66326200	4.87127300
N	1.07611600	2.90725000	6.71693700
N	1.39759700	4.21533700	4.39297900
N	-1.30707100	0.89218300	5.55567400
C	0.89830800	2.17576400	7.83004800
H	0.05710600	1.48915500	7.81341600
C	1.71810000	2.25797300	8.95901300
C	2.78445000	3.16466200	8.88523300
H	3.46471600	3.27299800	9.72539100
C	2.98057900	3.92519200	7.73837000
H	3.81536900	4.61349400	7.69123400
C	2.10475200	3.78398600	6.65538000
C	2.23733000	4.55831700	5.39529100
C	3.16478600	5.59335200	5.22602700
H	3.83022900	5.88143800	6.03053700
C	3.22507200	6.26914200	4.01280200
H	3.94274800	7.07371400	3.87936000
C	2.36150500	5.91811100	2.96651200
C	1.46517500	4.87661000	3.22653800
H	0.76416700	4.55663600	2.46084800
C	1.46796000	1.41385900	10.17970600
H	2.32910300	0.77261800	10.39498500
H	0.59262900	0.77219300	10.05397900
H	1.30448900	2.04007300	11.06297100
C	2.38939000	6.62103100	1.63601400
H	2.18099100	7.68961600	1.75375300
H	1.65051200	6.20736400	0.94554200

H	3.37547100	6.53559300	1.16762200
C	-2.50267600	0.95678300	6.16453400
H	-2.84913400	1.95497000	6.41665300
C	-3.28693800	-0.15906300	6.47204100
C	-2.76373600	-1.40482000	6.09990800
H	-3.32552700	-2.31260300	6.30164700
C	-1.52864000	-1.48591600	5.46693900
H	-1.14354500	-2.45424100	5.17194200
C	-0.80672200	-0.31504900	5.20549500
C	-4.61898900	-0.02305500	7.15924800
H	-5.42230900	-0.43782000	6.54141000
H	-4.85972800	1.02185400	7.36894100
H	-4.62846900	-0.56945700	8.10817500
N	-1.36199300	2.90720700	3.02559700
N	-1.68352800	4.21528800	5.34957300
N	1.02111400	0.89216100	4.18684400
C	-1.18417100	2.17573200	1.91248000
H	-0.34296400	1.48913000	1.92911400
C	-2.00395700	2.25793800	0.78351100
C	-3.07032000	3.16461200	0.85729200
H	-3.75058400	3.27294300	0.01713300
C	-3.26646400	3.92513100	2.00415900
H	-4.10126500	4.61342000	2.05129500
C	-2.39064000	3.78393300	3.08715400
C	-2.52323900	4.55826500	4.34724000
C	-3.45069700	5.59330400	4.51647900
H	-4.11612200	5.88138700	3.71195300
C	-3.51100500	6.26910300	5.72969700
H	-4.22868200	7.07367900	5.86311700
C	-2.64746200	5.91807700	6.77600700
C	-1.75113300	4.87656900	6.51600800
H	-1.05014500	4.55659600	7.28171800
C	-1.75379900	1.41383500	-0.43718600
H	-2.61493400	0.77258600	-0.65247500
H	-0.87846200	0.77217900	-0.31145700
H	-1.59032900	2.04005700	-1.32044600
C	-2.67537000	6.62100800	8.10649900
H	-2.46695400	7.68958900	7.98875600
H	-1.93651600	6.20733600	8.79699200
H	-3.66146400	6.53558900	8.57486600
C	2.21672500	0.95674400	3.57799300
H	2.56318200	1.95492300	3.32583900
C	3.00099400	-0.15911100	3.27053300
C	2.47778800	-1.40485800	3.64269400
H	3.03958100	-2.31264600	3.44098700
C	1.24268400	-1.48593500	4.27565100

H	0.85758500	-2.45425200	4.57067000
C	0.52076500	-0.31506000	4.53705600
C	4.33305400	-0.02312200	2.58334000
H	5.13636900	-0.43785000	3.20121100
H	4.57378600	1.02178000	2.37360200
H	4.34255500	-0.56956900	1.63444000

[Fe(5,5'-dmb)₃]²⁺ singlet in methanol, applied by CPCM

Fe	-0.14295900	2.64970600	4.87126900
N	0.89520200	2.74174900	6.58376700
N	1.16008400	4.08356500	4.36248100
N	-1.29821600	1.13774700	5.47446900
C	0.69513600	1.99126800	7.67885200
H	-0.10849700	1.26732900	7.62279400
C	1.45171000	2.11141900	8.84509800
C	2.46799400	3.07294600	8.84833400
H	3.08358100	3.20373700	9.72946200
C	2.68304000	3.85734200	7.72412500
H	3.46572800	4.60597400	7.72260400
C	1.88364500	3.66961000	6.59479900
C	2.02027400	4.43675500	5.34890900
C	2.95047000	5.46083900	5.16102600
H	3.63320700	5.72758100	5.95542400
C	2.99882100	6.12601100	3.94387600
H	3.71626100	6.92312300	3.78862300
C	2.11338600	5.76865500	2.92056200
C	1.21880600	4.73237100	3.18867800
H	0.51866200	4.41520200	2.42675400
C	1.17377200	1.24167200	10.03691200
H	2.07981300	0.72675300	10.36243500
H	0.41492600	0.49305700	9.80773200
H	0.81803300	1.83830300	10.88038500
C	2.11231900	6.44587700	1.58113900
H	1.92628600	7.51748500	1.68615200
H	1.34136400	6.02520100	0.93438900
H	3.07818600	6.33209700	1.08147100
C	-2.47435100	1.23968200	6.11453200
H	-2.83211500	2.24493000	6.29924800
C	-3.20678800	0.13648700	6.55480900
C	-2.67597800	-1.13050700	6.28597500
H	-3.20775400	-2.01817300	6.60723200
C	-1.46811300	-1.24819500	5.61339400
H	-1.05341000	-2.22397700	5.40229500
C	-0.79123400	-0.09293100	5.21765200
C	-4.51071300	0.31723400	7.27737000
H	-5.33742100	-0.09695800	6.69558800
H	-4.71442500	1.37427600	7.45437100

H	-4.49952500	-0.20029500	8.23992100
N	-1.18112100	2.74175100	3.15877100
N	-1.44600200	4.08356400	5.38005900
N	1.01229800	1.13774800	4.26806800
C	-0.98105600	1.99127100	2.06368600
H	-0.17742400	1.26733000	2.11974300
C	-1.73763200	2.11142200	0.89744100
C	-2.75391600	3.07294900	0.89420600
H	-3.36950400	3.20374000	0.01307900
C	-2.96895900	3.85734500	2.01841500
H	-3.75164700	4.60597700	2.01993800
C	-2.16956400	3.66961200	3.14774000
C	-2.30619200	4.43675600	4.39363100
C	-3.23638800	5.46084000	4.58151600
H	-3.91912500	5.72758400	3.78711800
C	-3.28473800	6.12601000	5.79866700
H	-4.00217800	6.92312300	5.95392100
C	-2.39930300	5.76865200	6.82198000
C	-1.50472300	4.73236900	6.55386300
H	-0.80458000	4.41519800	7.31578600
C	-1.45969700	1.24167300	-0.29437300
H	-2.36573900	0.72675500	-0.61989400
H	-0.70085100	0.49305800	-0.06519300
H	-1.10395800	1.83830300	-1.13784700
C	-2.39823600	6.44587200	8.16140400
H	-2.21220200	7.51748100	8.05639400
H	-1.62728100	6.02519500	8.80815400
H	-3.36410200	6.33209200	8.66107200
C	2.18843200	1.23968300	3.62800500
H	2.54619600	2.24493100	3.44328800
C	2.92087000	0.13648800	3.18772700
C	2.39006100	-1.13050600	3.45656200
H	2.92183700	-2.01817200	3.13530600
C	1.18219500	-1.24819500	4.12914300
H	0.76749300	-2.22397700	4.34024300
C	0.50531600	-0.09293100	4.52488500
C	4.22479500	0.31723600	2.46516600
H	5.05150300	-0.09695600	3.04694800
H	4.42850600	1.37427700	2.28816400
H	4.21360700	-0.20029400	1.50261600

[Fe(5,5'-dmb)₃]²⁺ quintet in methanol, applied by CPCM, <S²> = 6.0209

Fe	-0.14295300	2.57909600	4.87127300
N	0.95132900	2.86951800	6.72957400
N	1.31873700	4.14531600	4.39785000
N	-1.29121100	0.86924500	5.56621400
C	0.76424400	2.14147200	7.84018100

H	-0.03098100	1.40385000	7.79620000
C	1.53208300	2.28820800	8.99527700
C	2.53966100	3.25846500	8.95940000
H	3.17354000	3.40740500	9.82519200
C	2.73458700	4.02344400	7.81723000
H	3.52443200	4.76226500	7.78942200
C	1.91924500	3.81332400	6.70204100
C	2.06207500	4.57403300	5.44040200
C	2.90640200	5.68102500	5.30965500
H	3.47458000	6.04383500	6.15501300
C	2.98993800	6.33243100	4.08613300
H	3.63383400	7.19613300	3.97388400
C	2.24748800	5.87103500	2.99372800
C	1.41577200	4.77293600	3.21829900
H	0.79126600	4.38526400	2.41984000
C	1.28688800	1.43812200	10.20760000
H	2.20907000	0.95250700	10.53277000
H	0.54614100	0.66485100	10.00203900
H	0.92488400	2.04222700	11.04293700
C	2.31402900	6.53095800	1.64706300
H	2.13663600	7.60575900	1.73008200
H	1.57329100	6.10984300	0.96603300
H	3.30259600	6.39898000	1.19796100
C	-2.43673400	0.95069100	6.25687300
H	-2.78859300	1.95522900	6.47164800
C	-3.15238700	-0.16532500	6.69336100
C	-2.61874800	-1.41676100	6.36600400
H	-3.13266300	-2.31852200	6.67798200
C	-1.43449700	-1.51129900	5.64695100
H	-1.03288700	-2.48263200	5.39561800
C	-0.77979000	-0.34138600	5.25191200
C	-4.43525100	-0.01606300	7.45801700
H	-5.27467200	-0.42200100	6.88869700
H	-4.64206100	1.03455500	7.66742500
H	-4.39141200	-0.55795900	8.40601600
N	-1.23724100	2.86948600	3.01296800
N	-1.60465100	4.14531200	5.34467800
N	1.00528900	0.86923600	4.17634100
C	-1.05015100	2.14143400	1.90236500
H	-0.25493000	1.40380900	1.94635400
C	-1.81798200	2.28816600	0.74726300
C	-2.82555600	3.25842700	0.78312700
H	-3.45942800	3.40736400	-0.08267000
C	-3.02048600	4.02341300	1.92529000
H	-3.81032700	4.76223900	1.95308800
C	-2.20515200	3.81329700	3.04048800

C	-2.34799000	4.57401400	4.30212000
C	-3.19232700	5.68099900	4.43285600
H	-3.76050700	6.04379800	3.58749500
C	-3.27587300	6.33241400	5.65637200
H	-3.91977700	7.19611100	5.76861300
C	-2.53342500	5.87103100	6.74878400
C	-1.70169800	4.77293800	6.52422500
H	-1.07719200	4.38527700	7.32268800
C	-1.57278100	1.43807200	-0.46505300
H	-2.49496000	0.95245300	-0.79022400
H	-0.83203300	0.66480500	-0.25948500
H	-1.21077500	2.04217200	-1.30039300
C	-2.59998500	6.53096200	8.09544500
H	-2.42259200	7.60576300	8.01242100
H	-1.85925500	6.10985200	8.77648800
H	-3.58855700	6.39898300	8.54453400
C	2.15081500	0.95067600	3.48568500
H	2.50267600	1.95521200	3.27090300
C	2.86646700	-0.16534500	3.04920700
C	2.33282300	-1.41677700	3.37657000
H	2.84673500	-2.31854200	3.06459800
C	1.14856800	-1.51130800	4.09562000
H	0.74695500	-2.48263800	4.34695600
C	0.49386400	-0.34139100	4.49065000
C	4.14933400	-0.01609100	2.28455600
H	4.98875100	-0.42203400	2.85387800
H	4.35615000	1.03452600	2.07514800
H	4.10549400	-0.55798700	1.33655600

[Fe(5,5'-dmb)₃]²⁺ singlet in ethanol, applied by CPCM

Fe	-0.14296000	2.65133200	4.87126900
N	0.89880300	2.74457500	6.58465300
N	1.16310200	4.08658600	4.36148100
N	-1.29868300	1.13579200	5.47486700
C	0.70144900	1.99316100	7.68006800
H	-0.10306200	1.27005200	7.62544300
C	1.46054600	2.11168200	8.84514100
C	2.47802600	3.07236000	8.84616400
H	3.09635500	3.20328700	9.72595000
C	2.69205200	3.85618700	7.72108600
H	3.47682400	4.60248600	7.71856400
C	1.88911900	3.67080800	6.59342400
C	2.02462800	4.43895500	5.34734800
C	2.95608700	5.46216800	5.15808300
H	3.63953900	5.73043400	5.95176700
C	3.00392100	6.12713500	3.94064700
H	3.72266000	6.92350700	3.78507300

C	2.11807500	5.77015400	2.91732700
C	1.22164100	4.73555300	3.18733600
H	0.52063100	4.41780300	2.42628200
C	1.18384000	1.24238800	10.03841000
H	2.09038600	0.72667100	10.36276800
H	0.42361400	0.49382900	9.81212300
H	0.83060500	1.84056300	10.88244400
C	2.11876400	6.44890000	1.57788100
H	1.93472600	7.52111500	1.68428900
H	1.34769200	6.03129200	0.92886000
H	3.08536100	6.33382500	1.07932900
C	-2.47698500	1.23653600	6.11155400
H	-2.83507500	2.24160900	6.29666200
C	-3.21295700	0.13336100	6.54683600
C	-2.68135600	-1.13353400	6.27823600
H	-3.21409100	-2.02233500	6.59603800
C	-1.47091300	-1.25048200	5.60963100
H	-1.05613700	-2.22682000	5.39971300
C	-0.79189100	-0.09499900	5.21694700
C	-4.51962600	0.31391200	7.26576600
H	-5.34456100	-0.10313400	6.68265600
H	-4.72631400	1.37088400	7.44106900
H	-4.50991600	-0.20186600	8.22963200
N	-1.18472300	2.74457700	3.15788500
N	-1.44902200	4.08658600	5.38105900
N	1.01276300	1.13579200	4.26767100
C	-0.98736900	1.99316300	2.06247100
H	-0.18285800	1.27005400	2.11709500
C	-1.74646500	2.11168700	0.89739700
C	-2.76394400	3.07236500	0.89637500
H	-3.38227300	3.20329500	0.01658800
C	-2.97797100	3.85619000	2.02145300
H	-3.76274200	4.60249100	2.02397600
C	-2.17503900	3.67081000	3.14911600
C	-2.31054800	4.43895600	4.39519200
C	-3.24200700	5.46216900	4.58445800
H	-3.92545800	5.73043600	3.79077500
C	-3.28984000	6.12713500	5.80189500
H	-4.00857900	6.92350800	5.95746900
C	-2.40399400	5.77015300	6.82521400
C	-1.50756000	4.73555200	6.55520400
H	-0.80655000	4.41780100	7.31625800
C	-1.46975800	1.24239400	-0.29587300
H	-2.37630500	0.72667900	-0.62023300
H	-0.70953400	0.49383400	-0.06958700
H	-1.11652200	1.84057000	-1.13990600

C	-2.40468200	6.44889800	8.16466100
H	-2.22064400	7.52111300	8.05825400
H	-1.63361100	6.03129000	8.81368100
H	-3.37128000	6.33382300	8.66321300
C	2.19106500	1.23653700	3.63098400
H	2.54915400	2.24161100	3.44587600
C	2.92703800	0.13336300	3.19570200
C	2.39543800	-1.13353200	3.46430300
H	2.92817400	-2.02233400	3.14650100
C	1.18499500	-1.25048200	4.13290700
H	0.77022000	-2.22681900	4.34282600
C	0.50597200	-0.09499900	4.52559100
C	4.23370700	0.31391400	2.47677300
H	5.05864200	-0.10313100	3.05988400
H	4.44039400	1.37088600	2.30146900
H	4.22399700	-0.20186500	1.51290700

[Fe(5,5'-dmb)₃]²⁺ quintet in ethanol, applied by CPCM, <S²> = 6.0146

Fe	-0.14296300	2.59398400	4.87127200
N	0.97671900	2.88074400	6.72902600
N	1.35003200	4.14797800	4.40139200
N	-1.29019300	0.87247600	5.56872100
C	0.78091600	2.15471000	7.83929600
H	-0.01777300	1.42111800	7.79228500
C	1.54391900	2.29899400	8.99873900
C	2.55508600	3.26589100	8.96661200
H	3.18501700	3.41497900	9.83580800
C	2.75847000	4.02953600	7.82428900
H	3.54881500	4.76833400	7.80183100
C	1.94907100	3.81926600	6.70476700
C	2.10007800	4.57493600	5.43939300
C	2.95581900	5.67193400	5.30126000
H	3.53478800	6.02987100	6.14167200
C	3.04044700	6.31813000	4.07439000
H	3.69430900	7.17433800	3.95692400
C	2.28804100	5.86103600	2.98684700
C	1.44940200	4.76899300	3.21867200
H	0.82124400	4.38107400	2.42299400
C	1.28855400	1.45032400	10.21098700
H	2.20574600	0.95568100	10.53817900
H	0.54052900	0.68395900	10.00409700
H	0.93080600	2.05805500	11.04612200
C	2.35527300	6.51400100	1.63614800
H	2.17814100	7.58959100	1.71337400
H	1.61410900	6.08976600	0.95709700
H	3.34406500	6.37926200	1.18783300
C	-2.43522400	0.95112100	6.26122900

H	-2.78887300	1.95446600	6.47803100
C	-3.15169700	-0.16538500	6.69622100
C	-2.61743800	-1.41650600	6.36804600
H	-3.13022800	-2.31967300	6.67915700
C	-1.43309200	-1.50900500	5.64847900
H	-1.03094100	-2.48051900	5.39749900
C	-0.77928000	-0.33817400	5.25309400
C	-4.43465400	-0.01722900	7.46237300
H	-5.27470900	-0.42408600	6.89373600
H	-4.64332400	1.03293800	7.67342800
H	-4.38949300	-0.55962200	8.41039300
N	-1.26263700	2.88073200	3.01351200
N	-1.63596100	4.14798500	5.34113200
N	1.00428200	0.87247100	4.17385000
C	-1.06682500	2.15469000	1.90325000
H	-0.26813400	1.42110000	1.95027100
C	-1.82982000	2.29896300	0.74380100
C	-2.84098900	3.26585900	0.77591400
H	-3.47091400	3.41493900	-0.09328800
C	-3.04438200	4.02951400	1.91822800
H	-3.83472800	4.76831000	1.94067600
C	-2.23498900	3.81925400	3.03775700
C	-2.38600300	4.57493300	4.30312500
C	-3.24174700	5.67193100	4.44124600
H	-3.82071100	6.02986200	3.60082900
C	-3.32638200	6.31813400	5.66811200
H	-3.98024600	7.17434200	5.78556900
C	-2.57398100	5.86104900	6.75566200
C	-1.73533800	4.76900600	6.52384800
H	-1.10718200	4.38109400	7.31953000
C	-1.57444600	1.45028400	-0.46844000
H	-2.49163200	0.95563200	-0.79563100
H	-0.82641600	0.68392700	-0.26154000
H	-1.21669800	2.05801100	-1.30357800
C	-2.64122500	6.51402200	8.10635600
H	-2.46409400	7.58961200	8.02912400
H	-1.90006700	6.08979400	8.78541700
H	-3.63002200	6.37928500	8.55466300
C	2.14931100	0.95111200	3.48133800
H	2.50296100	1.95445500	3.26453100
C	2.86578100	-0.16539800	3.04635000
C	2.33152200	-1.41651600	3.37453300
H	2.84431000	-2.31968600	3.06342600
C	1.14717800	-1.50901000	4.09410300
H	0.74502600	-2.48052300	4.34508900
C	0.49336700	-0.33817600	4.48948400

C	4.14873800	-0.01724700	2.28019500
H	4.98879300	-0.42410600	2.84883100
H	4.35741000	1.03291800	2.06913800
H	4.10357300	-0.55964200	1.33217600

[Fe(5,5'-dmb)₃]²⁺ singlet in 2-propanol, applied by CPCM

Fe	-0.14296100	2.65246700	4.87126900
N	0.90132600	2.74655200	6.58503300
N	1.16481100	4.08868100	4.36063400
N	-1.29905100	1.13451200	5.47505700
C	0.70581400	1.99461600	7.68071400
H	-0.09942100	1.27221500	7.62717600
C	1.46691900	2.11184800	8.84480100
C	2.48545900	3.07167300	8.84406700
H	3.10592300	3.20243500	9.72275400
C	2.69863800	3.85513600	7.71840200
H	3.48496700	4.59970800	7.71496300
C	1.89299000	3.67156200	6.59209000
C	2.02749300	4.44042600	5.34591000
C	2.95969400	5.46309800	5.15556900
H	3.64381200	5.73230000	5.94862700
C	3.00689700	6.12795700	3.93794900
H	3.72645500	6.92382700	3.78199600
C	2.12046800	5.77131800	2.91485600
C	1.22284500	4.73786000	3.18631100
H	0.52084300	4.41992500	2.42612300
C	1.19115000	1.24289300	10.03905800
H	2.09794100	0.72631500	10.36230600
H	0.42967600	0.49466400	9.81490300
H	0.84007400	1.84213100	10.88361600
C	2.12202300	6.45100200	1.57537800
H	1.93928000	7.52359700	1.68265400
H	1.35080100	6.03531800	0.92503200
H	3.08899900	6.33510600	1.07738300
C	-2.47900600	1.23444100	6.10910700
H	-2.83715700	2.23940600	6.29475800
C	-3.21776500	0.13126500	6.54018500
C	-2.68575300	-1.13555400	6.27146700
H	-3.21951200	-2.02509900	6.58628400
C	-1.47328400	-1.25198300	5.60612300
H	-1.05858000	-2.22867200	5.39672600
C	-0.79246200	-0.09633700	5.21621900
C	-4.52662700	0.31159600	7.25597300
H	-5.34997600	-0.10760300	6.67164700
H	-4.73558100	1.36850900	7.42981200
H	-4.51834300	-0.20282500	8.22080300
N	-1.18724700	2.74655300	3.15750500

N	-1.45073300	4.08868000	5.38190600
N	1.01312900	1.13451200	4.26748200
C	-0.99173400	1.99462000	2.06182300
H	-0.18649800	1.27222000	2.11536000
C	-1.75283600	2.11185600	0.89773400
C	-2.77137500	3.07168100	0.89846800
H	-3.39183600	3.20244700	0.01978100
C	-2.98455700	3.85514000	2.02413600
H	-3.77088600	4.59971200	2.02757500
C	-2.17891100	3.67156300	3.15044900
C	-2.31341500	4.44042500	4.39662900
C	-3.24561600	5.46309800	4.58697100
H	-3.92973400	5.73230000	3.79391300
C	-3.29281900	6.12795700	5.80459100
H	-4.01237600	6.92382600	5.96054500
C	-2.40639000	5.77131700	6.82768400
C	-1.50876700	4.73785900	6.55622900
H	-0.80676400	4.41992400	7.31641700
C	-1.47706100	1.24290700	-0.29652700
H	-2.38385100	0.72633200	-0.61978100
H	-0.71558900	0.49467800	-0.07237200
H	-1.12598200	1.84215000	-1.14108000
C	-2.40794400	6.45100100	8.16716200
H	-2.22520100	7.52359500	8.05988700
H	-1.63672200	6.03531700	8.81750800
H	-3.37492000	6.33510500	8.66515800
C	2.19308500	1.23444100	3.63343300
H	2.55123600	2.23940600	3.44778100
C	2.93184600	0.13126500	3.20235700
C	2.39983400	-1.13555400	3.47107600
H	2.93359400	-2.02510000	3.15626300
C	1.18736400	-1.25198300	4.13641900
H	0.77266100	-2.22867200	4.34581800
C	0.50654100	-0.09633700	4.52632100
C	4.24070800	0.31159600	2.48657200
H	5.06405700	-0.10760200	3.07090100
H	4.44966200	1.36850800	2.31273000
H	4.23242800	-0.20282800	1.52174300

[Fe(5,5'-dmb)₃]²⁺ quintet in 2-propanol, applied by CPCM, <S²> = 6.0130

Fe	-0.14297200	2.60454200	4.87127200
N	0.98974700	2.88330900	6.72938500
N	1.36554600	4.15268000	4.40314600
N	-1.28965900	0.87600400	5.56984200
C	0.79361700	2.15525500	7.83851200
H	-0.00730700	1.42418900	7.79103500
C	1.55712900	2.29573600	8.99844300

C	2.57090700	3.26014100	8.96738000
H	3.20138600	3.40740500	9.83681500
C	2.77633700	4.02441400	7.82564100
H	3.56889300	4.76093100	7.80442200
C	1.96566400	3.81793300	6.70606600
C	2.11872300	4.57476700	5.44110600
C	2.98022300	5.66744900	5.30335000
H	3.56267500	6.02130700	6.14325600
C	3.06815000	6.31418400	4.07686900
H	3.72742800	7.16673500	3.96028200
C	2.31260300	5.86254000	2.98911100
C	1.46847500	4.77445300	3.22079200
H	0.83938300	4.39005600	2.42419700
C	1.29871100	1.44655600	10.21028100
H	2.21383800	0.94684600	10.53652300
H	0.54628300	0.68411600	10.00375000
H	0.94493300	2.05566400	11.04650900
C	2.38480900	6.51530100	1.63811400
H	2.20812000	7.59123400	1.71451200
H	1.64568600	6.09188800	0.95605400
H	3.37531200	6.37976300	1.19351400
C	-2.43502900	0.95366300	6.26226700
H	-2.78926300	1.95658000	6.47984700
C	-3.15235700	-0.16293200	6.69629500
C	-2.61792600	-1.41406000	6.36791900
H	-3.13044600	-2.31789900	6.67833900
C	-1.43331400	-1.50578000	5.64838700
H	-1.03109200	-2.47751600	5.39758800
C	-0.77915000	-0.33470600	5.25351800
C	-4.43547500	-0.01508200	7.46312000
H	-5.27584400	-0.42268800	6.89493000
H	-4.64529500	1.03486500	7.67486600
H	-4.38962000	-0.55750200	8.41132100
N	-1.27566800	2.88332300	3.01315000
N	-1.65148600	4.15270900	5.33936600
N	1.00376300	0.87600000	4.17276000
C	-1.07952000	2.15525500	1.90403600
H	-0.27859400	1.42419200	1.95153300
C	-1.84301500	2.29572300	0.74409200
C	-2.85679200	3.26013000	0.77512900
H	-3.48725700	3.40738500	-0.09431700
C	-3.06223800	4.02441900	1.91685600
H	-3.85479100	4.76094000	1.93805300
C	-2.25158300	3.81794800	3.03644400
C	-2.40465700	4.57479000	4.30139900
C	-3.26616000	5.66747000	4.43914500

H	-3.84860400	6.02132500	3.59923200
C	-3.35409900	6.31420500	5.66562500
H	-4.01338200	7.16675400	5.78220500
C	-2.59856300	5.86256400	6.75339100
C	-1.75442600	4.77448100	6.52171900
H	-1.12534000	4.39008900	7.31831900
C	-1.58457900	1.44653000	-0.46773200
H	-2.49969900	0.94680900	-0.79397600
H	-0.83214800	0.68409900	-0.26118400
H	-1.23079800	2.05563000	-1.30396400
C	-2.67078900	6.51532500	8.10438700
H	-2.49410200	7.59125800	8.02799100
H	-1.93167500	6.09191500	8.78645700
H	-3.66129800	6.37978300	8.54897200
C	2.14912600	0.95365400	3.48032300
H	2.50336200	1.95657000	3.26274100
C	2.86644400	-0.16294300	3.04628600
C	2.33201500	-1.41406900	3.37467400
H	2.84453000	-2.31791000	3.06425300
C	1.14741000	-1.50578400	4.09421800
H	0.74518900	-2.47751900	4.34502600
C	0.49325100	-0.33470800	4.48908900
C	4.14955500	-0.01510000	2.27944900
H	4.98992800	-0.42270400	2.84763300
H	4.35937500	1.03484500	2.06769400
H	4.10368900	-0.55752500	1.33125100

[Fe(5,5'-dmb)₃]²⁺ singlet in 1-butanol, applied by CPCM

Fe	-0.14296000	2.65314700	4.87126900
N	0.90285200	2.74772100	6.58514800
N	1.16567900	4.08991700	4.36005500
N	-1.29928300	1.13379400	5.47513000
C	0.70842600	1.99551800	7.68099700
H	-0.09729900	1.27360500	7.62815200
C	1.47084200	2.11191400	8.84441800
C	2.49010700	3.07111900	8.84254900
H	3.11193800	3.20166900	9.72050900
C	2.70272200	3.85438500	7.71654500
H	3.49001800	4.59788800	7.71247000
C	1.89534300	3.67196200	6.59112300
C	2.02914100	4.44127000	5.34489900
C	2.96172300	5.46365100	5.15387600
H	3.64630600	5.73335600	5.94650900
C	3.00843200	6.12847200	3.93615800
H	3.72843300	6.92405700	3.77992100
C	2.12154000	5.77206400	2.91329500
C	1.22326600	4.73925900	3.18565100

H	0.52055100	4.42128900	2.42606300
C	1.19566700	1.24317200	10.03925700
H	2.10255600	0.72593300	10.36169600
H	0.43331100	0.49528000	9.81642700
H	0.84608000	1.84304600	10.88418900
C	2.12344400	6.45226600	1.57379700
H	1.94141100	7.52506600	1.68155900
H	1.35210300	6.03762800	0.92277400
H	3.09059100	6.33593500	1.07603100
C	-2.48029100	1.23325200	6.10746500
H	-2.83840400	2.23815600	6.29356900
C	-3.22086700	0.13007100	6.53569800
C	-2.68869200	-1.13670200	6.26676400
H	-3.22323000	-2.02667100	6.57951700
C	-1.47491000	-1.25282600	5.60358500
H	-1.06031700	-2.22971100	5.39434200
C	-0.79285600	-0.09708100	5.21566600
C	-4.53115600	0.31025200	7.24934500
H	-5.35341500	-0.11029200	6.66416700
H	-4.74152600	1.36712700	7.42219100
H	-4.52390100	-0.20330300	8.21477200
N	-1.18877200	2.74772300	3.15739000
N	-1.45159900	4.08991700	5.38248500
N	1.01336300	1.13379400	4.26740800
C	-0.99434500	1.99552100	2.06154000
H	-0.18862000	1.27360800	2.11438400
C	-1.75676100	2.11191900	0.89811900
C	-2.77602700	3.07112300	0.89999000
H	-3.39785700	3.20167500	0.02203000
C	-2.98864200	3.85438800	2.02599500
H	-3.77593800	4.59789100	2.03007100
C	-2.18126300	3.67196400	3.15141600
C	-2.31506100	4.44127100	4.39764100
C	-3.24764300	5.46365100	4.58866500
H	-3.93222600	5.73335600	3.79603300
C	-3.29435100	6.12847100	5.80638400
H	-4.01435200	6.92405500	5.96262200
C	-2.40745900	5.77206200	6.82924700
C	-1.50918500	4.73925700	6.55688900
H	-0.80647000	4.42128700	7.31647700
C	-1.48158500	1.24317900	-0.29672100
H	-2.38847400	0.72594100	-0.61916200
H	-0.71923000	0.49528700	-0.07389300
H	-1.13199800	1.84305500	-1.14165100
C	-2.40936300	6.45226300	8.16874500
H	-2.22733000	7.52506300	8.06098400

H	-1.63802100	6.03762400	8.81976700
H	-3.37651000	6.33593200	8.66651100
C	2.19437200	1.23325200	3.63507300
H	2.55248600	2.23815600	3.44896900
C	2.93494800	0.13007100	3.20684100
C	2.40277300	-1.13670200	3.47577500
H	2.93731200	-2.02667100	3.16302300
C	1.18899100	-1.25282600	4.13895300
H	0.77439800	-2.22971200	4.34819700
C	0.50693600	-0.09708100	4.52687200
C	4.24523800	0.31025100	2.49319400
H	5.06749600	-0.11029200	3.07837400
H	4.45560800	1.36712600	2.32034800
H	4.23798300	-0.20330500	1.52776800

[Fe(5,5'-dmb)₃]²⁺ quintet in 1-butanol, applied by CPCM, <S²> = 6.0126

Fe	-0.14297000	2.60903000	4.87127100
N	0.99542000	2.88403100	6.72993000
N	1.37164700	4.15559000	4.40440000
N	-1.28946200	0.87740200	5.57041900
C	0.79961100	2.15488200	7.83856600
H	-0.00245500	1.42509700	7.79116000
C	1.56379300	2.29332000	8.99845800
C	2.57902800	3.25632300	8.96753200
H	3.21021700	3.40256700	9.83680600
C	2.78512300	4.02089100	7.82603100
H	3.57897700	4.75604100	7.80515000
C	1.97323000	3.81669600	6.70674900
C	2.12681800	4.57460300	5.44229000
C	2.99125700	5.66514600	5.30492700
H	3.57580100	6.01650400	6.14452600
C	3.08057400	6.31274500	4.07895300
H	3.74265600	7.16342300	3.96305200
C	2.32287200	5.86459100	2.99116000
C	1.47595300	4.77848500	3.22255300
H	0.84612200	4.39629700	2.42551100
C	1.30417100	1.44397600	10.21023900
H	2.21833800	0.94167100	10.53572200
H	0.54939100	0.68354500	10.00427700
H	0.95276300	2.05389400	11.04709700
C	2.39703000	6.51809300	1.64037000
H	2.22053000	7.59415500	1.71709400
H	1.65870500	6.09553400	0.95676500
H	3.38821900	6.38253000	1.19711000
C	-2.43521800	0.95462800	6.26244200
H	-2.78957500	1.95741700	6.48037200
C	-3.15317000	-0.16198700	6.69573800

C	-2.61865200	-1.41312900	6.36722000
H	-3.13116000	-2.31732200	6.67708300
C	-1.43378100	-1.50449800	5.64788300
H	-1.03161400	-2.47638300	5.39712600
C	-0.77916900	-0.33332800	5.25361900
C	-4.43647300	-0.01430800	7.46276800
H	-5.27692200	-0.42246500	6.89479200
H	-4.64701800	1.03552900	7.67474500
H	-4.39029300	-0.55662200	8.41114200
N	-1.28134600	2.88403900	3.01260600
N	-1.65758600	4.15561300	5.33811400
N	1.00356500	0.87740100	4.17217200
C	-1.08552400	2.15487600	1.90398300
H	-0.28345800	1.42509200	1.95140700
C	-1.84969400	2.29330200	0.74408100
C	-2.86492700	3.25630700	0.77498400
H	-3.49610400	3.40254300	-0.09430000
C	-3.07103300	4.02089200	1.91647200
H	-3.86488500	4.75604400	1.93733600
C	-2.25915300	3.81670600	3.03576600
C	-2.41275200	4.57462200	4.30021900
C	-3.27719000	5.66516600	4.43757300
H	-3.86172700	6.01652200	3.59796800
C	-3.36651500	6.31276700	5.66354500
H	-4.02859700	7.16344600	5.77944000
C	-2.60882200	5.86461500	6.75134400
C	-1.76189900	4.77850900	6.51995900
H	-1.13207200	4.39632400	7.31700600
C	-1.59005800	1.44394400	-0.46768700
H	-2.50422100	0.94163200	-0.79317200
H	-0.83527800	0.68351800	-0.26170900
H	-1.23864600	2.05385300	-1.30455000
C	-2.68299100	6.51812000	8.10213300
H	-2.50649300	7.59418100	8.02540800
H	-1.94467100	6.09556400	8.78574500
H	-3.67418400	6.38255600	8.54538400
C	2.14931500	0.95462400	3.48014000
H	2.50367500	1.95741200	3.26221100
C	2.86726100	-0.16199300	3.04683800
C	2.33274300	-1.41313400	3.37536300
H	2.84524900	-2.31732800	3.06550000
C	1.14787800	-1.50450000	4.09470900
H	0.74571200	-2.47638400	4.34547200
C	0.49327000	-0.33332900	4.48897400
C	4.15055900	-0.01431800	2.27980000
H	4.99101000	-0.42247400	2.84777200

H	4.36110400	1.03551700	2.06781600
H	4.10437200	-0.55663600	1.33142800

[Fe(dtbppy)₃]²⁺ singlet in gas phase

Fe	18.64643400	1.98202600	4.71883100
N	16.63413600	2.08694900	4.87523000
C	15.84450400	1.34399300	5.66710400
H	16.34872200	0.64088100	6.31932400
C	14.45730500	1.44736500	5.67997600
H	13.89880800	0.81010800	6.35354800
C	13.81006200	2.35669800	4.83330900
C	14.64696800	3.12621400	4.00926400
H	14.20716100	3.84406200	3.32871100
C	16.03265300	2.98153600	4.04498500
C	16.96667500	3.76474800	3.20695200
C	16.56817900	4.77590600	2.33453500
H	15.51734900	5.02408500	2.25690700
C	17.50149200	5.48230200	1.55896700
C	18.84052500	5.10432300	1.72282800
H	19.63392400	5.58889800	1.16834100
C	19.17794500	4.09044700	2.61355800
H	20.21252500	3.79610000	2.74395300
N	18.27558400	3.42119400	3.34866500
C	12.28666200	2.52759400	4.77924400
C	11.56621400	1.59150800	5.76745900
H	11.75642600	0.53589600	5.54726000
H	10.48678700	1.74792300	5.69482600
H	11.85349700	1.78923500	6.80544600
C	11.79633100	2.20695000	3.34530600
H	12.23616400	2.87456300	2.59798300
H	10.71018800	2.32599600	3.29269600
H	12.03602900	1.17659700	3.06408900
C	11.93014800	3.99233500	5.13466700
H	12.26451600	4.24954000	6.14476400
H	10.84525600	4.12671400	5.09573900
H	12.37428400	4.70840100	4.43636100
C	17.04535700	6.59380400	0.60535400
C	18.22907400	7.22807600	-0.14857600
H	18.94758900	7.69577100	0.53258300
H	17.85779900	8.01103700	-0.81492000
H	18.75988200	6.49867800	-0.76927000
C	16.33141200	7.69698100	1.42555400
H	15.44722400	7.31840100	1.94760500
H	16.00002900	8.49651300	0.75653800
H	17.00312700	8.13722300	2.16928900
C	16.06039800	5.99756800	-0.43064100
H	16.53679000	5.21320000	-1.02735900

H	15.72570000	6.78302900	-1.11445400
H	15.16922700	5.57240900	0.04126800
N	18.43890000	0.43734500	3.43255000
C	18.19784400	0.51059300	2.11013300
H	18.14581500	1.50758000	1.68949500
C	18.02725000	-0.60595300	1.30549500
H	17.83934200	-0.45838000	0.24820800
C	18.09524300	-1.89699700	1.85680200
C	18.34378400	-1.95922800	3.23285300
H	18.40436400	-2.92130500	3.72180900
C	18.51172700	-0.79690600	3.99167400
C	17.90440900	-3.13892400	0.97770600
C	18.99299100	-3.14331300	-0.12442100
H	18.93644400	-2.25785200	-0.76442000
H	18.86420400	-4.02060600	-0.76502900
H	19.99763800	-3.18756800	0.30825300
C	18.01373700	-4.44615000	1.78428300
H	18.99870600	-4.56246300	2.24910100
H	17.87058600	-5.29858900	1.11521000
H	17.24705800	-4.51475700	2.56351800
C	16.50261800	-3.07682100	0.32144600
H	15.70978400	-3.07035600	1.07626000
H	16.35502000	-3.95483600	-0.31411800
H	16.38029500	-2.19082400	-0.30852100
N	20.65873200	2.08694800	4.56243200
C	21.44836300	1.34399100	3.77055700
H	20.94414500	0.64088000	3.11833800
C	22.83556200	1.44736300	3.75768600
H	23.39405900	0.81010600	3.08411400
C	23.48280600	2.35669600	4.60435200
C	22.64590100	3.12621300	5.42839700
H	23.08570700	3.84406000	6.10895000
C	21.26021500	2.98153500	5.39267600
C	20.32619300	3.76474800	6.23070900
C	20.72469000	4.77590700	7.10312500
H	21.77552000	5.02408500	7.18075400
C	19.79137700	5.48230300	7.87869300
C	18.45234400	5.10432400	7.71483200
H	17.65894500	5.58890000	8.26931900
C	18.11492400	4.09044900	6.82410300
H	17.08034300	3.79610100	6.69370800
N	19.01728400	3.42119400	6.08899600
C	25.00620600	2.52759100	4.65841800
C	25.72665300	1.59150400	3.67020300
H	25.53644100	0.53589200	3.89040200
H	26.80608100	1.74791800	3.74283600

H	25.43937100	1.78923100	2.63221600
C	25.49653700	2.20694700	6.09235500
H	25.05670400	2.87456100	6.83967800
H	26.58267900	2.32599300	6.14496600
H	25.25683800	1.17659500	6.37357300
C	25.36272000	3.99233100	4.30299400
H	25.02835300	4.24953600	3.29289700
H	26.44761300	4.12671000	4.34192200
H	24.91858500	4.70839800	5.00129900
C	20.24751300	6.59380500	8.83230600
C	19.06379600	7.22807800	9.58623500
H	18.34528200	7.69577300	8.90507700
H	19.43507100	8.01103900	10.25257900
H	18.53298800	6.49868000	10.20692900
C	20.96145800	7.69698100	8.01210500
H	21.84564600	7.31840100	7.49005500
H	21.29284200	8.49651400	8.68112100
H	20.28974300	8.13722300	7.26837000
C	21.23247200	5.99756900	9.86830100
H	20.75608000	5.21320100	10.46502000
H	21.56717000	6.78303000	10.55211300
H	22.12364200	5.57241000	9.39639200
N	18.85396700	0.43734500	6.00511200
C	19.09502300	0.51059400	7.32752900
H	19.14705200	1.50758200	7.74816700
C	19.26561600	-0.60595200	8.13216800
H	19.45352500	-0.45837800	9.18945500
C	19.19762300	-1.89699600	7.58086200
C	18.94908100	-1.95922800	6.20481000
H	18.88850100	-2.92130500	5.71585500
C	18.78113900	-0.79690500	5.44598900
C	19.38845700	-3.13892200	8.45995800
C	18.29987400	-3.14331000	9.56208500
H	18.35642200	-2.25784900	10.20208300
H	18.42866100	-4.02060300	10.20269400
H	17.29522800	-3.18756500	9.12941100
C	19.27912700	-4.44614900	7.65338200
H	18.29415900	-4.56246200	7.18856400
H	19.42227800	-5.29858800	8.32245500
H	20.04580600	-4.51475700	6.87414700
C	20.79024700	-3.07682000	9.11621800
H	21.58308100	-3.07035600	8.36140300
H	20.93784500	-3.95483500	9.75178200
H	20.91257000	-2.19082300	9.74618500

[Fe(dtbppy)₃]²⁺ quintet in gas phase, <S²> = 6.0104

Fe	18.64643100	1.97118600	4.71883100
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N	16.44314800	2.22899500	4.83642400
C	15.64292900	1.51308700	5.64004500
H	16.14146000	0.82949600	6.32016600
C	14.25578800	1.61440700	5.62798900
H	13.68240500	1.00324800	6.31302200
C	13.62951300	2.49215300	4.73326400
C	14.48146500	3.23183500	3.89541300
H	14.04964700	3.91447500	3.17523000
C	15.86722100	3.09439700	3.96529900
C	16.80611800	3.86620900	3.10353500
C	16.39286600	4.90046800	2.26428600
H	15.34737400	5.17867500	2.23515700
C	17.31000200	5.60088000	1.46246900
C	18.64797200	5.19927900	1.56571500
H	19.42689900	5.67914800	0.98718100
C	18.99596700	4.16608000	2.43065100
H	20.03099300	3.85171700	2.52547300
N	18.10943200	3.50484100	3.18760800
C	12.10765700	2.66035400	4.64100300
C	11.36531100	1.76059900	5.64662200
H	11.55900000	0.69770100	5.46859100
H	10.28787600	1.91485100	5.54533900
H	11.63063400	1.99538500	6.68269100
C	11.64670000	2.28902800	3.20951200
H	12.10170000	2.92949700	2.44779100
H	10.56190000	2.40620500	3.13124200
H	11.89117800	1.24931000	2.97005500
C	11.74569400	4.13720000	4.93679600
H	12.06064800	4.43038100	5.94326900
H	10.66181700	4.26983500	4.87186200
H	12.20409100	4.82759200	4.22213600
C	16.83610100	6.73485200	0.54420700
C	17.99999000	7.36249200	-0.24530600
H	18.75166300	7.80803900	0.41458200
H	17.61597100	8.16147800	-0.88492500
H	18.49469100	6.63471400	-0.89689400
C	16.17180200	7.83649800	1.40694800
H	15.30174700	7.46459300	1.95670700
H	15.82879400	8.65124000	0.76255300
H	16.87830500	8.25454100	2.13099600
C	15.80315100	6.16986400	-0.46226200
H	16.24362900	5.38663600	-1.08731500
H	15.45604600	6.97062800	-1.12176700
H	14.92369200	5.75194500	0.03721400
N	18.52681600	0.19890300	3.38336800
C	18.32049900	0.24868500	2.05590300

H	18.32336700	1.23965000	1.61260100
C	18.11236900	-0.87807600	1.27430200
H	17.95720800	-0.75486700	0.20865500
C	18.09864600	-2.15163900	1.86833300
C	18.31064000	-2.18731400	3.25283300
H	18.29356600	-3.13722500	3.76760000
C	18.52774600	-1.01356600	3.98262600
C	17.85922000	-3.40859200	1.02279700
C	18.96941600	-3.50422700	-0.05350900
H	18.97384300	-2.63743800	-0.72087200
H	18.80758700	-4.39314800	-0.67019100
H	19.96078300	-3.58759000	0.40322600
C	17.88084500	-4.69524100	1.86864100
H	18.84751800	-4.84907000	2.36009200
H	17.70776800	-5.55828200	1.22052900
H	17.09426600	-4.70078900	2.63083100
C	16.47704600	-3.29211700	0.33302600
H	15.66985100	-3.22030500	1.06901000
H	16.29606600	-4.18028900	-0.27940000
H	16.41609200	-2.42062600	-0.32536900
N	20.84972000	2.22897800	4.60125400
C	21.64993000	1.51305100	3.79764200
H	21.15139000	0.82945900	3.11752800
C	23.03707200	1.61435700	3.80969600
H	23.61044800	1.00318400	3.12467000
C	23.66335700	2.49211000	4.70440600
C	22.81141400	3.23181200	5.54225000
H	23.24323900	3.91445900	6.26242000
C	21.42565700	3.09438300	5.47236900
C	20.48676400	3.86620900	6.33412500
C	20.90002300	4.90045200	7.17339200
H	21.94552000	5.17863500	7.20254300
C	19.98288700	5.60087400	7.97520000
C	18.64491000	5.19930100	7.87192600
H	17.86598300	5.67918100	8.45045100
C	18.29690800	4.16611800	7.00697400
H	17.26187900	3.85177800	6.91212900
N	19.18344400	3.50486900	6.25002800
C	25.18521400	2.66030000	4.79666000
C	25.92755000	1.76052600	3.79105100
H	25.73385300	0.69763200	3.96909600
H	27.00498700	1.91477000	3.89232800
H	25.66222500	1.99530100	2.75497900
C	25.64617300	2.28898900	6.22815400
H	25.19118100	2.92947100	6.98986800
H	26.73097400	2.40615800	6.30642000

H	25.40168700	1.24927600	6.46762600
C	25.54718900	4.13714000	4.50084700
H	25.23223300	4.43031000	3.49437100
H	26.63106600	4.26976600	4.56577600
H	25.08880000	4.82754400	5.21549900
C	20.45679400	6.73482700	8.89348200
C	19.29290500	7.36247800	9.68298600
H	18.54125000	7.80804700	9.02309200
H	19.67692900	8.16144900	10.32262000
H	18.79818100	6.63470100	10.33455700
C	21.12112500	7.83647100	8.03076300
H	21.99118100	7.46455600	7.48101100
H	21.46413800	8.65120000	8.67517100
H	20.41463900	8.25453500	7.30671000
C	21.48972000	6.16980900	9.89995900
H	21.04921900	5.38658100	10.52499700
H	21.83683000	6.97056000	10.55947800
H	22.36917900	5.75188100	9.40049100
N	18.76599300	0.19889600	6.05429000
C	18.97231300	0.24867200	7.38175500
H	18.96943400	1.23963400	7.82506400
C	19.18045900	-0.87809100	8.16334900
H	19.33562300	-0.75488700	9.22899600
C	19.19418900	-2.15165100	7.56931200
C	18.98218900	-2.18732000	6.18481200
H	18.99926700	-3.13722900	5.67004000
C	18.76507200	-1.01356900	5.45502700
C	19.43363000	-3.40860600	8.41483900
C	18.32343900	-3.50425800	9.49115000
H	18.31900800	-2.63747300	10.15851800
H	18.48527900	-4.39318100	10.10782600
H	17.33207100	-3.58762600	9.03441900
C	19.41201300	-4.69525100	7.56898900
H	18.44533900	-4.84908600	7.07754100
H	19.58510000	-5.55829400	8.21709500
H	20.19858800	-4.70078800	6.80679500
C	20.81580500	-3.29212300	9.10460500
H	21.62299700	-3.22030000	8.36861800
H	20.99679700	-4.18029700	9.71702500
H	20.87675600	-2.42063500	9.76300500

[Fe(dtbbpy)₃]²⁺ singlet in methanol, applied by CPCM

Fe	18.64643300	1.97585000	4.71883100
N	16.65931800	2.08825000	4.86773600
C	15.87377000	1.35324700	5.66739400
H	16.37594500	0.63729900	6.30380100
C	14.49131300	1.48899000	5.69957800

H	13.92465100	0.85790800	6.36878600
C	13.86050200	2.43203300	4.88244700
C	14.69188000	3.20181200	4.05826000
H	14.25945800	3.95613400	3.41304100
C	16.07018500	3.00811300	4.05982300
C	17.00803200	3.74720200	3.19419500
C	16.61641800	4.72052400	2.28044000
H	15.56911800	4.97478800	2.18747300
C	17.56154600	5.36204000	1.46877300
C	18.89018800	4.95333100	1.61558800
H	19.67932000	5.37965100	1.01262600
C	19.21887400	3.97709100	2.54863600
H	20.24208300	3.64804800	2.66542000
N	18.30983500	3.38375000	3.33588200
C	12.34626000	2.63784000	4.86603900
C	11.62835500	1.63962100	5.78390200
H	11.83568600	0.60959300	5.48006500
H	10.55055300	1.79902000	5.71619100
H	11.92448200	1.76047000	6.82826200
C	11.81469000	2.43557600	3.43224700
H	12.28871000	3.11280800	2.71915500
H	10.73724700	2.62424500	3.42074200
H	11.98572700	1.40899400	3.10086200
C	12.03141200	4.07486800	5.33102900
H	12.36965500	4.23751900	6.35680400
H	10.95235200	4.24336400	5.29354800
H	12.50822900	4.82040300	4.68952200
C	17.12359600	6.44288200	0.48263700
C	18.30920300	7.01552000	-0.30560000
H	19.04431700	7.48044900	0.35669900
H	17.94177700	7.78137600	-0.99151600
H	18.81203000	6.24444700	-0.89466900
C	16.45406900	7.59344300	1.26286900
H	15.56329700	7.25399300	1.79609700
H	16.15238300	8.37522700	0.56088100
H	17.14672900	8.02947300	1.98645500
C	16.10138800	5.84207900	-0.50520300
H	16.53389900	5.00865600	-1.06284400
H	15.79131100	6.60870200	-1.21940200
H	15.21005200	5.48386300	0.01578400
N	18.45137400	0.45537900	3.43851600
C	18.23023000	0.54464100	2.11657800
H	18.18877500	1.54537800	1.70779300
C	18.06609600	-0.56797700	1.30788300
H	17.88610000	-0.41933400	0.25035100
C	18.12891100	-1.85785500	1.85639300

C	18.36690400	-1.93841000	3.23081000
H	18.42954600	-2.90072900	3.71940100
C	18.52117700	-0.77920600	3.99260500
C	17.93596600	-3.08393600	0.96665200
C	19.00626300	-3.07896600	-0.14656300
H	18.96290700	-2.17047400	-0.74972200
H	18.84047100	-3.93352000	-0.80711800
H	20.00807700	-3.16253900	0.27981100
C	18.05523600	-4.39752400	1.75117600
H	19.04059300	-4.50037300	2.21485100
H	17.91881600	-5.23336800	1.06232200
H	17.29202400	-4.47700100	2.53045800
C	16.53521800	-3.01538700	0.32146000
H	15.75016100	-3.01350600	1.08249200
H	16.39419200	-3.89094500	-0.31627200
H	16.41808600	-2.12049000	-0.29383100
N	20.63354900	2.08824900	4.56992500
C	21.41909600	1.35324500	3.77026800
H	20.91692200	0.63729700	3.13386200
C	22.80155400	1.48898700	3.73808400
H	23.36821500	0.85790500	3.06887600
C	23.43236500	2.43203100	4.55521400
C	22.60098700	3.20181100	5.37940100
H	23.03341000	3.95613400	6.02461900
C	21.22268200	3.00811300	5.37783800
C	20.28483600	3.74720300	6.24346500
C	20.67645000	4.72052500	7.15721900
H	21.72375100	4.97478900	7.25018600
C	19.73132200	5.36204100	7.96888600
C	18.40268000	4.95333300	7.82207200
H	17.61354800	5.37965400	8.42503400
C	18.07399400	3.97709300	6.88902400
H	17.05078500	3.64805100	6.77224000
N	18.98303300	3.38375100	6.10177900
C	24.94660700	2.63783800	4.57162200
C	25.66451200	1.63961800	3.65375900
H	25.45718000	0.60959100	3.95759600
H	26.74231400	1.79901700	3.72146900
H	25.36838500	1.76046700	2.60939900
C	25.47817800	2.43557400	6.00541400
H	25.00415700	3.11280700	6.71850600
H	26.55562000	2.62424300	6.01691800
H	25.30714000	1.40899200	6.33679900
C	25.26145500	4.07486600	4.10663200
H	24.92321300	4.23751600	3.08085700
H	26.34051600	4.24336200	4.14411200

H	24.78463800	4.82040100	4.74813800
C	20.16927300	6.44288400	8.95502100
C	18.98366600	7.01552200	9.74325900
H	18.24855200	7.48045100	9.08096000
H	19.35109200	7.78137800	10.42917500
H	18.48083900	6.24444900	10.33232900
C	20.83880000	7.59344500	8.17478900
H	21.72957100	7.25399400	7.64156100
H	21.14048600	8.37522800	8.87677700
H	20.14614000	8.02947400	7.45120300
C	21.19148100	5.84208100	9.94286200
H	20.75896900	5.00865800	10.50050400
H	21.50155800	6.60870400	10.65706000
H	22.08281700	5.48386400	9.42187500
N	18.84149300	0.45538000	5.99914700
C	19.06263600	0.54464300	7.32108500
H	19.10409000	1.54538000	7.72986900
C	19.22677000	-0.56797400	8.12978000
H	19.40676600	-0.41933100	9.18731300
C	19.16395600	-1.85785300	7.58127100
C	18.92596400	-1.93840900	6.20685500
H	18.86332200	-2.90072900	5.71826400
C	18.77169000	-0.77920500	5.44505900
C	19.35690200	-3.08393200	8.47101300
C	18.28660400	-3.07896300	9.58422700
H	18.32995900	-2.17047100	10.18738600
H	18.45239600	-3.93351700	10.24478300
H	17.28479000	-3.16253700	9.15785300
C	19.23763300	-4.39752200	7.68649100
H	18.25227600	-4.50037200	7.22281500
H	19.37405300	-5.23336500	8.37534500
H	20.00084500	-4.47699900	6.90720900
C	20.75764900	-3.01538300	9.11620700
H	21.54270600	-3.01350100	8.35517400
H	20.89867600	-3.89094000	9.75393900
H	20.87478000	-2.12048500	9.73149700

[Fe(dtbbpy)₃]²⁺ quintet in methanol, applied by CPCM, <S²> = 6.0121

Fe	18.64644200	1.91620700	4.71883400
N	16.47903000	2.23341600	4.86779900
C	15.68122000	1.59462800	5.73334000
H	16.16969000	0.90518400	6.41222900
C	14.30484400	1.78513800	5.77555300
H	13.72195500	1.23876600	6.50292000
C	13.70175500	2.67254600	4.87940200
C	14.54981800	3.33840700	3.98306300
H	14.13149700	4.04088100	3.27417000

C	15.92241900	3.10741300	3.99595300
C	16.86745200	3.78788300	3.07287900
C	16.47126600	4.76752900	2.16591900
H	15.43338400	5.06676900	2.11369800
C	17.40817800	5.38000200	1.32119700
C	18.73079300	4.93904900	1.42353600
H	19.51024900	5.34868300	0.79685000
C	19.05774100	3.95486600	2.34987300
H	20.07511600	3.59627800	2.44877100
N	18.15736900	3.39304400	3.16522900
C	12.19728400	2.93600400	4.84825100
C	11.44340800	2.10989500	5.89929100
H	11.59342200	1.03634600	5.75839600
H	10.37361700	2.31224200	5.81084400
H	11.75278900	2.37621100	6.91302100
C	11.65254700	2.57872400	3.44977700
H	12.13777100	3.16356000	2.66526100
H	10.57944500	2.78611800	3.41534500
H	11.80450300	1.51855600	3.23149900
C	11.94904900	4.43268800	5.13078500
H	12.34331500	4.70983300	6.11108900
H	10.87501200	4.63131500	5.12388400
H	12.41647500	5.07057800	4.37707700
C	16.96538600	6.46750300	0.34381200
C	18.14219700	7.01807700	-0.47297100
H	18.90122300	7.47078300	0.17079400
H	17.77347200	7.78978800	-1.15144300
H	18.61742900	6.23724100	-1.07196700
C	16.33116400	7.63030000	1.13533000
H	15.43823800	7.31110500	1.67742000
H	16.04036000	8.42146700	0.43921400
H	17.04159600	8.04662300	1.85328400
C	15.91431600	5.87869800	-0.62074000
H	16.32766900	5.04351800	-1.19015300
H	15.59377700	6.65000400	-1.32535100
H	15.03308000	5.52587700	-0.07945400
N	18.57318800	0.18133300	3.38783900
C	18.42232000	0.24688500	2.05615300
H	18.44277700	1.24073300	1.62401700
C	18.24397700	-0.87628600	1.26523500
H	18.12249800	-0.75614100	0.19618700
C	18.20612700	-2.14848900	1.85512100
C	18.37976700	-2.20420600	3.24178600
H	18.35285800	-3.15362000	3.75736800
C	18.55751500	-1.03169500	3.98041000
C	17.97647800	-3.38393300	0.98804500

C	19.11020700	-3.48589700	-0.05361200
H	19.15511100	-2.60073500	-0.69078300
H	18.93776200	-4.35718700	-0.69027000
H	20.07788100	-3.60768500	0.43937400
C	17.95346800	-4.68001200	1.80622700
H	18.90807200	-4.84972400	2.31043700
H	17.77794700	-5.51846800	1.12921700
H	17.15621600	-4.67682600	2.55500800
C	16.62407600	-3.23735500	0.25947300
H	15.80388500	-3.16985200	0.97683300
H	16.45915900	-4.11556000	-0.36924900
H	16.59836700	-2.34998100	-0.37632000
N	20.81385500	2.23343100	4.56987600
C	21.61165200	1.59462500	3.70433800
H	21.12317000	0.90518600	3.02545400
C	22.98803100	1.78511700	3.66212400
H	23.57091100	1.23873200	2.93475900
C	23.59113200	2.67252700	4.55826400
C	22.74307900	3.33840500	5.45460100
H	23.16141000	4.04088200	6.16348700
C	21.37047800	3.10742500	5.44171500
C	20.42544600	3.78790000	6.36478900
C	20.82163000	4.76753300	7.27176200
H	21.85951400	5.06676500	7.32399600
C	19.88471200	5.38000200	8.11648200
C	18.56209700	4.93905300	8.01413000
H	17.78263800	5.34868200	8.64081600
C	18.23515000	3.95488600	7.08777600
H	17.21777400	3.59630300	6.98886300
N	19.13552700	3.39307300	6.27242100
C	25.09560600	2.93597000	4.58940900
C	25.84947000	2.10984900	3.53836900
H	25.69944500	1.03630200	3.67926800
H	26.91926400	2.31218600	3.62681300
H	25.54009000	2.37616600	2.52463900
C	25.64034500	2.57869200	5.98788200
H	25.15512800	3.16353400	6.77239700
H	26.71344900	2.78607800	6.02230800
H	25.48838200	1.51852500	6.20616400
C	25.34385200	4.43265100	4.30686700
H	24.94958500	4.70979600	3.32656400
H	26.41789100	4.63126900	4.31376200
H	24.87643600	5.07054900	5.06057400
C	20.32749900	6.46749500	9.09387700
C	19.15068500	7.01806300	9.91065700
H	18.39166200	7.47077500	9.26689100

H	19.51940600	7.78977100	10.58913600
H	18.67544900	6.23722400	10.50964600
C	20.96172600	7.63029700	8.30237100
H	21.85465500	7.31110700	7.76028200
H	21.25252800	8.42145700	8.99849500
H	20.25129800	8.04662800	7.58441700
C	21.37856400	5.87868300	10.05842900
H	20.96520900	5.04350000	10.62783600
H	21.69910100	6.64998500	10.76304600
H	22.25980200	5.52586400	9.51714500
N	18.71963400	0.18132500	6.04981500
C	18.87051700	0.24687300	7.38149900
H	18.85006400	1.24072100	7.81363900
C	19.04887000	-0.87630100	8.17241200
H	19.17036200	-0.75616000	9.24145800
C	19.08670300	-2.14850300	7.58252200
C	18.91304900	-2.20421500	6.19585900
H	18.93994600	-3.15362700	5.68027300
C	18.73530100	-1.03170000	5.45724100
C	19.31634900	-3.38395100	8.44959200
C	18.18262300	-3.48591500	9.49125200
H	18.13772500	-2.60075500	10.12842700
H	18.35506500	-4.35720800	10.12790600
H	17.21494700	-3.60769700	8.99826800
C	19.33934900	-4.68002800	7.63140400
H	18.38474200	-4.84973400	7.12719900
H	19.51487000	-5.51848700	8.30841000
H	20.13659700	-4.67684300	6.88261900
C	20.66875400	-3.23738500	9.17816100
H	21.48894400	-3.16988100	8.46080000
H	20.83366800	-4.11559700	9.80687500
H	20.69446900	-2.35001700	9.81396100

[Fe(dtbppy)₃]²⁺ singlet in ethanol, applied by CPCM

Fe	18.64643400	1.97301800	4.71883000
N	16.65604700	2.08550000	4.86722100
C	15.86863100	1.34963100	5.66461900
H	16.36919300	0.63222100	6.30098400
C	14.48582400	1.48538300	5.69589100
H	13.91929700	0.85318700	6.36460600
C	13.85516600	2.42852700	4.87827800
C	14.68847500	3.19741200	4.05472500
H	14.25754700	3.95039300	3.40714600
C	16.06717700	3.00516100	4.05859100
C	17.00569200	3.74826600	3.19639000
C	16.61458000	4.72619500	2.28690400
H	15.56702900	4.98065400	2.19647200

C	17.55925700	5.37294400	1.47839400
C	18.88888000	4.96742800	1.62838200
H	19.67981500	5.39907200	1.03123300
C	19.21720500	3.98663200	2.55714500
H	20.24161400	3.66102200	2.67551800
N	18.30771100	3.38509000	3.33780100
C	12.34025500	2.63664400	4.86102200
C	11.61951300	1.64193400	5.78207400
H	11.82172600	0.60948600	5.48229200
H	10.54177000	1.80489400	5.71580100
H	11.91639100	1.76484500	6.82640500
C	11.80912900	2.43377800	3.42620200
H	12.27925200	3.11489000	2.71366900
H	10.73080100	2.61805000	3.41373000
H	11.98466500	1.40872200	3.09129400
C	12.02767200	4.07565000	5.32485500
H	12.36919000	4.23980800	6.34972800
H	10.94835900	4.24509700	5.29091500
H	12.50284800	4.82064200	4.68117200
C	17.12012100	6.45620800	0.49369100
C	18.30598200	7.03157700	-0.29390600
H	19.04057400	7.49773200	0.36848500
H	17.93893800	7.79771500	-0.98024800
H	18.81069800	6.26213800	-0.88409300
C	16.44853400	7.60471300	1.27676800
H	15.55947300	7.26266700	1.81176500
H	16.14235700	8.38727300	0.57721200
H	17.14096700	8.04235400	2.00015100
C	16.09937500	5.85577100	-0.49713400
H	16.53416400	5.02459800	-1.05719000
H	15.78796900	6.62368600	-1.20986800
H	15.20733900	5.49395100	0.02052000
N	18.44982800	0.44982000	3.43722500
C	18.22471300	0.53677400	2.11536000
H	18.18059100	1.53658000	1.70396800
C	18.06077400	-0.57677000	1.30730200
H	17.87927200	-0.42773600	0.24995600
C	18.12698100	-1.86644800	1.85640100
C	18.36593600	-1.94437200	3.23102200
H	18.42962100	-2.90633700	3.71991600
C	18.52050100	-0.78451700	3.99234200
C	17.93719100	-3.09576500	0.96836800
C	19.00802600	-3.08880800	-0.14525800
H	18.95896500	-2.18281600	-0.75248900
H	18.84811100	-3.94669300	-0.80339600
H	20.01132800	-3.16425700	0.28030400

C	18.06095100	-4.40805900	1.75616700
H	19.04680300	-4.50819100	2.21985700
H	17.92664600	-5.24697300	1.07014700
H	17.29820700	-4.48838100	2.53610200
C	16.53504200	-3.03342700	0.32362400
H	15.75030800	-3.03331800	1.08532000
H	16.39491900	-3.90981900	-0.31385000
H	16.41340900	-2.14011400	-0.29347300
N	20.63682100	2.08549900	4.57043900
C	21.42423700	1.34963000	3.77304100
H	20.92367500	0.63222000	3.13667600
C	22.80704400	1.48538200	3.74176900
H	23.37357100	0.85318500	3.07305400
C	23.43770200	2.42852500	4.55938200
C	22.60439300	3.19741100	5.38293400
H	23.03532100	3.95039300	6.03051200
C	21.22569100	3.00516100	5.37906800
C	20.28717600	3.74826700	6.24126800
C	20.67828900	4.72619500	7.15075500
H	21.72584100	4.98065300	7.24118600
C	19.73361200	5.37294400	7.95926500
C	18.40398900	4.96743000	7.80927700
H	17.61305500	5.39907400	8.40642600
C	18.07566400	3.98663400	6.88051300
H	17.05125400	3.66102400	6.76213900
N	18.98515700	3.38509100	6.09985700
C	24.95261300	2.63664200	4.57663700
C	25.67335400	1.64193300	3.65558300
H	25.47114500	0.60948500	3.95536800
H	26.75109700	1.80489600	3.72185200
H	25.37647200	1.76484200	2.61125400
C	25.48374000	2.43377500	6.01145700
H	25.01361800	3.11488600	6.72399100
H	26.56206800	2.61804800	6.02392700
H	25.30820600	1.40871900	6.34636400
C	25.26519600	4.07564900	4.11280500
H	24.92367600	4.23980800	3.08793200
H	26.34450900	4.24509500	4.14674200
H	24.79002100	4.82064100	4.75649000
C	20.17274800	6.45620600	8.94397000
C	18.98688900	7.03157200	9.73157000
H	18.25229900	7.49773400	9.06918200
H	19.35393400	7.79770300	10.41791900
H	18.48216900	6.26212900	10.32175000
C	20.84433300	7.60471400	8.16089500
H	21.73339200	7.26267000	7.62589300

H	21.15051200	8.38727200	8.86045100
H	20.15189700	8.04235800	7.43751600
C	21.19349700	5.85576800	9.93479100
H	20.75871000	5.02459300	10.49484500
H	21.50490300	6.62368100	10.64752700
H	22.08553300	5.49395100	9.41713500
N	18.84304000	0.44982200	6.00043700
C	19.06815400	0.53677700	7.32230100
H	19.11227600	1.53658400	7.73369200
C	19.23209200	-0.57676500	8.13036200
H	19.41359300	-0.42773000	9.18770700
C	19.16588600	-1.86644400	7.58126300
C	18.92693200	-1.94437000	6.20664300
H	18.86324700	-2.90633600	5.71775000
C	18.77236800	-0.78451600	5.44532100
C	19.35567400	-3.09576000	8.46929900
C	18.28483700	-3.08880000	9.58292300
H	18.33389800	-2.18280700	10.19015300
H	18.44475000	-3.94668400	10.24106300
H	17.28153600	-3.16424900	9.15735900
C	19.23191500	-4.40805500	7.68150300
H	18.24606400	-4.50818700	7.21781000
H	19.36621700	-5.24696800	8.36752500
H	19.99466100	-4.48838000	6.90157000
C	20.75782200	-3.03342100	9.11404500
H	21.54255700	-3.03331500	8.35235100
H	20.89794400	-3.90981100	9.75152200
H	20.87945500	-2.14010600	9.73113900

[Fe(dtbbpy)₃]²⁺ quintet in ethanol, applied by CPCM, <S²> = 6.0119

Fe	18.64643300	1.91503500	4.71882900
N	16.47547000	2.22741600	4.86047800
C	15.67589500	1.58129500	5.71913500
H	16.16334000	0.88619700	6.39317300
C	14.29928100	1.77176700	5.76203200
H	13.71671500	1.21843300	6.48477000
C	13.69692300	2.66795000	4.87357000
C	14.54673500	3.33841100	3.98181600
H	14.12922100	4.04451300	3.27620500
C	15.91963500	3.10724400	3.99375800
C	16.86531500	3.79250400	3.07398200
C	16.46888800	4.77559200	2.17039300
H	15.43060100	5.07411200	2.12051100
C	17.40428800	5.39159500	1.32607300
C	18.72785300	4.95286300	1.42929400
H	19.50835800	5.36543700	0.80546100
C	19.05548600	3.96611300	2.35305500

H	20.07441200	3.61094300	2.45149600
N	18.15591300	3.39847900	3.16547300
C	12.19181700	2.93456200	4.84458200
C	11.43771500	2.10904700	5.89718400
H	11.58021200	1.03477100	5.75216500
H	10.36837100	2.31764900	5.81546700
H	11.75349600	2.36933300	6.91082500
C	11.64473500	2.57745700	3.44592000
H	12.12763600	3.16340800	2.66037800
H	10.57125600	2.78395400	3.41241900
H	11.79704800	1.51739200	3.22607500
C	11.94484700	4.43228900	5.12744200
H	12.33896800	4.71065200	6.10791700
H	10.87061900	4.63191900	5.12040700
H	12.41190400	5.07095400	4.37385300
C	16.95898800	6.48057300	0.34971900
C	18.13510400	7.03434600	-0.46755800
H	18.89393200	7.48857300	0.17575300
H	17.76570000	7.80602800	-1.14625600
H	18.61197600	6.25530900	-1.06819400
C	16.32263000	7.64158700	1.14369300
H	15.43311600	7.31918500	1.69000700
H	16.02437400	8.43206400	0.44956600
H	17.03376100	8.06199800	1.85910300
C	15.90869500	5.89082600	-0.61642600
H	16.32357000	5.05669200	-1.18707100
H	15.58684400	6.66227000	-1.32078100
H	15.02677600	5.53570300	-0.07735700
N	18.57254900	0.17597700	3.38716200
C	18.42039000	0.24064700	2.05537000
H	18.44040000	1.23459700	1.62277300
C	18.24178100	-0.88276400	1.26422200
H	18.12069900	-0.76135500	0.19513400
C	18.20490300	-2.15522200	1.85419400
C	18.37742300	-2.20949300	3.24134600
H	18.34998000	-3.15915900	3.75631200
C	18.55684500	-1.03705400	3.98020700
C	17.97747900	-3.39331700	0.98807900
C	19.11268600	-3.49444000	-0.05344500
H	19.15484900	-2.61126500	-0.69421700
H	18.94407300	-4.36813900	-0.68830900
H	20.08170700	-3.61085000	0.43894200
C	17.95573900	-4.68890500	1.80930500
H	18.90937900	-4.85768400	2.31636600
H	17.78227200	-5.53011400	1.13469100
H	17.15694200	-4.68604600	2.55668400

C	16.62440100	-3.25000700	0.25810300
H	15.80269300	-3.18066800	0.97426600
H	16.45952100	-4.12966400	-0.36916300
H	16.59810700	-2.36473200	-0.38116100
N	20.81739900	2.22741100	4.57718300
C	21.61696800	1.58128500	3.71852400
H	21.12951500	0.88619700	3.04448100
C	22.99358300	1.77174300	3.67562900
H	23.57614400	1.21840500	2.95289100
C	23.59595100	2.66791400	4.56409700
C	22.74614400	3.33838200	5.45585300
H	23.16366600	4.04447700	6.16146700
C	21.37324200	3.10722900	5.44390800
C	20.42756600	3.79249300	6.36368500
C	20.82399800	4.77557300	7.26727900
H	21.86228700	5.07408500	7.31716500
C	19.88860000	5.39157800	8.11160000
C	18.56503200	4.95285400	8.00837400
H	17.78452800	5.36542900	8.63220800
C	18.23739400	3.96611200	7.08460500
H	17.21846600	3.61095000	6.98615800
N	19.13696600	3.39847900	6.27218600
C	25.10106000	2.93450800	4.59308900
C	25.85515500	2.10898200	3.54049300
H	25.71264000	1.03470700	3.68551000
H	26.92450200	2.31756600	3.62221600
H	25.53938500	2.36927200	2.52684900
C	25.64813200	2.57739900	5.99175500
H	25.16523600	3.16335800	6.77729300
H	26.72161400	2.78388400	6.02525800
H	25.49580600	1.51733700	6.21160100
C	25.34804600	4.43223200	4.31022800
H	24.95392800	4.71059700	3.32975200
H	26.42227600	4.63185200	4.31726400
H	24.88099500	5.07090300	5.06381500
C	20.33390300	6.48055100	9.08795800
C	19.15778900	7.03432900	9.90523300
H	18.39896300	7.48856000	9.26192100
H	19.52719500	7.80601000	10.58393100
H	18.68091200	6.25529400	10.50586900
C	20.97027000	7.64156400	8.29398800
H	21.85978300	7.31915800	7.74767500
H	21.26852900	8.43203600	8.98811700
H	20.25914300	8.06198100	7.57857700
C	21.38419100	5.89079600	10.05410300
H	20.96931100	5.05666300	10.62474600

H	21.70604500	6.66223700	10.75846100
H	22.26610900	5.53567000	9.51503500
N	18.72029700	0.17597200	6.05048900
C	18.87246200	0.24063900	7.38228000
H	18.85245700	1.23458700	7.81488100
C	19.05107100	-0.88277600	8.17342600
H	19.17215800	-0.76137000	9.24251300
C	19.08794000	-2.15523200	7.58345000
C	18.91541500	-2.20949900	6.19629800
H	18.94285200	-3.15916400	5.68133000
C	18.73599600	-1.03705700	5.45744200
C	19.31535900	-3.39333100	8.44956200
C	18.18015200	-3.49445100	9.49108500
H	18.13799300	-2.61127700	10.13185900
H	18.34876200	-4.36815200	10.12594800
H	17.21113100	-3.61085600	8.99869900
C	19.33709200	-4.68891600	7.62833200
H	18.38345000	-4.85769000	7.12127100
H	19.51055600	-5.53012800	8.30294400
H	20.13588800	-4.68605900	6.88095200
C	20.66843800	-3.25002900	9.17953700
H	21.49014700	-3.18069000	8.46337500
H	20.83331400	-4.12969100	9.80679900
H	20.69473600	-2.36475700	9.81880600

[Fe(dtbbpy)₃]²⁺ singlet in 2-propanol, applied by CPCM

Fe	18.64643400	1.97189700	4.71883000
N	16.65391100	2.08345500	4.86703500
C	15.86562500	1.34650600	5.66283600
H	16.36560700	0.62914700	6.29992800
C	14.48242000	1.48063700	5.69254900
H	13.91631400	0.84751400	6.36103500
C	13.85128600	2.42260600	4.87362600
C	14.68546000	3.19118900	4.05034000
H	14.25499900	3.94213300	3.40019600
C	16.06465500	3.00173300	4.05694500
C	17.00333700	3.74890500	3.19796200
C	16.61208900	4.73040300	2.29211500
H	15.56410100	4.98373100	2.20279200
C	17.55636800	5.38282900	1.48739800
C	18.88714000	4.98163300	1.64093100
H	19.67927300	5.41897300	1.04931300
C	19.21569200	3.99726000	2.56606700
H	20.24131000	3.67574600	2.68673400
N	18.30584400	3.38747700	3.34001100
C	12.33581800	2.63109500	4.85524900
C	11.61356400	1.63871800	5.77864100

H	11.81300500	0.60467400	5.48206200
H	10.53581900	1.80343800	5.71290000
H	11.91048100	1.76368100	6.82299100
C	11.80552900	2.42700700	3.41970000
H	12.27298100	3.11062600	2.70745800
H	10.72656200	2.60784300	3.40616600
H	11.98464400	1.40294600	3.08288900
C	12.02371800	4.07136100	5.31769800
H	12.36691200	4.23708500	6.34203000
H	10.94416200	4.24076300	5.28568400
H	12.49759100	4.81603200	4.67248500
C	17.11592900	6.46804000	0.50431600
C	18.30169600	7.04658800	-0.28219200
H	19.03536800	7.51386800	0.38065800
H	17.93442700	7.81291000	-0.96854200
H	18.80843000	6.27891300	-0.87333100
C	16.44209100	7.61411600	1.29004600
H	15.55452600	7.26927200	1.82610000
H	16.13226800	8.39738200	0.59265900
H	17.13410100	8.05290300	2.01349100
C	16.09684100	5.86792900	-0.48919300
H	16.53387200	5.03901000	-1.05136500
H	15.78429500	6.63701800	-1.20046000
H	15.20442100	5.50268500	0.02561700
N	18.44854600	0.44682000	3.43641100
C	18.22080700	0.53218800	2.11460500
H	18.17476600	1.53126000	1.70132500
C	18.05686100	-0.58199600	1.30706400
H	17.87426200	-0.43289000	0.24983900
C	18.12510300	-1.87151200	1.85660600
C	18.36491900	-1.94768300	3.23130800
H	18.42922500	-2.90940400	3.72044100
C	18.51986800	-0.78735000	3.99220900
C	17.93697300	-3.10279700	0.96968300
C	19.00838600	-3.09492500	-0.14397300
H	18.95575300	-2.19085100	-0.75423000
H	18.85258300	-3.95523700	-0.80020500
H	20.01248700	-3.16486700	0.28138100
C	18.06298600	-4.41430000	1.75952900
H	19.04913200	-4.51317800	2.22314200
H	17.92959400	-5.25506300	1.07528700
H	17.30054600	-4.49484700	2.53991900
C	16.53404400	-3.04385100	0.32510500
H	15.74947000	-3.04483500	1.08716700
H	16.39431700	-3.92063000	-0.31234500
H	16.40979900	-2.15134100	-0.29289500

N	20.63895700	2.08345400	4.57062600
C	21.42724200	1.34650500	3.77482400
H	20.92726000	0.62914700	3.13773100
C	22.81044800	1.48063600	3.74511100
H	23.37655300	0.84751200	3.07662500
C	23.44158200	2.42260300	4.56403400
C	22.60740800	3.19118600	5.38732100
H	23.03787000	3.94213100	6.03746500
C	21.22821300	3.00173200	5.38071600
C	20.28953200	3.74890400	6.23969900
C	20.68078000	4.73040100	7.14554600
H	21.72876800	4.98372700	7.23487100
C	19.73650100	5.38282900	7.95026200
C	18.40572800	4.98163500	7.79672700
H	17.61359600	5.41897600	8.38834400
C	18.07717600	3.99726200	6.87159100
H	17.05155800	3.67575100	6.75092200
N	18.98702400	3.38747800	6.09764800
C	24.95705000	2.63109300	4.58241100
C	25.67930400	1.63871600	3.65901900
H	25.47986200	0.60467200	3.95559600
H	26.75705000	1.80343500	3.72476100
H	25.38238800	1.76368000	2.61466900
C	25.48733900	2.42700500	6.01796000
H	25.01988600	3.11062300	6.73020200
H	26.56630700	2.60784300	6.03149300
H	25.30822600	1.40294400	6.35477100
C	25.26915000	4.07135900	4.11996300
H	24.92595600	4.23708300	3.09563000
H	26.34870600	4.24076200	4.15197600
H	24.79527600	4.81603000	4.76517500
C	20.17694100	6.46803900	8.93334500
C	18.99117400	7.04658800	9.71985300
H	18.25750300	7.51386800	9.05700300
H	19.35844300	7.81290900	10.40620300
H	18.48443900	6.27891300	10.31099100
C	20.85078000	7.61411400	8.14761500
H	21.73834500	7.26927000	7.61156100
H	21.16060400	8.39738000	8.84500300
H	20.15877000	8.05290200	7.42417100
C	21.19602800	5.86792700	9.92685400
H	20.75899600	5.03900700	10.48902500
H	21.50857400	6.63701500	10.63812100
H	22.08844800	5.50268200	9.41204400
N	18.84432100	0.44682100	6.00125100
C	19.07206000	0.53219100	7.32305700

H	19.11810000	1.53126300	7.73633600
C	19.23600600	-0.58199300	8.13059900
H	19.41860300	-0.43288600	9.18782400
C	19.16776300	-1.87150900	7.58105800
C	18.92794900	-1.94768100	6.20635600
H	18.86364300	-2.90940300	5.71722300
C	18.77300000	-0.78735000	5.44545400
C	19.35589300	-3.10279400	8.46798300
C	18.28447800	-3.09491900	9.58163800
H	18.33711200	-2.19084400	10.19189300
H	18.44028000	-3.95523000	10.23787100
H	17.28037800	-3.16486100	9.15628300
C	19.22987800	-4.41429800	7.67813800
H	18.24373300	-4.51317500	7.21452500
H	19.36326900	-5.25505900	8.36238200
H	19.99232000	-4.49484700	6.89775000
C	20.75882100	-3.04384800	9.11256200
H	21.54339500	-3.04483400	8.35049900
H	20.89854700	-3.92062500	9.75001300
H	20.88306700	-2.15133700	9.73055900

[Fe(dtbppy)₃]²⁺ quintet in 2-propanol, applied by CPCM, <S²> = 6.0117

Fe	18.64642300	1.91789900	4.71882300
N	16.47270500	2.22641100	4.85755400
C	15.67286200	1.57644000	5.71320600
H	16.16061800	0.88041600	6.38621100
C	14.29570200	1.76424800	5.75536200
H	13.71401500	1.20714600	6.47616800
C	13.69235900	2.66204100	4.86884900
C	14.54252200	3.33562300	3.97946100
H	14.12452100	4.04181400	3.27430400
C	15.91608100	3.10731100	3.99227100
C	16.86137100	3.79651800	3.07450900
C	16.46361000	4.78126000	2.17300600
H	15.42469500	5.07809200	2.12472000
C	17.39733600	5.40066500	1.32899800
C	18.72201700	4.96488300	1.43284400
H	19.50270300	5.38018700	0.81081900
C	19.05129100	3.97712900	2.35518600
H	20.07164200	3.62552600	2.45355000
N	18.15291000	3.40477700	3.16576900
C	12.18622200	2.92652400	4.83885200
C	11.43257600	2.09863600	5.89068200
H	11.57410400	1.02444900	5.74276000
H	10.36299300	2.30766500	5.81121200
H	11.74933100	2.35551700	6.90508800
C	11.64055600	2.56872700	3.43914300

H	12.12194200	3.15636600	2.65367800
H	10.56647400	2.77260100	3.40465300
H	11.79539400	1.50903400	3.21833300
C	11.93623300	4.42420400	5.12220100
H	12.32812100	4.70372400	6.10350600
H	10.86151600	4.62244800	5.11339500
H	12.40306000	5.06460700	4.36972500
C	16.94929300	6.49027800	0.35350400
C	18.12429600	7.04734000	-0.46419600
H	18.88271800	7.50315000	0.17872500
H	17.75357800	7.81880600	-1.14277100
H	18.60278800	6.27004700	-1.06618800
C	16.31071100	7.64945900	1.14938500
H	15.42392200	7.32412500	1.69870900
H	16.00673000	8.43923200	0.45671900
H	17.02213300	8.07312400	1.86292600
C	15.89991200	5.89915200	-0.61361200
H	16.31645600	5.06621400	-1.18529300
H	15.57643300	6.67051500	-1.31761100
H	15.01794800	5.54158500	-0.07597700
N	18.57139200	0.17603900	3.38671400
C	18.41811000	0.23995800	2.05488600
H	18.43745700	1.23389500	1.62182800
C	18.23949600	-0.88369300	1.26367400
H	18.11843500	-0.76155400	0.19456900
C	18.20373800	-2.15629200	1.85377600
C	18.37582100	-2.20945200	3.24120100
H	18.34845600	-3.15927900	3.75578900
C	18.55619300	-1.03698100	3.98011100
C	17.97818700	-3.39627100	0.98847200
C	19.11442200	-3.49653700	-0.05290100
H	19.15446900	-2.61475500	-0.69613900
H	18.94871300	-4.37195800	-0.68645100
H	20.08429700	-3.60898400	0.43918700
C	17.95782400	-4.69138400	1.81187500
H	18.91092200	-4.85896500	2.32081200
H	17.78614700	-5.53456200	1.13896200
H	17.15798100	-4.68899800	2.55830000
C	16.62463100	-3.25572700	0.25761200
H	15.80192600	-3.18576800	0.97302500
H	16.46024400	-4.13634100	-0.36878700
H	16.59745300	-2.37174000	-0.38374500
N	20.82014800	2.22637800	4.58009200
C	21.61999600	1.57641600	3.72443700
H	21.13224100	0.88040300	3.05141900
C	22.99715700	1.76421500	3.68229500

H	23.57884700	1.20712000	2.96148500
C	23.60050000	2.66198500	4.56883100
C	22.75033300	3.33556000	5.45822000
H	23.16833300	4.04173500	6.16339400
C	21.37677100	3.10726300	5.44539300
C	20.43148500	3.79647400	6.36315400
C	20.82925600	4.78122100	7.26464900
H	21.86817200	5.07805000	7.31292500
C	19.89553800	5.40063600	8.10865800
C	18.57085400	4.96486100	8.00482100
H	17.79017300	5.38017400	8.62684800
C	18.24157100	3.97710200	7.08248900
H	17.22121800	3.62550400	6.98413300
N	19.13994300	3.40473700	6.27190400
C	25.10663900	2.92644900	4.59885200
C	25.86029100	2.09855300	3.54703300
H	25.71874300	1.02436700	3.69495000
H	26.92987600	2.30756400	3.62652200
H	25.54355900	2.35544000	2.53262200
C	25.65228000	2.56864300	5.99856800
H	25.17088600	3.15628100	6.78402900
H	26.72636400	2.77250900	6.03307700
H	25.49743200	1.50895000	6.21937200
C	25.35664800	4.42412600	4.31550900
H	24.96477700	4.70365100	3.33419900
H	26.43136600	4.62236200	4.32433200
H	24.88981400	5.06453200	5.06798000
C	20.34359300	6.49025300	9.08414300
C	19.16859700	7.04732700	9.90184600
H	18.41017400	7.50313800	9.25892500
H	19.53932300	7.81879600	10.58041300
H	18.69010200	6.27004200	10.50384600
C	20.98217800	7.64942500	8.28825200
H	21.86896100	7.32408100	7.73892500
H	21.28617100	8.43920000	8.98091200
H	20.27075500	8.07309100	7.57471300
C	21.39297400	5.89912500	10.05125900
H	20.97642700	5.06619300	10.62294500
H	21.71645900	6.67049000	10.75525300
H	22.27493400	5.54155200	9.51362200
N	18.72149300	0.17603500	6.05093500
C	18.87476500	0.23994800	7.38276400
H	18.85542400	1.23388300	7.81582700
C	19.05336600	-0.88370700	8.17397400
H	19.17441800	-0.76157400	9.24308000
C	19.08912800	-2.15630300	7.58386600

C	18.91705500	-2.20945600	6.19644000
H	18.94442300	-3.15928100	5.68184800
C	18.73668800	-1.03698300	5.45753300
C	19.31467400	-3.39628600	8.44916600
C	18.17843500	-3.49655500	9.49053400
H	18.13838500	-2.61477500	10.13377500
H	18.34414100	-4.37197800	10.12408100
H	17.20856100	-3.60899900	8.99844200
C	19.33503800	-4.69139600	7.62575800
H	18.38194300	-4.85897400	7.11681600
H	19.50671100	-5.53457600	8.29866900
H	20.13488500	-4.68900800	6.87933700
C	20.66822600	-3.25574600	9.18003200
H	21.49093500	-3.18578400	8.46462300
H	20.83261000	-4.13636300	9.80642700
H	20.69540200	-2.37176200	9.82139400

[Fe(dtbppy)₃]²⁺ singlet in 1-butanol, applied by CPCM

Fe	18.64643400	1.97208600	4.71883000
N	16.65270300	2.08246200	4.86715700
C	15.86423900	1.34466600	5.66215400
H	16.36425800	0.62817700	6.30031000
C	14.48068800	1.47668700	5.69034400
H	13.91511400	0.84299300	6.35890600
C	13.84881100	2.41690600	4.86980500
C	14.68312800	3.18544600	4.04643500
H	14.25251000	3.93430000	3.39403200
C	16.06277400	2.99892700	4.05542400
C	17.00130000	3.74927300	3.19875600
C	16.60959600	4.73291500	2.29529000
H	15.56116200	4.98462500	2.20608800
C	17.55355600	5.39003600	1.49385300
C	18.88534000	4.99296200	1.65053400
H	19.67814500	5.43504000	1.06323000
C	19.21438600	4.00633600	2.57323100
H	20.24099400	3.68853500	2.69620000
N	18.30434200	3.39004800	3.34184000
C	12.33290800	2.62461400	4.85034000
C	11.61015900	1.63333400	5.77507400
H	11.80881300	0.59845400	5.48063500
H	10.53233600	1.79833300	5.70919900
H	11.90659500	1.75995400	6.81951800
C	11.80353800	2.41927400	3.41431200
H	12.26946700	3.10423600	2.70216900
H	10.72416800	2.59783200	3.39982300
H	11.98508500	1.39574300	3.07676800
C	12.02015700	4.06548400	5.31170700

H	12.36396300	4.23243800	6.33578500
H	10.94037700	4.23425500	5.28052600
H	12.49304000	4.81013400	4.66563700
C	17.11197600	6.47643400	0.51197700
C	18.29750800	7.05764400	-0.27353000
H	19.03024700	7.52587300	0.38980100
H	17.92979200	7.82397600	-0.95981400
H	18.80594800	6.29136200	-0.86522200
C	16.43619500	7.62048900	1.29956700
H	15.54974800	7.27333500	1.83618900
H	16.12378100	8.40415900	0.60366600
H	17.12774300	8.06014000	2.02312400
C	16.09431300	5.87641200	-0.48346600
H	16.53312300	5.04920500	-1.04706400
H	15.78093100	6.64628700	-1.19367500
H	15.20172400	5.50860000	0.02934500
N	18.44758900	0.44589800	3.43598600
C	18.21827200	0.53034300	2.11423500
H	18.17106200	1.52895000	1.69982100
C	18.05425100	-0.58421700	1.30702400
H	17.87093600	-0.43511800	0.24987900
C	18.12365200	-1.87362900	1.85682500
C	18.36412400	-1.94879700	3.23153900
H	18.42882700	-2.91037500	3.72081600
C	18.51938300	-0.78817700	3.99215800
C	17.93630400	-3.10599000	0.97054200
C	19.00804000	-3.09770000	-0.14312700
H	18.95340100	-2.19478500	-0.75518200
H	18.85459800	-3.95944100	-0.79819200
H	20.01256400	-3.16447600	0.28214200
C	18.06345000	-4.41705900	1.76151600
H	19.04977800	-4.51537100	2.22501100
H	17.93040500	-5.25882800	1.07827200
H	17.30122400	-4.49763800	2.54221300
C	16.53293700	-3.04878500	0.32609700
H	15.74847800	-3.05036100	1.08838800
H	16.39335800	-3.92574700	-0.31136000
H	16.40727700	-2.15667200	-0.29234000
N	20.64016500	2.08246100	4.57050400
C	21.42862800	1.34466500	3.77550700
H	20.92860900	0.62817700	3.13735000
C	22.81217900	1.47668600	3.74731600
H	23.37775300	0.84299200	3.07875500
C	23.44405700	2.41690500	4.56785600
C	22.60974000	3.18544500	5.39122500
H	23.04035800	3.93429900	6.04362900

C	21.23009400	2.99892600	5.38223600
C	20.29156800	3.74927400	6.23890300
C	20.68327200	4.73291500	7.14237000
H	21.73170600	4.98462400	7.23157300
C	19.73931200	5.39003800	7.94380600
C	18.40752700	4.99296500	7.78712300
H	17.61472300	5.43504500	8.37442600
C	18.07848200	4.00633900	6.86442600
H	17.05187300	3.68853900	6.74145600
N	18.98852500	3.39005000	6.09581800
C	24.95995900	2.62461300	4.58732000
C	25.68270900	1.63333400	3.66258600
H	25.48405500	0.59845300	3.95702500
H	26.76053200	1.79833300	3.72846200
H	25.38627300	1.75995400	2.61814200
C	25.48933000	2.41927400	6.02334900
H	25.02340000	3.10423400	6.73549200
H	26.56869900	2.59783200	6.03783700
H	25.30778400	1.39574100	6.36089200
C	25.27271000	4.06548400	4.12595400
H	24.92890500	4.23243700	3.10187600
H	26.35249000	4.23425500	4.15713500
H	24.79982700	4.81013300	4.77202400
C	20.18089300	6.47643500	8.92568200
C	18.99536100	7.05764600	9.71118800
H	18.26262200	7.52587500	9.04785700
H	19.36307600	7.82397900	10.39747100
H	18.48692000	6.29136500	10.30288100
C	20.85667500	7.62048900	8.13809200
H	21.74312200	7.27333400	7.60147100
H	21.16909000	8.40415800	8.83399400
H	20.16512800	8.06014100	7.41453500
C	21.19855400	5.87641200	9.92112600
H	20.75974300	5.04920600	10.48472400
H	21.51193600	6.64628700	10.63133500
H	22.09114300	5.50859900	9.40831600
N	18.84527800	0.44589900	6.00167600
C	19.07459500	0.53034500	7.32342800
H	19.12180400	1.52895300	7.73784000
C	19.23861600	-0.58421400	8.13064000
H	19.42193000	-0.43511300	9.18778400
C	19.16921600	-1.87362600	7.58084000
C	18.92874500	-1.94879500	6.20612600
H	18.86404100	-2.91037400	5.71685000
C	18.77348500	-0.78817700	5.44550500
C	19.35656300	-3.10598600	8.46712400

C	18.28482600	-3.09769400	9.58079200
H	18.33946400	-2.19477800	10.19284600
H	18.43826700	-3.95943400	10.23585900
H	17.28030200	-3.16447000	9.15552300
C	19.22941700	-4.41705600	7.67615200
H	18.24309000	-4.51536800	7.21265600
H	19.36246000	-5.25882400	8.35939700
H	19.99164400	-4.49763700	6.89545600
C	20.75992900	-3.04878000	9.11157100
H	21.54438900	-3.05035800	8.34928000
H	20.89950800	-3.92574100	9.74902900
H	20.88558900	-2.15666700	9.73000600

[Fe(dtbppy)₃]²⁺ quintet in 1-butanol, applied by CPCM, <S²> = 6.0117

Fe	18.64642700	1.92026100	4.71882600
N	16.47109400	2.22660400	4.85625800
C	15.67126500	1.57478100	5.71060200
H	16.15936000	0.87887500	6.38356800
C	14.29372000	1.76052000	5.75201300
H	13.71265700	1.20156300	6.47203000
C	13.68953500	2.65824400	4.86581900
C	14.53975000	3.33350700	3.97757500
H	14.12126900	4.03917800	3.27221800
C	15.91378000	3.10744300	3.99126600
C	16.85872400	3.79899600	3.07462500
C	16.46003700	4.78454600	2.17424400
H	15.42071200	5.08020900	2.12678300
C	17.39274400	5.40608500	1.33049900
C	18.71814200	4.97227600	1.43480600
H	19.49886600	5.38930000	0.81385000
C	19.04851500	3.98407000	2.35639800
H	20.06973000	3.63469700	2.45481700
N	18.15087900	3.40887900	3.16589000
C	12.18268500	2.92062600	4.83468900
C	11.42940300	2.09090600	5.88576000
H	11.57125400	1.01687300	5.73628200
H	10.35956900	2.29936600	5.80701000
H	11.74595800	2.34612500	6.90076000
C	11.63850100	2.56212900	3.43421100
H	12.11899400	3.15091400	2.64892000
H	10.56399300	2.76398700	3.39878300
H	11.79536600	1.50272000	3.21294700
C	11.93011200	4.41813600	5.11823300
H	12.32019700	4.69846800	6.10016700
H	10.85503700	4.61510800	5.10797600
H	12.39684300	5.05973300	4.36658700
C	16.94300200	6.49598300	0.35549300

C	18.11727800	7.05503400	-0.46247900
H	18.87544000	7.51184500	0.18018300
H	17.74568700	7.82632600	-1.14096600
H	18.59674700	6.27878300	-1.06524700
C	16.30308200	7.65406100	1.15247900
H	15.41788100	7.32700900	1.70352300
H	15.99583100	8.44340400	0.46064600
H	17.01465300	8.07960300	1.86494500
C	15.89419800	5.90396500	-0.61215700
H	16.31181900	5.07184000	-1.18451700
H	15.56962600	6.67527700	-1.31587100
H	15.01230800	5.54478400	-0.07533700
N	18.57049600	0.17676800	3.38644000
C	18.41644700	0.24017100	2.05460100
H	18.43534800	1.23404600	1.62117800
C	18.23783300	-0.88365600	1.26341300
H	18.11668800	-0.76114900	0.19430300
C	18.20284200	-2.15630900	1.85364000
C	18.37479900	-2.20875800	3.24120000
H	18.34758500	-3.15865700	3.75561100
C	18.55571600	-1.03623100	3.98007400
C	17.97844800	-3.39741800	0.98888800
C	19.11526300	-3.49712900	-0.05239700
H	19.15402300	-2.61616900	-0.69706500
H	18.95130600	-4.37357100	-0.68515200
H	20.08561200	-3.60720700	0.43954800
C	17.95906200	-4.69219400	1.81361100
H	18.91189100	-4.85888000	2.32360400
H	17.78854400	-5.53655500	1.14172500
H	17.15862900	-4.69014900	2.55949700
C	16.62459500	-3.25865100	0.25757000
H	15.80134500	-3.18845900	0.97258800
H	16.46059600	-4.13984600	-0.36830400
H	16.59676400	-2.37540900	-0.38497400
N	20.82176500	2.22658100	4.58139300
C	21.62159400	1.57476200	3.72704600
H	21.13349900	0.87886600	3.05407100
C	22.99914100	1.76049000	3.68564500
H	23.58020400	1.20153700	2.96562500
C	23.60332900	2.65819500	4.57185600
C	22.75311400	3.33345600	5.46010100
H	23.17159700	4.03911400	6.16546900
C	21.37908200	3.10740600	5.44639800
C	20.43414100	3.79896300	6.36303900
C	20.83283600	4.78451300	7.26341700
H	21.87216200	5.08017200	7.31087300

C	19.90013500	5.40605900	8.10716400
C	18.57473400	4.97225800	8.00286200
H	17.79401400	5.38928700	8.62381800
C	18.24435400	3.98405100	7.08127200
H	17.22313700	3.63468400	6.98285700
N	19.14198300	3.40885300	6.27177800
C	25.11018100	2.92056000	4.60300100
C	25.86346500	2.09083200	3.55193800
H	25.72159600	1.01680100	3.70141200
H	26.93330000	2.29927600	3.63070200
H	25.54692600	2.34605700	2.53693400
C	25.65434800	2.56205600	6.00348400
H	25.17385100	3.15084200	6.78877200
H	26.72885700	2.76390500	6.03892500
H	25.49747200	1.50264700	6.22474400
C	25.36277100	4.41806800	4.31946200
H	24.97269900	4.69840400	3.33752400
H	26.43784800	4.61503100	4.32973100
H	24.89603700	5.05966800	5.07110400
C	20.34988600	6.49595700	9.08216500
C	19.17561500	7.05501800	9.90013900
H	18.41745400	7.51183000	9.25747800
H	19.54721300	7.82630900	10.57862300
H	18.69614400	6.27877100	10.50291100
C	20.98981000	7.65402900	8.28517500
H	21.87500700	7.32697100	7.73412800
H	21.29706900	8.44337200	8.97700600
H	20.27824000	8.07957500	7.57271100
C	21.39868800	5.90393600	10.04981500
H	20.98106500	5.07181400	10.62217700
H	21.72326600	6.67524800	10.75352700
H	22.28057700	5.54475000	9.51299300
N	18.72237600	0.17676400	6.05121100
C	18.87642000	0.24016100	7.38305100
H	18.85752400	1.23403500	7.81647800
C	19.05502500	-0.88366900	8.17423500
H	19.17616600	-0.76116700	9.24334700
C	19.09001600	-2.15632000	7.58400400
C	18.91806300	-2.20876300	6.19644200
H	18.94527700	-3.15866000	5.68202800
C	18.73715100	-1.03623300	5.45757200
C	19.31440400	-3.39743300	8.44875200
C	18.17758700	-3.49714500	9.49003300
H	18.13882700	-2.61618700	10.13470500
H	18.34154100	-4.37359000	10.12278600
H	17.20723900	-3.60722000	8.99808700

C	19.33378800	-4.69220600	7.62402300
H	18.38096100	-4.85888800	7.11402800
H	19.50430300	-5.53657000	8.29590800
H	20.13422400	-4.69016100	6.87814000
C	20.66825600	-3.25867200	9.18007300
H	21.49150800	-3.18847800	8.46505700
H	20.83225200	-4.13987100	9.80594300
H	20.69608700	-2.37543300	9.82262100