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## Input Files for Vanadium Complexes

For unsymmetrical phosphine complexes,  $\Delta H^\circ$  values for both amides were calculated. The average enthalpy for rotating the amides was used as the modeling input value.

### NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>3</sub>) – Ground State

%chk=VPM3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

```
0 1
V      -1.27022938  -0.00000024  -0.04179306
N      -1.87744805   1.68483873   0.55252600
H      -2.14820327   2.46700145  -0.03337890
H      -2.14298899   1.90635553   1.50880845
N      -1.87744548  -1.68484013   0.55252545
H      -2.14820214  -2.46700366  -0.03337777
H      -2.14298610  -1.90635517   1.50880853
N      -1.18516512  -0.00000038  -1.60271377
P      1.19457970   0.00000015   0.08664002
C      1.88173090   1.43574330  -0.81131239
H      1.59006356   2.36170045  -0.30326367
H      2.97646538   1.38578909  -0.87473074
H      1.45029517   1.45115895  -1.81792431
C      1.88173772  -1.43576940  -0.81126529
H      2.97646865  -1.38578711  -0.87472388
H      1.59011565  -2.36170902  -0.30315865
H      1.45026957  -1.45124831  -1.81786231
C      2.14162494   0.00002784   1.65856117
H      1.88583094   0.88733813   2.24895525
H      1.88581608  -0.88724953   2.24899817
H      3.22348499   0.00001449   1.47222526
```

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### NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>3</sub>) – Transition State

%chk=VPM<sub>3</sub>\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -1.27022938 -0.00000024 -0.04179306  
 N -1.87744805 1.68483873 0.55252600  
 H -2.14085965 1.90237047 1.50733788  
 H -2.15033261 2.47098651 -0.03190833  
 N -1.87744548 -1.68484013 0.55252545  
 H -2.14820214 -2.46700366 -0.03337777  
 H -2.14298610 -1.90635517 1.50880853  
 N -1.18516512 -0.00000038 -1.60271377  
 P 1.19457970 0.00000015 0.08664002  
 C 1.88173090 1.43574330 -0.81131239  
 H 1.59006356 2.36170045 -0.30326367  
 H 2.97646538 1.38578909 -0.87473074  
 H 1.45029517 1.45115895 -1.81792431  
 C 1.88173772 -1.43576940 -0.81126529  
 H 2.97646865 -1.38578711 -0.87472388  
 H 1.59011565 -2.36170902 -0.30315865  
 H 1.45026957 -1.45124831 -1.81786231  
 C 2.14162494 0.00002784 1.65856117  
 H 1.88583094 0.88733813 2.24895525  
 H 1.88581608 -0.88724953 2.24899817  
 H 3.22348499 0.00001449 1.47222526

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#### Title Card Required

0 1			
V	-1.27022938	-0.00000024	-0.04179306
N	-1.87744805	1.68483873	0.55252600
H	-2.14820327	2.46700145	-0.03337890
H	-2.14298899	1.90635553	1.50880845
N	-1.87744548	-1.68484013	0.55252545
H	-2.14820214	-2.46700366	-0.03337777
H	-2.14298610	-1.90635517	1.50880853
N	-1.18516512	-0.00000038	-1.60271377
P	1.19457970	0.00000015	0.08664002
C	1.88173090	1.43574330	-0.81131239
H	1.59006356	2.36170045	-0.30326367
H	2.97646538	1.38578909	-0.87473074
H	1.45029517	1.45115895	-1.81792431
C	1.88173772	-1.43576940	-0.81126529
H	2.97646865	-1.38578711	-0.87472388
H	1.59011565	-2.36170902	-0.30315865
H	1.45026957	-1.45124831	-1.81786231



C	2.14162494	0.00002784	1.65856117
H	1.88583094	0.88733813	2.24895525
H	1.88581608	-0.88724953	2.24899817
H	3.22348499	0.00001449	1.47222526

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Title Card Required

0 1			
V	-1.25038626	0.01101218	-0.05346932
N	-2.27764059	1.50993423	0.63052392
H	-3.19176420	1.67769084	0.20923796
H	-1.81293382	2.41495722	0.52441594
N	-1.70578748	-1.70357722	0.54730054
H	-1.85113027	-2.53335472	-0.01587751
H	-2.09446681	-1.86276631	1.47391254
N	-1.10407363	-0.09224066	-1.61480599
P	1.22030566	0.06119525	0.09925915
C	1.93430113	1.44212654	-0.86437689
H	1.67413570	2.40176965	-0.40299220
H	3.02734787	1.36362877	-0.92470687
H	1.50473090	1.41901246	-1.87171060

C	1.87655945	-1.42663508	-0.73041331
H	2.97251705	-1.40236207	-0.78610105
H	1.55934215	-2.32002363	-0.18153797
H	1.44806906	-1.47489978	-1.73696134
C	2.15612255	0.11394570	1.67574169
H	1.91602210	1.02951452	2.22809474
H	1.87422343	-0.74131232	2.30034566
H	3.23881914	0.08149881	1.49794965

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### **NV(NH<sub>2</sub>)<sub>2</sub>(PEt<sub>3</sub>) – Ground State**

%chk=VPet3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	1.54574473	-0.00071124	-0.08612854
N	2.09613779	-1.68540491	0.56842539
H	2.42060026	-2.47475033	0.02037173
H	2.27310847	-1.89583176	1.54763860
N	2.10129456	1.68511887	0.55993022

H	2.41024479	2.47569314	0.00463077
H	2.28977615	1.90152525	1.53562140
N	1.57467315	-0.00579165	-1.64851887
P	-0.92045066	0.00384071	0.04382387
C	-1.67221953	-1.64663817	-0.28464512
H	-1.47330830	-2.25997978	0.60543548
H	-2.76412558	-1.51752857	-0.34663469
C	-1.69738700	1.10250786	-1.21060269
H	-2.78332358	1.12314494	-1.02987707
H	-1.53566141	0.60850959	-2.17809523
C	-1.70172037	0.51951356	1.63432765
H	-1.58872258	1.61057583	1.70139697
H	-2.78188236	0.31500142	1.58228235
C	-1.11737057	-2.32227508	-1.52696042
H	-0.03163659	-2.45211265	-1.45003010
H	-1.57841122	-3.30693721	-1.67126250
H	-1.30529597	-1.73099007	-2.43153136
C	-1.10193826	2.49965778	-1.23404587
H	-0.03321709	2.45387282	-1.47481889
H	-1.59811742	3.12106291	-1.98924874
H	-1.20649637	3.00853986	-0.26677467
C	-1.06963351	-0.15217826	2.84229694
H	-0.00248460	0.09644070	2.91897159
H	-1.55139701	0.16737060	3.77416182
H	-1.14814165	-1.24584099	2.79028092

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### NV(NH<sub>2</sub>)<sub>2</sub>(PEt<sub>3</sub>) – Transition State

%chk=VPet3\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	-1.54582872	-0.00086906	0.08637885
N	-2.09623842	-1.68628425	-0.56631126
H	-2.42057104	-2.47499643	-0.01726966
H	-2.27293035	-1.89807019	-1.54527844
N	-2.10143905	1.68436726	-0.56116270
H	-2.41030745	2.47545474	-0.00655181
H	-2.28975579	1.89999800	-1.53705869
N	-1.57460144	-0.00434671	1.64877907
P	0.92030644	0.00406175	-0.04396656
C	1.67249567	-1.64606671	0.28536702
H	1.47274465	-2.26026036	-0.60393333
H	2.76445548	-1.51685566	0.34620678
C	1.69774475	1.10381467	1.20919146
H	2.78353711	1.12464111	1.02764124
H	1.53690888	0.61044286	2.17715086
C	1.70084398	0.51852738	-1.63523939
H	1.58691168	1.60941055	-1.70362833
H	2.78118208	0.31496024	-1.58318595
C	1.11887166	-2.32061067	1.52882037
H	0.03300973	-2.45022874	1.45324693
H	1.57979963	-3.30529681	1.67333176
H	1.30803121	-1.72873775	2.43275071

C	1.10185831	2.50079594	1.23212560
H	0.03330446	2.45478732	1.47360620
H	1.59829252	3.12284841	1.98663085
H	1.20562593	3.00911041	0.26447425
C	1.06900098	-0.15511507	-2.84225269
H	0.00163440	0.09257429	-2.91896333
H	1.55027061	0.16370644	-3.77462402
H	1.14838055	-1.24865365	-2.78897124

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Title Card Required

0 1

V	-1.54582872	-0.00086906	0.08637885
N	-2.09623842	-1.68628425	-0.56631126
H	-2.27092716	-1.89407002	-1.54355952
H	-2.42257423	-2.47899660	-0.01898858
N	-2.10143905	1.68436726	-0.56116270
H	-2.41030745	2.47545474	-0.00655181
H	-2.28975579	1.89999800	-1.53705869
N	-1.57460144	-0.00434671	1.64877907
P	0.92030644	0.00406175	-0.04396656
C	1.67249567	-1.64606671	0.28536702
H	1.47274465	-2.26026036	-0.60393333
H	2.76445548	-1.51685566	0.34620678
C	1.69774475	1.10381467	1.20919146
H	2.78353711	1.12464111	1.02764124
H	1.53690888	0.61044286	2.17715086
C	1.70084398	0.51852738	-1.63523939
H	1.58691168	1.60941055	-1.70362833
H	2.78118208	0.31496024	-1.58318595
C	1.11887166	-2.32061067	1.52882037
H	0.03300973	-2.45022874	1.45324693
H	1.57979963	-3.30529681	1.67333176
H	1.30803121	-1.72873775	2.43275071
C	1.10185831	2.50079594	1.23212560
H	0.03330446	2.45478732	1.47360620
H	1.59829252	3.12284841	1.98663085
H	1.20562593	3.00911041	0.26447425
C	1.06900098	-0.15511507	-2.84225269
H	0.00163440	0.09257429	-2.91896333
H	1.55027061	0.16370644	-3.77462402
H	1.14838055	-1.24865365	-2.78897124

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#### Title Card Required

0 1

V	1.54018829	0.02995733	-0.11177881
N	2.26477165	-1.67611192	0.48757495
H	1.69948466	-2.49170409	0.24140876
H	3.19253663	-1.93779739	0.15215495
N	2.04831419	1.62216465	0.74151890
H	2.28068041	2.50834110	0.30760357
H	2.36495273	1.64289011	1.70832434
N	1.51629336	0.30779912	-1.65738865
P	-0.92580974	-0.01301526	0.05499153
C	-1.62998335	-1.63053208	-0.48339932
H	-1.37883257	-2.35794409	0.30191170
H	-2.72735404	-1.54066018	-0.48660627
C	-1.73579129	1.22198457	-1.03827808
H	-2.82103013	1.18576510	-0.85626338
H	-1.56101759	0.86990112	-2.06361821
C	-1.68151490	0.26431959	1.71267286
H	-1.52798801	1.32637719	1.94950411
H	-2.76863979	0.10907994	1.63843472
C	-1.10419373	-2.09667045	-1.83165175
H	-0.01022176	-2.17724846	-1.83073059
H	-1.52431443	-3.07500091	-2.09397500

H	-1.36663428	-1.39706242	-2.63432289
C	-1.18037600	2.62574866	-0.86948484
H	-0.11279886	2.64300028	-1.11828001
H	-1.69893353	3.32896611	-1.53197086
H	-1.29517965	2.99422250	0.15822974
C	-1.06494708	-0.61306800	2.78996593
H	0.01787247	-0.44978031	2.86600621
H	-1.50576656	-0.40234994	3.77146966
H	-1.21881643	-1.68044197	2.58587408

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## NV(NH<sub>2</sub>)<sub>2</sub>(P<sup>t</sup>Bu<sub>3</sub>) – Ground State

%Mem=4GB



%Nprocs=4

%chk=M\_PtBu3\_freq2.chk

# opt=calcall freq m06l/cc-pvdz pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

V	2.13824356	0.01728833	-0.24076676
N	2.76614548	-1.63462311	0.41863313
H	3.15343445	-2.39574775	-0.13642660
H	2.99469764	-1.82558348	1.39513727
N	2.75484085	1.67298173	0.41866274
H	3.16476481	2.43230920	-0.12206150
H	2.94907210	1.86119860	1.40337036
N	2.23044680	0.01522077	-1.79617314
P	-0.36579222	-0.00313200	0.00155990
C	-0.78296851	-0.53768881	1.80035772
C	0.25351046	0.13366130	2.71331331
H	0.07916626	-0.18387485	3.75406881
H	1.27592523	-0.18154884	2.44715246
H	0.22530826	1.22837712	2.69460451
C	-2.19635136	-0.19863586	2.27203178
H	-2.97128330	-0.64933826	1.63728577
H	-2.34323476	-0.59396875	3.29064072
H	-2.38619140	0.88114546	2.32160827
C	-0.55742496	-2.04443667	1.95681895
H	-1.31393262	-2.65295408	1.44617288
H	0.43798315	-2.34421760	1.59761825
H	-0.61578344	-2.29510583	3.02834917
C	-1.07676418	1.75623265	-0.31683269
C	-0.72662693	2.67201566	0.85939061
H	-1.00502969	3.70235251	0.58661797
H	-1.26909157	2.43170454	1.78254715
H	0.35480602	2.66857386	1.06014684
C	-2.58823284	1.79153321	-0.54354517
H	-3.16039389	1.36349337	0.29064761
H	-2.90774337	2.84112024	-0.64969246
H	-2.89187694	1.27656413	-1.46390357
C	-0.35244413	2.34645743	-1.53412597
H	0.73440314	2.37541160	-1.37637437
H	-0.53337438	1.80346888	-2.46647803
H	-0.70581115	3.38011958	-1.67953277
C	-1.15337124	-1.24279103	-1.23412238
C	-0.25891823	-2.48794971	-1.29340527
H	-0.17937770	-3.02723507	-0.34387037

H	-0.68458532	-3.18531388	-2.03285826
H	0.75572785	-2.22356520	-1.62315179
C	-2.58792997	-1.64392839	-0.89034853
H	-3.27001033	-0.78631445	-0.81870631
H	-2.97572866	-2.29834300	-1.68798760
H	-2.66085268	-2.21351223	0.04544145
C	-1.11756508	-0.63995331	-2.64121706
H	-1.39288133	-1.42931909	-3.35848253
H	-1.83283658	0.18027960	-2.78206365
H	-0.10749853	-0.29298243	-2.90333373

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$END

```

### NV(NH<sub>2</sub>)<sub>2</sub>(P'Bu<sub>3</sub>) – Transition State

```

%Mem=4GB
%Nprocs=4
%chk=M_PtBu3_QST32.chk
# opt=(calcall,qst3) freq m06l/cc-pvdz pop=(nbo6,savenbos)
geom=connectivity
Title Card Required
0 1
V      2.13824356  0.01728833 -0.24076676
N      2.76614548 -1.63462311  0.41863313
H      3.15343445 -2.39574775 -0.13642660
H      2.99469764 -1.82558348  1.39513727
N      2.75484085  1.67298173  0.41866274
H      3.16476481  2.43230920 -0.12206150
H      2.94907210  1.86119860  1.40337036
N      2.23044680  0.01522077 -1.79617314
P     -0.36579222 -0.00313200  0.00155990
C     -0.78296851 -0.53768881  1.80035772
C      0.25351046  0.13366130  2.71331331
H      0.07916626 -0.18387485  3.75406881
H      1.27592523 -0.18154884  2.44715246
H      0.22530826  1.22837712  2.69460451
C     -2.19635136 -0.19863586  2.27203178
H     -2.97128330 -0.64933826  1.63728577
H     -2.34323476 -0.59396875  3.29064072
H     -2.38619140  0.88114546  2.32160827

```

C	-0.55742496	-2.04443667	1.95681895
H	-1.31393262	-2.65295408	1.44617288
H	0.43798315	-2.34421760	1.59761825
H	-0.61578344	-2.29510583	3.02834917
C	-1.07676418	1.75623265	-0.31683269
C	-0.72662693	2.67201566	0.85939061
H	-1.00502969	3.70235251	0.58661797
H	-1.26909157	2.43170454	1.78254715
H	0.35480602	2.66857386	1.06014684
C	-2.58823284	1.79153321	-0.54354517
H	-3.16039389	1.36349337	0.29064761
H	-2.90774337	2.84112024	-0.64969246
H	-2.89187694	1.27656413	-1.46390357
C	-0.35244413	2.34645743	-1.53412597
H	0.73440314	2.37541160	-1.37637437
H	-0.53337438	1.80346888	-2.46647803
H	-0.70581115	3.38011958	-1.67953277
C	-1.15337124	-1.24279103	-1.23412238
C	-0.25891823	-2.48794971	-1.29340527
H	-0.17937770	-3.02723507	-0.34387037
H	-0.68458532	-3.18531388	-2.03285826
H	0.75572785	-2.22356520	-1.62315179
C	-2.58792997	-1.64392839	-0.89034853
H	-3.27001033	-0.78631445	-0.81870631
H	-2.97572866	-2.29834300	-1.68798760
H	-2.66085268	-2.21351223	0.04544145
C	-1.11756508	-0.63995331	-2.64121706
H	-1.39288133	-1.42931909	-3.35848253
H	-1.83283658	0.18027960	-2.78206365
H	-0.10749853	-0.29298243	-2.90333373

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# Title Card Required

0 1

V	2.13824356	0.01728833	-0.24076676
N	2.76614548	-1.63462311	0.41863313
H	2.99264916	-1.82241656	1.39373542
H	3.15548293	-2.39891467	-0.13502475
N	2.75484085	1.67298173	0.41866274
H	3.16476481	2.43230920	-0.12206150

H	2.94907210	1.86119860	1.40337036
N	2.23044680	0.01522077	-1.79617314
P	-0.36579222	-0.00313200	0.00155990
C	-0.78296851	-0.53768881	1.80035772
C	0.25351046	0.13366130	2.71331331
H	0.07916626	-0.18387485	3.75406881
H	1.27592523	-0.18154884	2.44715246
H	0.22530826	1.22837712	2.69460451
C	-2.19635136	-0.19863586	2.27203178
H	-2.97128330	-0.64933826	1.63728577
H	-2.34323476	-0.59396875	3.29064072
H	-2.38619140	0.88114546	2.32160827
C	-0.55742496	-2.04443667	1.95681895
H	-1.31393262	-2.65295408	1.44617288
H	0.43798315	-2.34421760	1.59761825
H	-0.61578344	-2.29510583	3.02834917
C	-1.07676418	1.75623265	-0.31683269
C	-0.72662693	2.67201566	0.85939061
H	-1.00502969	3.70235251	0.58661797
H	-1.26909157	2.43170454	1.78254715
H	0.35480602	2.66857386	1.06014684
C	-2.58823284	1.79153321	-0.54354517
H	-3.16039389	1.36349337	0.29064761
H	-2.90774337	2.84112024	-0.64969246
H	-2.89187694	1.27656413	-1.46390357
C	-0.35244413	2.34645743	-1.53412597
H	0.73440314	2.37541160	-1.37637437
H	-0.53337438	1.80346888	-2.46647803
H	-0.70581115	3.38011958	-1.67953277
C	-1.15337124	-1.24279103	-1.23412238
C	-0.25891823	-2.48794971	-1.29340527
H	-0.17937770	-3.02723507	-0.34387037
H	-0.68458533	-3.18531388	-2.03285826
H	0.75572785	-2.22356520	-1.62315179
C	-2.58792997	-1.64392839	-0.89034853
H	-3.27001033	-0.78631445	-0.81870631
H	-2.97572866	-2.29834300	-1.68798760
H	-2.66085268	-2.21351223	0.04544145
C	-1.11756508	-0.63995331	-2.64121706
H	-1.39288133	-1.42931909	-3.35848253
H	-1.83283658	0.18027960	-2.78206365
H	-0.10749853	-0.29298243	-2.90333373

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Title Card Required

0 1

V	2.13824356	0.01728833	-0.24076676
N	2.76614548	-1.63462311	0.41863313
H	2.22448786	-2.49285656	0.50487195
H	3.74992863	-1.88574300	0.52527178
N	2.75484085	1.67298173	0.41866274
H	3.16476481	2.43230920	-0.12206150
H	2.94907210	1.86119860	1.40337036
N	2.23044680	0.01522077	-1.79617314
P	-0.36579222	-0.00313200	0.00155990
C	-0.78296851	-0.53768881	1.80035772
C	0.25351046	0.13366130	2.71331331
H	0.07916626	-0.18387485	3.75406881
H	1.27592523	-0.18154884	2.44715246
H	0.22530826	1.22837712	2.69460451
C	-2.19635136	-0.19863586	2.27203178
H	-2.97128330	-0.64933826	1.63728577
H	-2.34323476	-0.59396875	3.29064072
H	-2.38619140	0.88114546	2.32160827
C	-0.55742496	-2.04443667	1.95681895
H	-1.31393262	-2.65295408	1.44617288
H	0.43798315	-2.34421760	1.59761825
H	-0.61578344	-2.29510583	3.02834917
C	-1.07676418	1.75623265	-0.31683269
C	-0.72662693	2.67201566	0.85939061
H	-1.00502969	3.70235251	0.58661797
H	-1.26909157	2.43170454	1.78254715
H	0.35480602	2.66857386	1.06014684
C	-2.58823284	1.79153321	-0.54354517
H	-3.16039389	1.36349337	0.29064761
H	-2.90774337	2.84112024	-0.64969246
H	-2.89187694	1.27656413	-1.46390357
C	-0.35244413	2.34645743	-1.53412597
H	0.73440314	2.37541160	-1.37637437
H	-0.53337438	1.80346888	-2.46647803
H	-0.70581115	3.38011958	-1.67953277
C	-1.15337124	-1.24279103	-1.23412238
C	-0.25891823	-2.48794971	-1.29340527



H	-0.17937770	-3.02723507	-0.34387037
H	-0.68458532	-3.18531388	-2.03285826
H	0.75572785	-2.22356520	-1.62315179
C	-2.58792997	-1.64392839	-0.89034853
H	-3.27001033	-0.78631445	-0.81870631
H	-2.97572866	-2.29834300	-1.68798760
H	-2.66085268	-2.21351223	0.04544145
C	-1.11756508	-0.63995331	-2.64121706
H	-1.39288133	-1.42931909	-3.35848253
H	-1.83283658	0.18027960	-2.78206365
H	-0.10749853	-0.29298243	-2.90333373

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 \$END

### NV(NH<sub>2</sub>)<sub>2</sub>(P<sup>i</sup>Bu<sub>3</sub>) – Ground State

%chk=VPiBu3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V           2.82529040   0.01192586   0.06119924  
 N           3.39092219   -1.65698642   0.72675901  
 H           3.71661664   -2.45120488   0.17909731  
 H           3.60162102   -1.85728438   1.70526905  
 N           3.40444798   1.69937862   0.66584245  
 H           3.73952374   2.46925731   0.08977522  
 H           3.61766505   1.93220060   1.63658548  
 N           2.84776658   -0.01780861   -1.49704315  
 P           0.34961896   0.00790092   0.11815924  
 C           -0.19030020   -1.59345347   -0.62879581  
 H           0.02134187   -2.32973789   0.16510988  
 H           0.57077803   -1.79402955   -1.40221729  
 C           -0.18947187   1.40439151   -0.96384117  
 H           0.45689596   2.24974262   -0.67081098  
 H           0.20217072   1.10275908   -1.94940482  
 C           -0.44334011   0.19313520   1.78257522  
 H           0.16102846   -0.43229778   2.46335817  
 H           -0.19517185   1.23021770   2.06760633

C	-1.93336393	-0.09703597	2.03143714
H	-2.51817866	0.23108490	1.15249490
C	-2.41894748	0.68980493	3.24334516
H	-2.31656740	1.77569242	3.10300607
H	-3.47613951	0.48050273	3.46142773
H	-1.83894537	0.41909158	4.14001831
C	-2.18320118	-1.58292644	2.25171241
H	-1.81041560	-2.20522229	1.42859822
H	-1.68157476	-1.92514555	3.17099268
H	-3.25592575	-1.79533204	2.36599087
C	-1.59607281	-1.80189835	-1.21543494
H	-2.33759231	-1.26581269	-0.59394880
C	-1.68850154	-1.27641985	-2.64176533
H	-1.01780374	-1.84496745	-3.30467550
H	-2.70888045	-1.37654041	-3.03929443
H	-1.40247676	-0.22084361	-2.72686304
C	-1.94653651	-3.28546362	-1.19161846
H	-2.93547729	-3.47206657	-1.63469452
H	-1.21143469	-3.86625289	-1.77075319
H	-1.95566361	-3.69531775	-0.17098556
C	-1.64893121	1.87658906	-1.05247147
H	-2.32192782	1.00094175	-0.99218113
C	-1.88528086	2.56096873	-2.39418891
H	-2.91491521	2.93805575	-2.47728301
H	-1.20811397	3.42116527	-2.51488760
H	-1.70691538	1.88495649	-3.24262147
C	-1.99861304	2.83493207	0.07853315
H	-3.05835915	3.12664187	0.04446179
H	-1.80612120	2.41187293	1.07278101
H	-1.40159744	3.75723614	-0.00175294

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### **NV(NH<sub>2</sub>)<sub>2</sub>(P<sup>i</sup>Bu<sub>3</sub>) – Transition State**

%chk=VPiBu3\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	2.82529040	0.01192586	0.06119924
N	3.39092219	-1.65698642	0.72675901
H	3.71661664	-2.45120488	0.17909731
H	3.60162102	-1.85728438	1.70526905
N	3.40444798	1.69937862	0.66584245
H	3.73952374	2.46925731	0.08977522
H	3.61766505	1.93220060	1.63658548
N	2.84776658	-0.01780861	-1.49704315
P	0.34961896	0.00790092	0.11815924
C	-0.19030020	-1.59345347	-0.62879581
H	0.02134187	-2.32973789	0.16510988
H	0.57077803	-1.79402955	-1.40221729
C	-0.18947187	1.40439151	-0.96384117
H	0.45689596	2.24974262	-0.67081098
H	0.20217072	1.10275908	-1.94940482
C	-0.44334011	0.19313520	1.78257522
H	0.16102846	-0.43229778	2.46335817
H	-0.19517185	1.23021770	2.06760633
C	-1.93336393	-0.09703597	2.03143714
H	-2.51817866	0.23108490	1.15249490
C	-2.41894748	0.68980493	3.24334516
H	-2.31656740	1.77569242	3.10300607
H	-3.47613951	0.48050273	3.46142773
H	-1.83894537	0.41909158	4.14001831
C	-2.18320118	-1.58292644	2.25171241
H	-1.81041560	-2.20522229	1.42859822
H	-1.68157476	-1.92514555	3.17099268
H	-3.25592575	-1.79533204	2.36599087
C	-1.59607281	-1.80189835	-1.21543494
H	-2.33759231	-1.26581269	-0.59394880
C	-1.68850154	-1.27641985	-2.64176533
H	-1.01780374	-1.84496745	-3.30467550
H	-2.70888045	-1.37654041	-3.03929443
H	-1.40247676	-0.22084361	-2.72686304
C	-1.94653651	-3.28546362	-1.19161846
H	-2.93547729	-3.47206657	-1.63469452
H	-1.21143469	-3.86625289	-1.77075319
H	-1.95566361	-3.69531775	-0.17098556
C	-1.64893121	1.87658906	-1.05247147
H	-2.32192782	1.00094175	-0.99218113
C	-1.88528086	2.56096873	-2.39418891
H	-2.91491521	2.93805575	-2.47728301

H	-1.20811397	3.42116527	-2.51488760
H	-1.70691538	1.88495649	-3.24262147
C	-1.99861304	2.83493207	0.07853315
H	-3.05835915	3.12664187	0.04446179
H	-1.80612120	2.41187293	1.07278101
H	-1.40159744	3.75723614	-0.00175294

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# Title Card Required

0 1  
 V 2.82529040 0.01192586 0.06119924  
 N 3.39092219 -1.65698642 0.72675901  
 H 3.59971300 -1.85374675 1.70373646  
 H 3.71852466 -2.45474251 0.18062990  
 N 3.40444798 1.69937862 0.66584245  
 H 3.73952374 2.46925731 0.08977522  
 H 3.61766505 1.93220060 1.63658548  
 N 2.84776658 -0.01780861 -1.49704315  
 P 0.34961896 0.00790092 0.11815924  
 C -0.19030020 -1.59345347 -0.62879581  
 H 0.02134187 -2.32973789 0.16510988  
 H 0.57077803 -1.79402955 -1.40221729  
 C -0.18947187 1.40439151 -0.96384117  
 H 0.45689596 2.24974262 -0.67081098  
 H 0.20217072 1.10275908 -1.94940482  
 C -0.44334011 0.19313520 1.78257522  
 H 0.16102846 -0.43229778 2.46335817  
 H -0.19517185 1.23021770 2.06760633  
 C -1.93336393 -0.09703597 2.03143714  
 H -2.51817866 0.23108490 1.15249490  
 C -2.41894748 0.68980493 3.24334516  
 H -2.31656740 1.77569242 3.10300607  
 H -3.47613951 0.48050273 3.46142773  
 H -1.83894537 0.41909158 4.14001831  
 C -2.18320118 -1.58292644 2.25171241  
 H -1.81041560 -2.20522229 1.42859822  
 H -1.68157476 -1.92514555 3.17099268

H	-3.25592575	-1.79533204	2.36599087
C	-1.59607281	-1.80189835	-1.21543494
H	-2.33759231	-1.26581269	-0.59394880
C	-1.68850154	-1.27641985	-2.64176533
H	-1.01780374	-1.84496745	-3.30467550
H	-2.70888045	-1.37654041	-3.03929443
H	-1.40247676	-0.22084361	-2.72686304
C	-1.94653651	-3.28546362	-1.19161846
H	-2.93547729	-3.47206657	-1.63469452
H	-1.21143469	-3.86625289	-1.77075319
H	-1.95566361	-3.69531775	-0.17098556
C	-1.64893121	1.87658906	-1.05247147
H	-2.32192782	1.00094175	-0.99218113
C	-1.88528086	2.56096873	-2.39418891
H	-2.91491521	2.93805575	-2.47728301
H	-1.20811397	3.42116527	-2.51488760
H	-1.70691538	1.88495649	-3.24262147
C	-1.99861304	2.83493207	0.07853315
H	-3.05835915	3.12664187	0.04446179
H	-1.80612120	2.41187293	1.07278101
H	-1.40159744	3.75723614	-0.00175294

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Title Card Required

0 1  
 V        2.82529040   0.01192586   0.06119924  
 N        3.48288076   -1.92831272   0.83496354  
 H        2.99863002   -2.81844191   0.73514162  
 H        4.43638352   -2.28871138   0.78073756  
 N        3.40444798   1.69937862   0.66584245  
 H        3.73952374   2.46925731   0.08977522  
 H        3.61766505   1.93220060   1.63658548  
 N        2.84776658   -0.01780861   -1.49704315  
 P        0.34961896   0.00790092   0.11815924  
 C        -0.19030020   -1.59345347   -0.62879581  
 H        0.02134187   -2.32973789   0.16510988  
 H        0.57077803   -1.79402955   -1.40221729

C	-0.18947187	1.40439151	-0.96384117
H	0.45689596	2.24974262	-0.67081098
H	0.20217072	1.10275908	-1.94940482
C	-0.44334011	0.19313520	1.78257522
H	0.16102846	-0.43229778	2.46335817
H	-0.19517185	1.23021770	2.06760633
C	-1.93336393	-0.09703597	2.03143714
H	-2.51817866	0.23108490	1.15249490
C	-2.41894748	0.68980493	3.24334516
H	-2.31656740	1.77569242	3.10300607
H	-3.47613951	0.48050273	3.46142773
H	-1.83894537	0.41909158	4.14001831
C	-2.18320118	-1.58292644	2.25171241
H	-1.81041560	-2.20522229	1.42859822
H	-1.68157476	-1.92514555	3.17099268
H	-3.25592575	-1.79533204	2.36599087
C	-1.59607281	-1.80189835	-1.21543494
H	-2.33759231	-1.26581269	-0.59394880
C	-1.68850154	-1.27641985	-2.64176533
H	-1.01780374	-1.84496745	-3.30467550
H	-2.70888045	-1.37654041	-3.03929443
H	-1.40247676	-0.22084361	-2.72686304
C	-1.94653651	-3.28546362	-1.19161846
H	-2.93547729	-3.47206657	-1.63469452
H	-1.21143469	-3.86625289	-1.77075319
H	-1.95566361	-3.69531775	-0.17098556
C	-1.64893121	1.87658906	-1.05247147
H	-2.32192782	1.00094175	-0.99218113
C	-1.88528086	2.56096873	-2.39418891
H	-2.91491521	2.93805575	-2.47728301
H	-1.20811397	3.42116527	-2.51488760
H	-1.70691538	1.88495649	-3.24262147
C	-1.99861304	2.83493207	0.07853315
H	-3.05835915	3.12664187	0.04446179
H	-1.80612120	2.41187293	1.07278101
H	-1.40159744	3.75723614	-0.00175294

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## NV(NH<sub>2</sub>)<sub>2</sub>(P<sup>i</sup>Pr<sub>3</sub>) – Ground State

%chk=VPiPr3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	1.79183900	-0.05306692	-0.24705019
N	2.31333052	-1.76391461	0.36464299
H	2.55101436	-2.56461963	-0.21093679
H	2.56010700	-1.98984150	1.32501589
N	2.46099271	1.59469708	0.39625467
H	2.80757711	2.37048033	-0.15768511
H	2.70309766	1.77538843	1.36755705
N	1.74029013	-0.03985888	-1.81003074
P	-0.65385487	0.01875533	0.07120383
C	-1.57423590	-1.15173771	-1.06143528
H	-2.55094092	-1.32422592	-0.57786894
C	-1.39877108	1.70354661	-0.26726307
H	-2.45510795	1.50852720	-0.51878746
C	-1.23098039	-0.41313455	1.80096057
H	-2.20711938	0.08006827	1.93941156
C	-1.40858223	-1.90867645	2.02426587
H	-0.45844326	-2.44086232	1.88122987
H	-1.73180867	-2.08904038	3.05844488
H	-2.15828562	-2.35722965	1.36310315
C	-0.23169128	0.13412645	2.81696515
H	-0.59150009	-0.03415647	3.84107557
H	0.72957047	-0.39118102	2.71721678
H	-0.03545387	1.20457855	2.70112639
C	-0.82106935	-2.47146808	-1.20056053
H	-0.57409576	-2.93995602	-0.24366381
H	-1.42388602	-3.18212935	-1.78222023
H	0.12083521	-2.30088286	-1.73737646
C	-1.80902940	-0.56695913	-2.44772243
H	-0.85121319	-0.34133286	-2.93475557
H	-2.32719980	-1.31083757	-3.06764359
H	-2.42663088	0.33814000	-2.43820272
C	-0.69976683	2.37633565	-1.44500724
H	-0.62739221	1.74601098	-2.33432127
H	-1.23241345	3.29858271	-1.71465186
H	0.32678494	2.64249173	-1.16438253
C	-1.35050207	2.63429595	0.93704122

H	-1.79926029	3.59911917	0.66549043
H	-1.89685620	2.25455241	1.80793509
H	-0.31037529	2.83312751	1.22945268

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## NV(NH<sub>2</sub>)<sub>2</sub>(P<sup>i</sup>Pr<sub>3</sub>) – Transition State

%chk=VPiPr3\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	1.79172306	-0.05005269	-0.24851155
N	2.31810275	-1.75941129	0.36312030
H	2.55937960	-2.55940544	-0.21192405
H	2.56541590	-1.98378022	1.32373732
N	2.45635935	1.59968662	0.39449243
H	2.80145205	2.37616353	-0.15939044
H	2.69850866	1.78056198	1.36576251
N	1.74051622	-0.03692399	-1.81148927
P	-0.65400152	0.01753438	0.07159681
C	-1.57334018	-1.15526865	-1.05943869
H	-2.54911268	-1.32955641	-0.57461178
C	-1.40233336	1.70073048	-0.26696227
H	-2.45851680	1.50336955	-0.51736006
C	-1.22833889	-0.41447789	1.80211835
H	-2.20513776	0.07723450	1.94125167
C	-1.40324537	-1.91012911	2.02661423
H	-0.45238110	-2.44084156	1.88292086
H	-1.72505146	-2.09037965	3.06126134
H	-2.15288995	-2.36042795	1.36656880
C	-0.22870546	0.13511815	2.81652293
H	-0.58695536	-0.03269242	3.84125536
H	0.73314170	-0.38903873	2.71605041
H	-0.03383992	1.20569730	2.69949337
C	-0.81744052	-2.47341690	-1.19864309
H	-0.56848415	-2.94102102	-0.24183017
H	-1.41910444	-3.18571658	-1.77949711
H	0.12365778	-2.30097157	-1.73632484
C	-1.81099075	-0.57177119	-2.44572787
H	-0.85425369	-0.34459591	-2.93416471
H	-2.32848984	-1.31695453	-3.06464570
H	-2.43027213	0.33218608	-2.43601639
C	-0.70566882	2.37398736	-1.44581793
H	-0.63246134	1.74312748	-2.33468085
H	-1.24040927	3.29488061	-1.71596661
H	0.32048807	2.64259497	-1.16607309
C	-1.35478263	2.63233807	0.93665863

H	-1.80603436	3.59597947	0.66504081
H	-1.89926311	2.25192683	1.80844286
H	-0.31476641	2.83373463	1.22770406

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# Title Card Required

0 1

V	1.79172306	-0.05005269	-0.24851155
N	2.31810275	-1.75941129	0.36312030
H	2.56357639	-1.97992356	1.32228567
H	2.56121911	-2.56326209	-0.21047240
N	2.45635935	1.59968661	0.39449243
H	2.80145205	2.37616353	-0.15939044
H	2.69850866	1.78056198	1.36576250
N	1.74051622	-0.03692399	-1.81148927
P	-0.65400152	0.01753438	0.07159681
C	-1.57334018	-1.15526865	-1.05943869
H	-2.54911268	-1.32955641	-0.57461178
C	-1.40233336	1.70073048	-0.26696227
H	-2.45851680	1.50336955	-0.51736006
C	-1.22833889	-0.41447788	1.80211835
H	-2.20513776	0.07723450	1.94125167
C	-1.40324537	-1.91012911	2.02661423
H	-0.45238110	-2.44084156	1.88292086
H	-1.72505146	-2.09037965	3.06126134
H	-2.15288995	-2.36042795	1.36656880
C	-0.22870546	0.13511815	2.81652293
H	-0.58695536	-0.03269242	3.84125536
H	0.73314170	-0.38903874	2.71605041
H	-0.03383992	1.20569730	2.69949337
C	-0.81744052	-2.47341690	-1.19864309
H	-0.56848415	-2.94102102	-0.24183017
H	-1.41910444	-3.18571658	-1.77949711
H	0.12365778	-2.30097157	-1.73632484
C	-1.81099075	-0.57177119	-2.44572787
H	-0.85425369	-0.34459591	-2.93416471
H	-2.32848984	-1.31695453	-3.06464570
H	-2.43027213	0.33218608	-2.43601639
C	-0.70566882	2.37398736	-1.44581793
H	-0.63246134	1.74312748	-2.33468085
H	-1.24040927	3.29488061	-1.71596661
H	0.32048807	2.64259497	-1.16607309
C	-1.35478263	2.63233807	0.93665863
H	-1.80603436	3.59597947	0.66504081
H	-1.89926311	2.25192683	1.80844286
H	-0.31476641	2.83373463	1.22770406



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Title Card Required

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V	1.77861956	0.07307604	-0.22957527
N	2.64422066	-1.54280426	0.42703485
H	2.11528593	-2.39879637	0.24497847
H	3.56540757	-1.76504216	0.04820430
N	2.25343622	1.71631513	0.54844926
H	2.49229628	2.57958743	0.07380324
H	2.57857185	1.77450793	1.51107678
N	1.73370715	0.28426465	-1.78558543
P	-0.67702745	-0.04113059	0.06015637
C	-1.46860736	-1.22468252	-1.14999691
H	-2.44077031	-1.50807825	-0.71285864
C	-1.52205636	1.60771496	-0.21432366
H	-2.55856959	1.34856846	-0.49025306
C	-1.24190371	-0.58891959	1.76050210
H	-2.24513012	-0.15629528	1.90667066
C	-1.34461939	-2.10000081	1.91664130
H	-0.36251815	-2.57738568	1.80037923
H	-1.69610445	-2.33798388	2.92942496
H	-2.04350292	-2.56198693	1.21035779
C	-0.27893285	-0.03344275	2.80756402
H	-0.63934760	-0.26302545	3.81932938
H	0.71078538	-0.49892318	2.69303679
H	-0.14248875	1.05019896	2.73636823
C	-0.58857025	-2.46193315	-1.31064094
H	-0.38361414	-2.97639678	-0.36621871
H	-1.07433401	-3.18444141	-1.97999590
H	0.37134628	-2.17854676	-1.76484361
C	-1.70376899	-0.59674436	-2.51692010
H	-0.75293477	-0.26703559	-2.95614543
H	-2.13649276	-1.34962985	-3.18919638
H	-2.39611637	0.25208773	-2.48754793
C	-0.86282606	2.38506982	-1.34892935
H	-0.73843888	1.80756085	-2.26757376
H	-1.46007641	3.27845327	-1.57687183
H	0.13959099	2.70980040	-1.04558528
C	-1.55395491	2.47717330	1.03556096
H	-2.06986986	3.41843319	0.80424946
H	-2.07956325	2.01573883	1.87909047
H	-0.53435899	2.73500230	1.35197124

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### **NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Ph) – Ground State**

%chk=VPM<sub>2</sub>Ph<sub>2</sub>\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	2.14459738	-0.48194224	0.26294899
N	2.04153878	-2.06970029	-0.74647669
H	2.56245631	-2.28321848	-1.59505359
H	1.60424140	-2.93697439	-0.43158104
N	2.37753038	-0.34853256	2.12279060
H	3.04406606	0.24307221	2.61500877
H	1.95882313	-0.97594272	2.81062095
N	3.09669471	0.52639324	-0.44831449
P	0.15907756	0.84519990	-0.36820904
C	0.17327783	2.52111516	0.34927881
H	-0.62267366	3.15718344	-0.06260758
H	0.07584211	2.46307042	1.44072888
H	1.15121569	2.96402474	0.12155558
C	0.17257841	1.14302946	-2.17361194
H	0.09470056	0.18221288	-2.69786923
H	-0.65501726	1.79625181	-2.48236889
H	1.13838902	1.59431686	-2.43495476
C	-1.52477059	0.19131279	-0.06187954
C	-1.81256980	-1.10401778	-0.51993713
C	-2.51687366	0.90543806	0.62027964
C	-3.07142959	-1.66241750	-0.31756778
H	-1.03446345	-1.67742080	-1.03425964
C	-3.77469535	0.33947572	0.83120465
H	-2.31425104	1.91130359	0.99456913
C	-4.05575073	-0.94134087	0.36020055
H	-3.28392484	-2.66881567	-0.68356491
H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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 25 28 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Ph) – Transition State 1

%chk=VPM<sub>2</sub>Ph<sub>2</sub>\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1			
V	2.14459738	-0.48194224	0.26294899
N	2.04153878	-2.06970029	-0.74647669
H	2.56245631	-2.28321848	-1.59505359
H	1.60424140	-2.93697439	-0.43158104
N	2.37753038	-0.34853256	2.12279060
H	3.04406606	0.24307221	2.61500877
H	1.95882313	-0.97594272	2.81062095
N	3.09669471	0.52639324	-0.44831449
P	0.15907756	0.84519990	-0.36820904
C	0.17327783	2.52111516	0.34927881
H	-0.62267366	3.15718344	-0.06260758
H	0.07584211	2.46307042	1.44072888
H	1.15121569	2.96402474	0.12155558
C	0.17257841	1.14302946	-2.17361194
H	0.09470056	0.18221288	-2.69786923
H	-0.65501726	1.79625181	-2.48236889
H	1.13838902	1.59431686	-2.43495476
C	-1.52477059	0.19131279	-0.06187954
C	-1.81256980	-1.10401778	-0.51993713

C	-2.51687366	0.90543806	0.62027964
C	-3.07142959	-1.66241750	-0.31756778
H	-1.03446345	-1.67742080	-1.03425964
C	-3.77469535	0.33947572	0.83120465
H	-2.31425104	1.91130359	0.99456913
C	-4.05575073	-0.94134087	0.36020055
H	-3.28392484	-2.66881567	-0.68356491
H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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Title Card Required

0 1

V	2.14459738	-0.48194224	0.26294899
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N	2.04153878	-2.06970029	-0.74647669
H	1.60424140	-2.93697439	-0.43158104
H	2.56245631	-2.28321848	-1.59505359
N	2.37753038	-0.34853256	2.12279060
H	3.04406606	0.24307221	2.61500877
H	1.95882313	-0.97594272	2.81062095
N	3.09669471	0.52639324	-0.44831449
P	0.15907756	0.84519990	-0.36820904
C	0.17327783	2.52111516	0.34927881
H	-0.62267366	3.15718344	-0.06260758
H	0.07584211	2.46307042	1.44072888
H	1.15121569	2.96402474	0.12155558
C	0.17257841	1.14302946	-2.17361194
H	0.09470056	0.18221288	-2.69786923
H	-0.65501726	1.79625181	-2.48236889
H	1.13838902	1.59431686	-2.43495476
C	-1.52477059	0.19131279	-0.06187954
C	-1.81256980	-1.10401778	-0.51993713
C	-2.51687366	0.90543806	0.62027964
C	-3.07142959	-1.66241750	-0.31756778
H	-1.03446345	-1.67742080	-1.03425964
C	-3.77469535	0.33947572	0.83120465
H	-2.31425104	1.91130359	0.99456913
C	-4.05575073	-0.94134087	0.36020055
H	-3.28392484	-2.66881567	-0.68356491
H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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Title Card Required

0 1  
 V 2.14459738 -0.48194224 0.26294899  
 N 2.02578628 -2.31238904 -0.90076736  
 H 1.56785292 -2.42830772 -1.80292463  
 H 2.72726410 -3.05433194 -0.89927387  
 N 2.37753038 -0.34853256 2.12279060  
 H 3.04406606 0.24307221 2.61500877  
 H 1.95882313 -0.97594272 2.81062095  
 N 3.09669471 0.52639324 -0.44831449  
 P 0.15907756 0.84519990 -0.36820904  
 C 0.17327783 2.52111516 0.34927881  
 H -0.62267366 3.15718344 -0.06260758  
 H 0.07584211 2.46307042 1.44072888  
 H 1.15121569 2.96402474 0.12155558  
 C 0.17257841 1.14302946 -2.17361194  
 H 0.09470056 0.18221288 -2.69786923  
 H -0.65501726 1.79625181 -2.48236889  
 H 1.13838902 1.59431686 -2.43495476  
 C -1.52477059 0.19131279 -0.06187954  
 C -1.81256980 -1.10401778 -0.51993713  
 C -2.51687366 0.90543806 0.62027964  
 C -3.07142959 -1.66241750 -0.31756778  
 H -1.03446345 -1.67742080 -1.03425964  
 C -3.77469535 0.33947572 0.83120465  
 H -2.31425104 1.91130359 0.99456913  
 C -4.05575073 -0.94134087 0.36020055  
 H -3.28392484 -2.66881567 -0.68356491



H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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20 23 1.5 24 1.0
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23 25 1.5 27 1.0
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### **NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Ph) – Transition State 2**

%chk=VPMc2Ph2\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1			
V	2.14459738	-0.48194224	0.26294899
N	2.04153878	-2.06970029	-0.74647669
H	2.56245631	-2.28321848	-1.59505359
H	1.60424140	-2.93697439	-0.43158104

N	2.37753038	-0.34853256	2.12279060
H	3.04406606	0.24307221	2.61500877
H	1.95882313	-0.97594272	2.81062095
N	3.09669471	0.52639324	-0.44831449
P	0.15907756	0.84519990	-0.36820904
C	0.17327783	2.52111516	0.34927881
H	-0.62267366	3.15718344	-0.06260758
H	0.07584211	2.46307042	1.44072888
H	1.15121569	2.96402474	0.12155558
C	0.17257841	1.14302946	-2.17361194
H	0.09470056	0.18221288	-2.69786923
H	-0.65501726	1.79625181	-2.48236889
H	1.13838902	1.59431686	-2.43495476
C	-1.52477059	0.19131279	-0.06187954
C	-1.81256980	-1.10401778	-0.51993713
C	-2.51687366	0.90543806	0.62027964
C	-3.07142959	-1.66241750	-0.31756778
H	-1.03446345	-1.67742080	-1.03425964
C	-3.77469535	0.33947572	0.83120465
H	-2.31425104	1.91130359	0.99456913
C	-4.05575073	-0.94134087	0.36020055
H	-3.28392484	-2.66881567	-0.68356491
H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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# Title Card Required

0 1

V	2.14459738	-0.48194224	0.26294899
N	2.04153878	-2.06970029	-0.74647669
H	2.56245631	-2.28321848	-1.59505359
H	1.60424140	-2.93697439	-0.43158104
N	2.37753038	-0.34853256	2.12279060
H	1.95882313	-0.97594272	2.81062095
H	3.04406606	0.24307221	2.61500877
N	3.09669471	0.52639324	-0.44831449
P	0.15907756	0.84519990	-0.36820904
C	0.17327783	2.52111516	0.34927881
H	-0.62267366	3.15718344	-0.06260758
H	0.07584211	2.46307042	1.44072888
H	1.15121569	2.96402474	0.12155558
C	0.17257841	1.14302946	-2.17361194
H	0.09470056	0.18221288	-2.69786923
H	-0.65501726	1.79625181	-2.48236889
H	1.13838902	1.59431686	-2.43495476
C	-1.52477059	0.19131279	-0.06187954
C	-1.81256980	-1.10401778	-0.51993713
C	-2.51687366	0.90543806	0.62027964
C	-3.07142959	-1.66241750	-0.31756778
H	-1.03446345	-1.67742080	-1.03425964
C	-3.77469535	0.33947572	0.83120465
H	-2.31425104	1.91130359	0.99456913
C	-4.05575073	-0.94134087	0.36020055
H	-3.28392484	-2.66881567	-0.68356491
H	-4.53925360	0.90629095	1.36615124
H	-5.04099981	-1.38137486	0.52513446

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 2 3 1.0 4 1.0  
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 5 7 1.0 6 1.0  
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 9 10 1.0 14 1.0 18 1.0  
 10 11 1.0 12 1.0 13 1.0  
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 14 15 1.0 16 1.0 17 1.0  
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 18 19 1.5 20 1.5  
 19 21 1.5 22 1.0  
 20 23 1.5 24 1.0  
 21 25 1.5 26 1.0  
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 23 25 1.5 27 1.0  
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 25 28 1.0  
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Title Card Required

0 1  
 V 2.12679149 -0.49214036 0.12077880  
 N 2.02373289 -2.07989841 -0.88864688  
 H 2.54465042 -2.29341660 -1.73722378  
 H 1.58643551 -2.94717251 -0.57375123  
 N 2.39533627 -0.33833444 2.26496079  
 H 3.23308387 -0.57062106 2.79483495  
 H 1.91834362 0.33418589 2.86684473  
 N 3.07888882 0.51619512 -0.59048468  
 P 0.14127167 0.83500178 -0.51037923  
 C 0.15547194 2.51091704 0.20710862  
 H -0.64047955 3.14698532 -0.20477777

H	0.05803622	2.45287230	1.29855869
H	1.13340980	2.95382662	-0.02061461
C	0.15477252	1.13283134	-2.31578213
H	0.07689467	0.17201476	-2.84003942
H	-0.67282315	1.78605369	-2.62453908
H	1.12058313	1.58411874	-2.57712495
C	-1.54257648	0.18111467	-0.20404973
C	-1.83037569	-1.11421590	-0.66210732
C	-2.53467955	0.89523994	0.47810945
C	-3.08923548	-1.67261562	-0.45973797
H	-1.05226934	-1.68761892	-1.17642983
C	-3.79250124	0.32927760	0.68903446
H	-2.33205693	1.90110547	0.85239894
C	-4.07355662	-0.95153899	0.21803036
H	-3.30173073	-2.67901379	-0.82573510
H	-4.55705949	0.89609283	1.22398105
H	-5.05880570	-1.39157298	0.38296427

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21 25 1.5 26 1.0

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23 25 1.5 27 1.0

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25 28 1.0

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### NV(NH<sub>2</sub>)<sub>2</sub>(PH<sub>3</sub>) – Ground State

%chk=VPH3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	0.52857708	0.00000035	0.06529323
N	1.17749438	1.66768997	-0.49413844
H	1.43393764	2.44844983	0.10723561
H	1.47724651	1.89954288	-1.44209357
N	1.17750245	-1.66768596	-0.49413953
H	1.43394031	-2.44844610	0.10723681
H	1.47725047	-1.89954467	-1.44209457
N	0.40344558	-0.00000066	1.61575141
P	-1.95571394	-0.00000193	-0.18339898
H	-2.70890444	-0.00000018	-1.39126393
H	-2.62206643	-1.07329363	0.45895181
H	-2.62206472	1.07328937	0.45895416

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### NV(NH<sub>2</sub>)<sub>2</sub>(PH<sub>3</sub>) – Transition State

%chk=VPH3\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	0.52857708	0.00000035	0.06529323
N	1.17749438	1.66768997	-0.49413844
H	1.47524852	1.89590534	-1.44084857
H	1.43593563	2.45208737	0.10599061
N	1.17750245	-1.66768596	-0.49413953
H	1.43394031	-2.44844610	0.10723681
H	1.47725047	-1.89954467	-1.44209457
N	0.40344558	-0.00000066	1.61575141
P	-1.95571394	-0.00000193	-0.18339898
H	-2.70890444	-0.00000018	-1.39126393
H	-2.62206643	-1.07329363	0.45895181
H	-2.62206472	1.07328937	0.45895416

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Title Card Required

0 1

V	0.52857708	0.00000035	0.06529323
N	1.17749438	1.66768997	-0.49413844
H	1.43393764	2.44844983	0.10723561
H	1.47724651	1.89954288	-1.44209357
N	1.17750245	-1.66768596	-0.49413953
H	1.43394031	-2.44844610	0.10723681
H	1.47725047	-1.89954467	-1.44209457
N	0.40344558	-0.00000066	1.61575141
P	-1.95571394	-0.00000193	-0.18339898
H	-2.70890444	-0.00000018	-1.39126393
H	-2.62206643	-1.07329363	0.45895181
H	-2.62206472	1.07328937	0.45895416

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 2 3 1.0 4 1.0  
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 5 6 1.0 7 1.0  
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 9 10 1.0 11 1.0 12 1.0  
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# Title Card Required

0 1  
 V            0.47406491   -0.14009359   0.11228818  
 N            1.23200655   1.80778391   -0.54113339  
 H            2.15409126   2.19330709   -0.34586049  
 H            0.72287609   2.69093298   -0.48581684  
 N            1.12299028   -1.80777990   -0.44714458  
 H            1.37942814   -2.58854004   0.15423176  
 H            1.42273830   -2.03963861   -1.39509962  
 N            0.34893341   -0.14009460   1.66274636  
 P            -2.01022611   -0.14009587   -0.13640403  
 H            -2.76341661   -0.14009412   -1.34426898  
 H            -2.67657860   -1.21338757   0.50594676  
 H            -2.67657689   0.93319543   0.50594911

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## NV(NH<sub>2</sub>)<sub>2</sub>(POMe<sub>3</sub>) – Ground State

%chk=VPOMe32\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	-1.84367325	-0.03584734	0.05370969
N	-2.30254583	1.75975455	0.33726869
H	-2.54118291	2.45000499	-0.37214890
H	-2.46283880	2.18892907	1.24965829
N	-2.50703513	-1.51993666	0.98141075
H	-2.81603711	-2.40109035	0.57547352
H	-2.71246481	-1.55170241	1.98068742
N	-1.85068875	-0.32804076	-1.47951822
P	0.61250727	-0.03551959	0.14569133
O	1.21850852	-1.56132532	0.00727551
O	1.41685661	0.83385886	-1.00866094
O	1.34985459	0.61818646	1.46532682
C	2.62869055	-1.77268004	0.06314743
H	3.00931704	-1.60808087	1.08233472
H	2.80437404	-2.81634737	-0.21884436
H	3.16565452	-1.11505106	-0.63785543
C	1.13790261	0.56213552	-2.39173371
H	1.58982861	-0.39449392	-2.69450430
H	0.05529216	0.52505651	-2.57883628
H	1.59722100	1.37719682	-2.96131457
C	2.52814986	1.42463675	1.39273536
H	2.33863566	2.35572569	0.84323333
H	2.79728540	1.65868123	2.42879766
H	3.36346294	0.89570110	0.91207191

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 21 22 1.0 23 1.0 24 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(POMe<sub>3</sub>) – Transition State 1

%chk=VPOMe32\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1			
V	-1.84367325	-0.03584734	0.05370969
N	-2.30254583	1.75975455	0.33726869
H	-2.54118291	2.45000499	-0.37214890
H	-2.46283880	2.18892907	1.24965829
N	-2.50703513	-1.51993666	0.98141075
H	-2.81603711	-2.40109035	0.57547352
H	-2.71246481	-1.55170241	1.98068742
N	-1.85068875	-0.32804076	-1.47951822
P	0.61250727	-0.03551959	0.14569133
O	1.21850852	-1.56132532	0.00727551
O	1.41685661	0.83385886	-1.00866094
O	1.34985459	0.61818646	1.46532682
C	2.62869055	-1.77268004	0.06314743
H	3.00931704	-1.60808087	1.08233472
H	2.80437404	-2.81634737	-0.21884436
H	3.16565452	-1.11505106	-0.63785543
C	1.13790261	0.56213552	-2.39173371
H	1.58982861	-0.39449392	-2.69450430
H	0.05529216	0.52505651	-2.57883628
H	1.59722100	1.37719682	-2.96131457
C	2.52814986	1.42463675	1.39273536
H	2.33863566	2.35572569	0.84323333

H	2.79728540	1.65868123	2.42879766
H	3.36346294	0.89570110	0.91207191

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 9 10 1.0 11 1.0 12 1.0  
 10 13 1.0  
 11 17 1.0  
 12 21 1.0  
 13 14 1.0 15 1.0 16 1.0  
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 17 18 1.0 19 1.0 20 1.0  
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 21 22 1.0 23 1.0 24 1.0  
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Title Card Required

0 1			
V	-1.84367325	-0.03584734	0.05370969
N	-2.30254583	1.75975455	0.33726869
H	-2.46283880	2.18892907	1.24965829
H	-2.54118291	2.45000499	-0.37214890
N	-2.50703513	-1.51993666	0.98141075
H	-2.81603711	-2.40109035	0.57547352
H	-2.71246481	-1.55170241	1.98068742
N	-1.85068875	-0.32804076	-1.47951822
P	0.61250727	-0.03551959	0.14569133
O	1.21850852	-1.56132532	0.00727551
O	1.41685661	0.83385886	-1.00866094
O	1.34985459	0.61818646	1.46532682

C	2.62869055	-1.77268004	0.06314743
H	3.00931704	-1.60808087	1.08233472
H	2.80437404	-2.81634737	-0.21884436
H	3.16565452	-1.11505106	-0.63785543
C	1.13790261	0.56213552	-2.39173371
H	1.58982861	-0.39449392	-2.69450430
H	0.05529216	0.52505651	-2.57883628
H	1.59722100	1.37719682	-2.96131457
C	2.52814986	1.42463675	1.39273536
H	2.33863566	2.35572569	0.84323333
H	2.79728540	1.65868123	2.42879766
H	3.36346294	0.89570110	0.91207191

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Title Card Required

0 1

V -1.84367325 -0.03584734 0.05370969

N -2.37820369 2.05580929 0.38402125

H	-1.83710619	2.87561044	0.11605442
H	-3.32700129	2.43183044	0.35699136
N	-2.50703513	-1.51993666	0.98141075
H	-2.81603711	-2.40109035	0.57547352
H	-2.71246481	-1.55170241	1.98068742
N	-1.85068875	-0.32804076	-1.47951822
P	0.61250727	-0.03551959	0.14569133
O	1.21850852	-1.56132532	0.00727551
O	1.41685661	0.83385886	-1.00866094
O	1.34985459	0.61818646	1.46532682
C	2.62869055	-1.77268004	0.06314743
H	3.00931704	-1.60808087	1.08233472
H	2.80437404	-2.81634737	-0.21884436
H	3.16565452	-1.11505106	-0.63785543
C	1.13790261	0.56213552	-2.39173371
H	1.58982861	-0.39449392	-2.69450430
H	0.05529216	0.52505651	-2.57883628
H	1.59722100	1.37719682	-2.96131457
C	2.52814986	1.42463675	1.39273536
H	2.33863566	2.35572569	0.84323333
H	2.79728540	1.65868123	2.42879766
H	3.36346294	0.89570110	0.91207191

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## NV(NH<sub>2</sub>)<sub>2</sub>(POMe<sub>3</sub>) – Transition State 2

%chk=VPOMe32\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
V -1.84367325 -0.03584734 0.05370969  
N -2.30254583 1.75975455 0.33726869  
H -2.54118291 2.45000499 -0.37214890  
H -2.46283880 2.18892907 1.24965829  
N -2.50703513 -1.51993666 0.98141075  
H -2.81603711 -2.40109035 0.57547352  
H -2.71246481 -1.55170241 1.98068742  
N -1.85068875 -0.32804076 -1.47951822  
P 0.61250727 -0.03551959 0.14569133  
O 1.21850852 -1.56132532 0.00727551  
O 1.41685661 0.83385886 -1.00866094  
O 1.34985459 0.61818646 1.46532682  
C 2.62869055 -1.77268004 0.06314743  
H 3.00931704 -1.60808087 1.08233472  
H 2.80437404 -2.81634737 -0.21884436  
H 3.16565452 -1.11505106 -0.63785543  
C 1.13790261 0.56213552 -2.39173371  
H 1.58982861 -0.39449392 -2.69450430  
H 0.05529216 0.52505651 -2.57883628  
H 1.59722100 1.37719682 -2.96131457  
C 2.52814986 1.42463675 1.39273536  
H 2.33863566 2.35572569 0.84323333  
H 2.79728540 1.65868123 2.42879766  
H 3.36346294 0.89570110 0.91207191

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 13 14 1.0 15 1.0 16 1.0  
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 17 18 1.0 19 1.0 20 1.0  
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 21 22 1.0 23 1.0 24 1.0  
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#### Title Card Required

0 1  
 V -1.84367325 -0.03584734 0.05370969  
 N -2.30254583 1.75975455 0.33726869  
 H -2.54118291 2.45000499 -0.37214890  
 H -2.46283880 2.18892907 1.24965829  
 N -2.50703513 -1.51993666 0.98141075  
 H -2.71246481 -1.55170241 1.98068742  
 H -2.81603711 -2.40109035 0.57547352  
 N -1.85068875 -0.32804076 -1.47951822  
 P 0.61250727 -0.03551959 0.14569133  
 O 1.21850852 -1.56132532 0.00727551  
 O 1.41685661 0.83385886 -1.00866094  
 O 1.34985459 0.61818646 1.46532682  
 C 2.62869055 -1.77268004 0.06314743  
 H 3.00931704 -1.60808087 1.08233472  
 H 2.80437404 -2.81634737 -0.21884436  
 H 3.16565452 -1.11505106 -0.63785543  
 C 1.13790261 0.56213552 -2.39173371  
 H 1.58982861 -0.39449392 -2.69450430  
 H 0.05529216 0.52505651 -2.57883628  
 H 1.59722100 1.37719682 -2.96131457  
 C 2.52814986 1.42463675 1.39273536

H	2.33863566	2.35572569	0.84323333
H	2.79728540	1.65868123	2.42879766
H	3.36346294	0.89570110	0.91207191

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Title Card Required

0 1

V	-1.78937321	0.08563403	-0.02222805
N	-2.24824579	1.88123592	0.26133095
H	-2.48688287	2.57148636	-0.44808664
H	-2.40853876	2.31041044	1.17372055
N	-2.56133517	-1.64141803	1.05734849
H	-3.51259544	-2.00288584	1.02352531
H	-2.02639030	-2.47526259	1.30291218
N	-1.79638871	-0.20655939	-1.55545596
P	0.66680731	0.08596178	0.06975359
O	1.27280856	-1.43984395	-0.06866223
O	1.47115665	0.95534023	-1.08459868



O	1.40415463	0.73966783	1.38938908
C	2.68299059	-1.65119867	-0.01279031
H	3.06361708	-1.48659950	1.00639698
H	2.85867408	-2.69486600	-0.29478210
H	3.21995456	-0.99356969	-0.71379317
C	1.19220265	0.68361689	-2.46767145
H	1.64412865	-0.27301255	-2.77044204
H	0.10959220	0.64653788	-2.65477402
H	1.65152104	1.49867819	-3.03725231
C	2.58244990	1.54611812	1.31679762
H	2.39293570	2.47720706	0.76729559
H	2.85158544	1.78016260	2.35285992
H	3.41776298	1.01718247	0.83613417

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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9 10 1.0 11 1.0 12 1.0

10 13 1.0

11 17 1.0

12 21 1.0

13 14 1.0 15 1.0 16 1.0

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# NV(NH<sub>2</sub>)<sub>2</sub>(POEt<sub>3</sub>) – Ground State

%chk=VPOEt3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

# Title Card Required

0 1

V	-1.82679040	-0.78455110	-0.46660488
N	-1.59591271	-2.64913887	-0.47468375
H	-1.83872085	-3.30328501	0.26740915
H	-1.34184388	-3.20085001	-1.29551139
N	-2.59174503	0.26914534	-1.81339644
H	-3.28418927	1.00628976	-1.69536411
H	-2.45780817	0.13106872	-2.81597824
N	-2.39726903	-0.33892552	0.91697833
P	0.35441479	0.24615437	0.00812429
O	1.02097232	-0.11628727	1.47747116
O	1.54602367	-0.00516415	-1.08817029
O	0.40597081	1.88264882	0.10485819
C	0.78316522	-1.42862229	2.03708037
H	1.02492134	-1.31945718	3.10284511
H	-0.29225677	-1.66335200	1.95938305
C	1.63569948	-2.47953960	1.37476596
H	2.70180350	-2.21433264	1.42107449
H	1.50417885	-3.44955134	1.87436314
H	1.35604257	-2.60914670	0.31873294
C	2.84440938	0.60463431	-0.88785391
H	3.08212785	0.60578816	0.18817593
H	2.78796897	1.65282987	-1.21907539
C	3.84903279	-0.18176547	-1.68087241
H	4.84749194	0.26401559	-1.57980525
H	3.90163832	-1.22251598	-1.33402606
H	3.58717127	-0.19286537	-2.74711171
C	-0.43536600	2.52624990	1.09727068
H	-1.33129840	1.90855127	1.27757631
H	0.13536364	2.57611569	2.03811220
C	-0.79409457	3.89075289	0.58255245
H	-1.38856783	4.43302220	1.32967709
H	0.10536904	4.48301818	0.36624897
H	-1.38575971	3.81961228	-0.33989670

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 12 27 1.0  
 13 14 1.0 15 1.0 16 1.0  
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 16 17 1.0 18 1.0 19 1.0  
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 20 21 1.0 22 1.0 23 1.0  
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 23 24 1.0 25 1.0 26 1.0  
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 27 28 1.0 29 1.0 30 1.0  
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 30 31 1.0 32 1.0 33 1.0  
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# **NV(NH<sub>2</sub>)<sub>2</sub>(POEt<sub>3</sub>) – Transition State**

%chk=VPOEt32\_OPT\_M06L.chk

# opt m06l/cc-pvdz geom=connectivity

Title Card Required

0 1			
V	-2.14426531	0.00000400	-0.05481473
N	-2.70950552	1.68404059	0.54282772
H	-2.93336726	2.48927671	-0.03906952
H	-2.93160979	1.93070382	1.50823365
N	-2.70947535	-1.68405199	0.54279968
H	-2.93331577	-2.48927915	-0.03911853
H	-2.93157194	-1.93074630	1.50819908
N	-2.07628326	0.00001506	-1.61026976

P	0.30294750	-0.00001295	0.05559132
O	1.02606770	-1.28753941	-0.69049556
O	1.02602942	1.28704679	-0.69133628
O	1.08874961	0.00044288	1.52368710
C	3.71613219	-0.00267634	1.38203791
H	4.04410102	-0.87684118	0.85937905
H	4.04615240	0.87046057	0.85895226
H	4.12659033	-0.00291687	2.37017963
C	3.65599592	1.21510126	-0.72757815
H	4.00987419	0.67672482	0.12671746
H	3.98715380	0.72594498	-1.61974438
H	4.04045772	2.21337678	-0.70444558
C	3.65585858	-1.21230360	-0.73236353
H	4.04517621	-2.02907239	-0.16120634
H	3.99880095	-1.28835798	-1.74305946
H	3.99302511	-0.28888513	-0.30985074
C	2.51667493	-0.00125235	1.44670384
H	2.51878173	1.06863303	1.46222223
H	2.51456815	-1.07113775	1.43118591
C	2.45535904	1.24794596	-0.71103295
H	2.42693742	0.65866195	-1.60368998
H	2.48378067	1.83723034	0.18162383
C	2.45530188	-1.24665039	-0.71324990
H	2.48545556	-1.78696435	0.20981650
H	2.42514821	-0.70633683	-1.63631653

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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10 31 1.0

11 28 1.0

12 25 1.0

13 14 1.0 15 1.0 16 1.0 25 1.0

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 21 22 1.0 23 1.0 24 1.0 31 1.0  
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 25 26 1.0 27 1.0  
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 28 29 1.0 30 1.0  
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 31 32 1.0 33 1.0  
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# **NV(NH<sub>2</sub>)<sub>2</sub>(PMePh<sub>2</sub>) – Ground State**

%chk=VPMcPh2\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -1.09332082 2.24607007 -0.26755926  
 N -1.28363172 1.97279835 -2.11837062  
 H -2.14036855 1.74942542 -2.62135692  
 H -0.56540206 2.17506895 -2.81522818  
 N -0.18890338 3.66908946 0.56348668  
 H -0.53505560 4.25038737 1.32445603  
 H 0.67464694 4.09333266 0.22223085  
 N -2.46686394 2.02557258 0.43621431  
 P -0.04778048 0.19202978 0.64984640  
 C -0.01076564 0.22000555 2.47668040  
 H 0.41961799 -0.70159187 2.89236143  
 H 0.55517235 1.09433440 2.82323675  
 H -1.04704086 0.32986218 2.81974690  
 C -0.93656649 -1.36222590 0.25021366  
 C -0.29763273 -2.60689483 0.34320650  
 C -2.28545186 -1.29991470 -0.12177252  
 C -1.00249077 -3.77644002 0.06905185  
 H 0.75792920 -2.66231371 0.62465009  
 C -2.98520089 -2.47587180 -0.39160220

H	-2.77630930	-0.32434296	-0.18910304
C	-2.34714319	-3.71178893	-0.29900016
H	-0.49900934	-4.74258219	0.14142784
H	-4.03668899	-2.42237440	-0.68038702
H	-2.89734927	-4.62966223	-0.51623185
C	1.67635929	-0.15616022	0.14194173
C	2.75163163	-0.14678462	1.03781856
C	1.92500047	-0.39418953	-1.21934431
C	4.05052590	-0.37839220	0.58254557
H	2.58288755	0.04116849	2.10031456
C	3.22004304	-0.63208152	-1.66884552
H	1.09022836	-0.39761892	-1.92676889
C	4.28704224	-0.62357694	-0.76818666
H	4.88071412	-0.36966058	1.29154594
H	3.39937131	-0.82279429	-2.72873200
H	5.30342958	-0.80702547	-1.12154955

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2 3 1.0 4 1.0

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15 17 1.5 18 1.0

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17 21 1.5 22 1.0

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26 28 1.5 29 1.0

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 28 32 1.5 33 1.0  
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 30 32 1.5 34 1.0  
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 32 35 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(PMePh<sub>2</sub>) – Transition State 1

%chk=VPMcPh2\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

```
0 1
V      -1.09332082   2.24607007  -0.26755926
N      -1.28363172   1.97279835  -2.11837062
H      -0.56488106   2.17514833  -2.81071494
H      -2.14088955   1.74934604  -2.62587016
N      -0.18890338   3.66908946   0.56348668
H      -0.53505560   4.25038737   1.32445603
H      0.67464694   4.09333266   0.22223085
N      -2.46686394   2.02557258   0.43621431
P      -0.04778048   0.19202978   0.64984640
C      -0.01076564   0.22000555   2.47668040
H      0.41961799   -0.70159187   2.89236143
H      0.55517235   1.09433440   2.82323675
H      -1.04704086   0.32986218   2.81974690
C      -0.93656649  -1.36222590   0.25021366
C      -0.29763273  -2.60689483   0.34320650
C      -2.28545186  -1.29991470  -0.12177252
C      -1.00249077  -3.77644002   0.06905185
H      0.75792920  -2.66231371   0.62465009
C      -2.98520089  -2.47587180  -0.39160220
H      -2.77630930  -0.32434296  -0.18910304
C      -2.34714319  -3.71178893  -0.29900016
H      -0.49900934  -4.74258219   0.14142784
H      -4.03668899  -2.42237440  -0.68038702
H      -2.89734927  -4.62966223  -0.51623185
C      1.67635929  -0.15616022   0.14194173
C      2.75163163  -0.14678462   1.03781856
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C	1.92500047	-0.39418953	-1.21934431
C	4.05052590	-0.37839220	0.58254557
H	2.58288755	0.04116849	2.10031456
C	3.22004304	-0.63208152	-1.66884552
H	1.09022836	-0.39761892	-1.92676889
C	4.28704224	-0.62357694	-0.76818666
H	4.88071412	-0.36966058	1.29154594
H	3.39937131	-0.82279429	-2.72873200
H	5.30342958	-0.80702547	-1.12154955

1 2 1.0 5 1.0 8 3.0 9 1.0

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10 11 1.0 12 1.0 13 1.0

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14 15 1.5 16 1.5

15 17 1.5 18 1.0

16 19 1.5 20 1.0

17 21 1.5 22 1.0

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19 21 1.5 23 1.0

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21 24 1.0

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25 26 1.5 27 1.5

26 28 1.5 29 1.0

27 30 1.5 31 1.0

28 32 1.5 33 1.0

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30 32 1.5 34 1.0

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32 35 1.0

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Title Card Required

0 1

V	-1.09332082	2.24607007	-0.26755926
N	-1.28363172	1.97279835	-2.11837062
H	-2.14036855	1.74942542	-2.62135692
H	-0.56540206	2.17506895	-2.81522818
N	-0.18890338	3.66908946	0.56348668
H	-0.53505560	4.25038737	1.32445603
H	0.67464694	4.09333266	0.22223085
N	-2.46686394	2.02557258	0.43621431
P	-0.04778048	0.19202978	0.64984640
C	-0.01076564	0.22000555	2.47668040
H	0.41961799	-0.70159187	2.89236143
H	0.55517235	1.09433440	2.82323675
H	-1.04704086	0.32986218	2.81974690
C	-0.93656649	-1.36222590	0.25021366
C	-0.29763273	-2.60689483	0.34320650
C	-2.28545186	-1.29991470	-0.12177252
C	-1.00249077	-3.77644002	0.06905185
H	0.75792920	-2.66231371	0.62465009
C	-2.98520089	-2.47587180	-0.39160220
H	-2.77630930	-0.32434296	-0.18910304
C	-2.34714319	-3.71178893	-0.29900016
H	-0.49900934	-4.74258219	0.14142784
H	-4.03668899	-2.42237440	-0.68038702
H	-2.89734927	-4.62966223	-0.51623185
C	1.67635929	-0.15616022	0.14194173
C	2.75163163	-0.14678462	1.03781856
C	1.92500047	-0.39418953	-1.21934431
C	4.05052590	-0.37839220	0.58254557
H	2.58288755	0.04116849	2.10031456
C	3.22004304	-0.63208152	-1.66884552
H	1.09022836	-0.39761892	-1.92676889
C	4.28704224	-0.62357694	-0.76818666
H	4.88071412	-0.36966058	1.29154594
H	3.39937131	-0.82279429	-2.72873200
H	5.30342958	-0.80702547	-1.12154955

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 14 15 1.5 16 1.5  
 15 17 1.5 18 1.0  
 16 19 1.5 20 1.0  
 17 21 1.5 22 1.0  
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 19 21 1.5 23 1.0  
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 21 24 1.0  
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 25 26 1.5 27 1.5  
 26 28 1.5 29 1.0  
 27 30 1.5 31 1.0  
 28 32 1.5 33 1.0  
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 30 32 1.5 34 1.0  
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 32 35 1.0  
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Title Card Required

0 1			
V	-1.07707465	2.26939831	-0.10956206
N	-1.29987789	1.94947011	-2.27636782
H	-1.91835548	2.45119311	-2.91091347
H	-1.32413675	1.03621658	-2.73217172
N	-0.17265721	3.69241770	0.72148388

H	-0.51880943	4.27371561	1.48245323
H	0.69089311	4.11666090	0.38022805
N	-2.45061777	2.04890082	0.59421151
P	-0.03153431	0.21535802	0.80784360
C	0.00548053	0.24333379	2.63467760
H	0.43586416	-0.67826363	3.05035863
H	0.57141852	1.11766264	2.98123395
H	-1.03079469	0.35319042	2.97774410
C	-0.92032032	-1.33889766	0.40821086
C	-0.28138656	-2.58356659	0.50120370
C	-2.26920569	-1.27658646	0.03622468
C	-0.98624460	-3.75311178	0.22704905
H	0.77417537	-2.63898547	0.78264729
C	-2.96895472	-2.45254356	-0.23360500
H	-2.76006313	-0.30101472	-0.03110584
C	-2.33089702	-3.68846069	-0.14100296
H	-0.48276317	-4.71925395	0.29942504
H	-4.02044282	-2.39904616	-0.52238982
H	-2.88110310	-4.60633399	-0.35823465
C	1.69260546	-0.13283198	0.29993893
C	2.76787780	-0.12345638	1.19581576
C	1.94124664	-0.37086129	-1.06134711
C	4.06677207	-0.35506396	0.74054277
H	2.59913372	0.06449673	2.25831176
C	3.23628921	-0.60875328	-1.51084832
H	1.10647453	-0.37429068	-1.76877169
C	4.30328841	-0.60024870	-0.61018946
H	4.89696029	-0.34633234	1.44954314
H	3.41561748	-0.79946605	-2.57073480
H	5.31967575	-0.78369723	-0.96355235

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 14 15 1.5 16 1.5  
 15 17 1.5 18 1.0  
 16 19 1.5 20 1.0  
 17 21 1.5 22 1.0  
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 19 21 1.5 23 1.0  
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 21 24 1.0  
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 25 26 1.5 27 1.5  
 26 28 1.5 29 1.0  
 27 30 1.5 31 1.0  
 28 32 1.5 33 1.0  
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 30 32 1.5 34 1.0  
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 32 35 1.0  
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## NV(NH<sub>2</sub>)<sub>2</sub>(PMePh<sub>2</sub>) – Transition State 2

%chk=VPMcPh2\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	-1.09332082	2.24607007	-0.26755926
N	-1.28363172	1.97279835	-2.11837062
H	-0.56488106	2.17514833	-2.81071494
H	-2.14088955	1.74934604	-2.62587016
N	-0.18890338	3.66908946	0.56348668
H	-0.53505560	4.25038737	1.32445603
H	0.67464694	4.09333266	0.22223085
N	-2.46686394	2.02557258	0.43621431
P	-0.04778048	0.19202978	0.64984640
C	-0.01076564	0.22000555	2.47668040
H	0.41961799	-0.70159187	2.89236143
H	0.55517235	1.09433440	2.82323675

H	-1.04704086	0.32986218	2.81974690
C	-0.93656649	-1.36222590	0.25021366
C	-0.29763273	-2.60689483	0.34320650
C	-2.28545186	-1.29991470	-0.12177252
C	-1.00249077	-3.77644002	0.06905185
H	0.75792920	-2.66231371	0.62465009
C	-2.98520089	-2.47587180	-0.39160220
H	-2.77630930	-0.32434296	-0.18910304
C	-2.34714319	-3.71178893	-0.29900016
H	-0.49900934	-4.74258219	0.14142784
H	-4.03668899	-2.42237440	-0.68038702
H	-2.89734927	-4.62966223	-0.51623185
C	1.67635929	-0.15616022	0.14194173
C	2.75163163	-0.14678462	1.03781856
C	1.92500047	-0.39418953	-1.21934431
C	4.05052590	-0.37839220	0.58254557
H	2.58288755	0.04116849	2.10031456
C	3.22004304	-0.63208152	-1.66884552
H	1.09022836	-0.39761892	-1.92676889
C	4.28704224	-0.62357694	-0.76818666
H	4.88071412	-0.36966058	1.29154594
H	3.39937131	-0.82279429	-2.72873200
H	5.30342958	-0.80702547	-1.12154955

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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10 11 1.0 12 1.0 13 1.0

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15 17 1.5 18 1.0

16 19 1.5 20 1.0

17 21 1.5 22 1.0

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19 21 1.5 23 1.0

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 21 24 1.0  
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 25 26 1.5 27 1.5  
 26 28 1.5 29 1.0  
 27 30 1.5 31 1.0  
 28 32 1.5 33 1.0  
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 30 32 1.5 34 1.0  
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 32 35 1.0  
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# Title Card Required

0 1  
 V -1.09332082 2.24607007 -0.26755926  
 N -1.28363172 1.97279835 -2.11837062  
 H -0.56488106 2.17514833 -2.81071494  
 H -2.14088955 1.74934604 -2.62587016  
 N -0.18890338 3.66908946 0.56348668  
 H 0.67274302 4.08963246 0.22068639  
 H -0.53315168 4.25408757 1.32600049  
 N -2.46686394 2.02557258 0.43621431  
 P -0.04778048 0.19202978 0.64984640  
 C -0.01076564 0.22000555 2.47668040  
 H 0.41961799 -0.70159187 2.89236143  
 H 0.55517235 1.09433440 2.82323675  
 H -1.04704086 0.32986218 2.81974690  
 C -0.93656649 -1.36222590 0.25021366  
 C -0.29763273 -2.60689483 0.34320650  
 C -2.28545186 -1.29991470 -0.12177252  
 C -1.00249077 -3.77644002 0.06905185  
 H 0.75792920 -2.66231371 0.62465009  
 C -2.98520089 -2.47587180 -0.39160220  
 H -2.77630930 -0.32434296 -0.18910304  
 C -2.34714319 -3.71178893 -0.29900016  
 H -0.49900934 -4.74258219 0.14142784  
 H -4.03668899 -2.42237440 -0.68038702

H	-2.89734927	-4.62966223	-0.51623185
C	1.67635929	-0.15616022	0.14194173
C	2.75163163	-0.14678462	1.03781856
C	1.92500047	-0.39418953	-1.21934431
C	4.05052590	-0.37839220	0.58254557
H	2.58288755	0.04116849	2.10031456
C	3.22004304	-0.63208152	-1.66884552
H	1.09022836	-0.39761892	-1.92676889
C	4.28704224	-0.62357694	-0.76818666
H	4.88071412	-0.36966058	1.29154594
H	3.39937131	-0.82279429	-2.72873200
H	5.30342958	-0.80702547	-1.12154955

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# Title Card Required

0 1			
V	-1.25099360	1.99798614	-0.41244073
N	-1.44130450	1.72471442	-2.26325209
H	-0.72255384	1.92706440	-2.95559641
H	-2.29856233	1.50126211	-2.77075163
N	-0.18890338	3.66908946	0.56348668
H	0.36636865	3.62412553	1.41580950
H	-0.52262676	4.63313646	0.60089096
N	-2.62453672	1.77748865	0.29133284
P	-0.20545326	-0.05605415	0.50496493
C	-0.16843842	-0.02807838	2.33179893
H	0.26194521	-0.94967580	2.74747996
H	0.39749957	0.84625047	2.67835528
H	-1.20471364	0.08177825	2.67486543
C	-1.09423927	-1.61030983	0.10533219
C	-0.45530551	-2.85497876	0.19832503
C	-2.44312464	-1.54799863	-0.26665399
C	-1.16016355	-4.02452395	-0.07582962
H	0.60025642	-2.91039764	0.47976862
C	-3.14287367	-2.72395573	-0.53648367
H	-2.93398208	-0.57242689	-0.33398451
C	-2.50481597	-3.95987286	-0.44388163
H	-0.65668212	-4.99066612	-0.00345363
H	-4.19436177	-2.67045833	-0.82526849
H	-3.05502205	-4.87774616	-0.66111332
C	1.51868651	-0.40424415	-0.00293974
C	2.59395885	-0.39486855	0.89293709
C	1.76732769	-0.64227346	-1.36422578
C	3.89285312	-0.62647613	0.43766410
H	2.42521477	-0.20691544	1.95543309
C	3.06237026	-0.88016545	-1.81372699
H	0.93255558	-0.64570285	-2.07165036
C	4.12936946	-0.87166087	-0.91306813
H	4.72304134	-0.61774451	1.14666447
H	3.24169853	-1.07087822	-2.87361347



H            5.14575680   -1.05510940   -1.26643102

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### **NV(NH<sub>2</sub>)<sub>2</sub>(PPh<sub>3</sub>) – Ground State**

%chk=VPPH3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	0.00152318	-0.08246652	-2.62524623
N	-1.79751276	-0.42436044	-3.04939455
H	-2.47336524	0.22430471	-3.44856146
H	-2.23310230	-1.34770500	-3.03230684
N	1.48115300	-1.16416137	-3.04272182
H	2.37127400	-0.86990410	-3.44022749
H	1.47797376	-2.18504996	-3.02400349
N	0.33961158	1.40828409	-2.93035702
P	0.00818015	0.01559166	-0.13888818
C	-1.22406742	1.16875863	0.57764278
C	-1.65154375	1.06382943	1.90883617
C	-1.70505731	2.20999441	-0.22611518
C	-2.55243959	1.98985989	2.42812885
H	-1.28915257	0.24776630	2.53997600
C	-2.60361514	3.13649067	0.30237008
H	-1.36327469	2.28683232	-1.26284602
C	-3.02856826	3.02784532	1.62535433
H	-2.88436513	1.90101550	3.46446202
H	-2.97475863	3.94676003	-0.32803197
H	-3.73519465	3.75275724	2.03460418
C	-0.37114027	-1.60992376	0.61694433
C	0.65469304	-2.52252529	0.90173726
C	-1.70558260	-2.01257695	0.77650512
C	0.35041393	-3.80227089	1.36246882
H	1.69844318	-2.22879816	0.76379569
C	-2.00442224	-3.29266663	1.23791378
H	-2.51489715	-1.31680369	0.53957931
C	-0.97805161	-4.18930350	1.53530720
H	1.15864675	-4.50078324	1.58782054
H	-3.04695270	-3.59074600	1.36535185
H	-1.21411238	-5.19113487	1.89894576
C	1.60525898	0.52832194	0.60017295
C	2.54135374	1.17292809	-0.21755433
C	1.88625649	0.33559867	1.96048254
C	3.74714610	1.61808375	0.32434164
H	2.30970389	1.32869724	-1.27543071
C	3.09368933	0.77825893	2.49357598
H	1.16269315	-0.17159018	2.60470690
C	4.02521914	1.42048173	1.67549250
H	4.47287715	2.12176751	-0.31696510
H	3.30850925	0.62269606	3.55267280

H 4.97130095 1.76733056 2.09612888

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**NV(NH<sub>2</sub>)<sub>2</sub>(PPh<sub>3</sub>) – Transition State**

%chk=VPPH3\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	0.00152318	-0.08246652	-2.62524623
N	-1.79751276	-0.42436044	-3.04939455
H	-2.47336524	0.22430471	-3.44856146
H	-2.23310230	-1.34770500	-3.03230684
N	1.48115300	-1.16416137	-3.04272182
H	2.37127400	-0.86990410	-3.44022749
H	1.47797376	-2.18504996	-3.02400349
N	0.33961158	1.40828409	-2.93035702
P	0.00818015	0.01559166	-0.13888818
C	-1.22406742	1.16875863	0.57764278
C	-1.65154375	1.06382943	1.90883617
C	-1.70505731	2.20999441	-0.22611518
C	-2.55243959	1.98985989	2.42812885
H	-1.28915257	0.24776630	2.53997600
C	-2.60361514	3.13649067	0.30237008
H	-1.36327469	2.28683232	-1.26284602
C	-3.02856826	3.02784532	1.62535433
H	-2.88436513	1.90101550	3.46446202
H	-2.97475863	3.94676003	-0.32803197
H	-3.73519465	3.75275724	2.03460418
C	-0.37114027	-1.60992376	0.61694433
C	0.65469304	-2.52252529	0.90173726
C	-1.70558260	-2.01257695	0.77650512
C	0.35041393	-3.80227089	1.36246882
H	1.69844318	-2.22879816	0.76379569
C	-2.00442224	-3.29266663	1.23791378
H	-2.51489715	-1.31680369	0.53957931
C	-0.97805161	-4.18930350	1.53530720
H	1.15864675	-4.50078324	1.58782054
H	-3.04695270	-3.59074600	1.36535185
H	-1.21411238	-5.19113487	1.89894576
C	1.60525898	0.52832194	0.60017295
C	2.54135374	1.17292809	-0.21755433
C	1.88625649	0.33559867	1.96048254

C	3.74714610	1.61808375	0.32434164
H	2.30970389	1.32869724	-1.27543071
C	3.09368933	0.77825893	2.49357598
H	1.16269315	-0.17159018	2.60470690
C	4.02521914	1.42048173	1.67549250
H	4.47287715	2.12176751	-0.31696510
H	3.30850925	0.62269606	3.55267280
H	4.97130095	1.76733056	2.09612888

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# Title Card Required

0 1

V	0.00152318	-0.08246652	-2.62524623
N	-1.79751276	-0.42436044	-3.04939455
H	-2.22873955	-1.34662680	-3.03080706
H	-2.47772799	0.22322651	-3.45006124
N	1.48115300	-1.16416137	-3.04272182
H	2.37127400	-0.86990410	-3.44022749
H	1.47797376	-2.18504996	-3.02400349
N	0.33961158	1.40828409	-2.93035702
P	0.00818015	0.01559166	-0.13888818
C	-1.22406742	1.16875863	0.57764278
C	-1.65154375	1.06382943	1.90883617
C	-1.70505731	2.20999441	-0.22611518
C	-2.55243959	1.98985989	2.42812885
H	-1.28915257	0.24776630	2.53997600
C	-2.60361514	3.13649067	0.30237008
H	-1.36327469	2.28683232	-1.26284602
C	-3.02856826	3.02784532	1.62535433
H	-2.88436513	1.90101550	3.46446202
H	-2.97475863	3.94676003	-0.32803197
H	-3.73519465	3.75275724	2.03460418
C	-0.37114027	-1.60992376	0.61694433
C	0.65469304	-2.52252529	0.90173726
C	-1.70558260	-2.01257695	0.77650512
C	0.35041393	-3.80227089	1.36246882
H	1.69844318	-2.22879816	0.76379569
C	-2.00442224	-3.29266663	1.23791378
H	-2.51489715	-1.31680369	0.53957931
C	-0.97805161	-4.18930350	1.53530720
H	1.15864675	-4.50078324	1.58782054
H	-3.04695270	-3.59074600	1.36535185
H	-1.21411238	-5.19113487	1.89894576

C	1.60525898	0.52832194	0.60017295
C	2.54135374	1.17292809	-0.21755433
C	1.88625649	0.33559867	1.96048254
C	3.74714610	1.61808375	0.32434164
H	2.30970389	1.32869724	-1.27543071
C	3.09368933	0.77825893	2.49357598
H	1.16269315	-0.17159018	2.60470690
C	4.02521914	1.42048173	1.67549250
H	4.47287715	2.12176751	-0.31696510
H	3.30850925	0.62269606	3.55267280
H	4.97130095	1.76733056	2.09612888

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 39 42 1.0  
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# Title Card Required

0 1

V	-0.79355609	0.62837178	2.41808655
N	-2.72394483	0.81181333	2.28873675
H	-3.10605660	0.09901861	1.65315524
H	-3.26559583	0.64595059	3.14227965
N	0.24218083	2.09152523	2.95331530
H	0.99715456	2.10527578	3.63557792
H	-0.06322760	3.05293904	2.79170671
N	-0.24320297	-0.63000519	3.16504740
P	0.00828714	0.03251762	0.13232702
C	-0.82284206	-1.48519954	-0.46619293
C	-1.33259237	-1.60459190	-1.76541754
C	-0.94001276	-2.55842578	0.43150229
C	-1.94280034	-2.79242885	-2.16688030
H	-1.25602108	-0.76848328	-2.46508656
C	-1.54633951	-3.74254070	0.01881126
H	-0.56496065	-2.44895609	1.45406365
C	-2.04736291	-3.86183874	-1.27807701
H	-2.33950096	-2.88045365	-3.18020725
H	-1.63538888	-4.57428395	0.72011365
H	-2.52760932	-4.78960906	-1.59548871
C	-0.36307201	1.30890802	-1.12562466
C	0.44472690	1.53500959	-2.24721442
C	-1.52304720	2.07560642	-0.93880952
C	0.08751417	2.50942305	-3.17804170
H	1.35766026	0.95067955	-2.39075715
C	-1.87771643	3.04271025	-1.87707439
H	-2.14604068	1.91831040	-0.04987379
C	-1.07403035	3.26036759	-2.99627745



H	0.72181281	2.68368749	-4.04942125
H	-2.78178215	3.63559615	-1.72653523
H	-1.34930284	4.02374393	-3.72670249
C	1.79881232	-0.29658657	-0.01792153
C	2.68125499	0.51526971	0.70721345
C	2.30282211	-1.31116757	-0.84069878
C	4.05554131	0.32115258	0.59496645
H	2.27728217	1.28842709	1.36746748
C	3.67998579	-1.50345731	-0.94311601
H	1.61874793	-1.95661679	-1.39783803
C	4.55634197	-0.68736130	-0.22887654
H	4.73941096	0.95379497	1.16389332
H	4.06858246	-2.29833292	-1.58262376
H	5.63398560	-0.84343044	-0.30793948

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 35 39 1.5 40 1.0  
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 37 39 1.5 41 1.0  
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 39 42 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(PF<sub>3</sub>) – Ground State

%chk=VPF3\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V 1.23044671 -0.00000004 -0.01879428  
 N 1.89654895 -1.68725670 0.40808961  
 H 1.92257165 -2.49892523 -0.20754481  
 H 2.37166927 -1.94193648 1.27551362  
 N 1.89654873 1.68725713 0.40808920  
 H 1.92257179 2.49892553 -0.20754585  
 H 2.37166915 1.94193737 1.27551332  
 N 0.71643357 -0.00000062 -1.50634744  
 P -1.12129644 0.00000002 0.12146194  
 F -1.81877189 -1.22930886 -0.63596778  
 F -2.09979276 0.00000023 1.41700081  
 F -1.81877182 1.22930872 -0.63596820

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# **NV(NH<sub>2</sub>)<sub>2</sub>(PF<sub>3</sub>) – Transition State**

%chk=VPF3\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V 1.23044671 -0.00000004 -0.01879428  
 N 1.89654895 -1.68725670 0.40808961  
 H 1.92257165 -2.49892523 -0.20754481  
 H 2.37166927 -1.94193648 1.27551362  
 N 1.89654873 1.68725713 0.40808920  
 H 1.92257179 2.49892553 -0.20754585  
 H 2.37166915 1.94193737 1.27551332  
 N 0.71643357 -0.00000062 -1.50634744  
 P -1.12129644 0.00000002 0.12146194  
 F -1.81877189 -1.22930886 -0.63596778  
 F -2.09979276 0.00000023 1.41700081  
 F -1.81877182 1.22930872 -0.63596820

1 2 1.0 5 1.0 8 3.0 9 1.0  
 2 3 1.0 4 1.0  
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 5 6 1.0 7 1.0  
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 9 10 1.0 11 1.0 12 1.0  
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Title Card Required

0 1  
 V 1.23044671 -0.00000004 -0.01879428  
 N 1.89654895 -1.68725670 0.40808961

H	2.37010305	-1.93860383	1.27472670
H	1.92413787	-2.50225788	-0.20675789
N	1.89654873	1.68725713	0.40808920
H	1.92257179	2.49892553	-0.20754585
H	2.37166915	1.94193737	1.27551332
N	0.71643357	-0.00000062	-1.50634744
P	-1.12129644	0.00000002	0.12146194
F	-1.81877189	-1.22930886	-0.63596778
F	-2.09979276	0.00000023	1.41700081
F	-1.81877182	1.22930872	-0.63596820

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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9 10 1.0 11 1.0 12 1.0

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Title Card Required

0 1

V	1.23044671	-0.00000004	-0.01879428
N	2.00691459	-1.96681612	0.47881946
H	1.50571886	-2.85065553	0.40059247
H	2.94995841	-2.30597773	0.28218966
N	1.89654873	1.68725713	0.40808920
H	1.92257179	2.49892553	-0.20754585
H	2.37166915	1.94193737	1.27551332
N	0.71643357	-0.00000062	-1.50634744
P	-1.12129644	0.00000002	0.12146194
F	-1.81877189	-1.22930886	-0.63596778
F	-2.09979276	0.00000023	1.41700081
F	-1.81877182	1.22930872	-0.63596820

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2 3 1.0 4 1.0

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 9 10 1.0 11 1.0 12 1.0  
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# **NV(NH<sub>2</sub>)<sub>2</sub>(P(CF<sub>3</sub>)<sub>3</sub>) – Ground State**

%mem=4GB

%Nprocs=4

%chk=PCF3\_freq.chk

# opt=calcfreq freq m06l/cc-pvdz pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

N	2.13413143	-0.11761419	-1.48151973
N	2.86665160	-1.67643458	0.73908447
H	3.12951239	-1.87546724	1.70550095
H	3.04541129	-2.51765455	0.19258623
N	2.79627567	1.71265851	0.53700877
H	2.95269251	2.48757982	-0.10609802
H	3.04115985	2.03595827	1.47420114
P	-0.12401185	-0.01604524	0.06432040
C	-0.91278237	-1.27220832	-1.12287714
C	-0.90496034	1.59456615	-0.57289499
C	-1.23181884	-0.29273770	1.58583945
F	-0.78479430	-0.84143817	-2.37834685
F	-0.30737764	-2.45591120	-0.99952560
F	-0.18189260	2.12035963	-1.55600713
F	-2.21951363	-1.44580556	-0.86672186
F	-2.15505155	1.41307219	-1.01833760
F	-0.94507014	2.46697547	0.44985661
F	-2.49507702	0.11847880	1.44648810
F	-0.69816786	0.35637267	2.63416225
F	-1.24056200	-1.60698839	1.86678627
V	2.28943133	-0.02712023	0.07223467

1 21 1.0

2 3 1.0 4 1.0 21 1.0

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5 6 1.0 7 1.0 21 1.0

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8 9 1.0 10 1.0 11 1.0 21 1.0
9 12 1.0 13 1.0 15 1.0
10 14 1.0 16 1.0 17 1.0
11 18 1.0 19 1.0 20 1.0
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$END

```

### **NV(NH<sub>2</sub>)<sub>2</sub>(P(CF<sub>3</sub>)<sub>3</sub>) – Transition State**

```

%mem=4GB
%Nprocs=4
%chk=PCF3_QST3_3.chk
# opt=(calcall,qst3) freq m06l/cc-pvdz pop=(nbo6,savenbos)
geom=connectivity
Title Card Required
0 1
N      2.13413143  -0.11761419  -1.48151973
N      2.86665160  -1.67643458   0.73908447
H      3.12951239  -1.87546724   1.70550095
H      3.04541129  -2.51765455   0.19258623
N      2.79627567   1.71265851   0.53700877
H      2.95269251   2.48757982  -0.10609802
H      3.04115985   2.03595827   1.47420114
P     -0.12401185  -0.01604524   0.06432040
C     -0.91278237  -1.27220832  -1.12287714
C     -0.90496034   1.59456615  -0.57289499
C     -1.23181884  -0.29273770   1.58583945
F     -0.78479430  -0.84143817  -2.37834685
F     -0.30737764  -2.45591120  -0.99952560
F     -0.18189260   2.12035963  -1.55600713
F     -2.21951363  -1.44580556  -0.86672186
F     -2.15505155   1.41307219  -1.01833760
F     -0.94507014   2.46697547   0.44985661

```

F	-2.49507702	0.11847880	1.44648810
F	-0.69816786	0.35637267	2.63416225
F	-1.24056200	-1.60698839	1.86678627
V	2.28943133	-0.02712023	0.07223467

1 21 1.0

2 3 1.0 4 1.0 21 1.0

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5 6 1.0 7 1.0 21 1.0

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8 9 1.0 10 1.0 11 1.0 21 1.0

9 12 1.0 13 1.0 15 1.0

10 14 1.0 16 1.0 17 1.0

11 18 1.0 19 1.0 20 1.0

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Title Card Required

0 1

N	2.13413143	-0.11761419	-1.48151973
N	2.86665160	-1.67643458	0.73908447
H	3.12951239	-1.87546724	1.70550095
H	3.04541129	-2.51765455	0.19258623
N	2.79627567	1.71265851	0.53700877
H	3.03998243	2.03273609	1.47333829
H	2.95386993	2.49080200	-0.10523517
P	-0.12401185	-0.01604524	0.06432040
C	-0.91278237	-1.27220832	-1.12287714
C	-0.90496034	1.59456615	-0.57289499
C	-1.23181884	-0.29273770	1.58583945
F	-0.78479430	-0.84143817	-2.37834685
F	-0.30737764	-2.45591120	-0.99952560
F	-0.18189260	2.12035963	-1.55600713
F	-2.21951363	-1.44580556	-0.86672186
F	-2.15505155	1.41307219	-1.01833760

F	-0.94507014	2.46697547	0.44985661
F	-2.49507702	0.11847880	1.44648810
F	-0.69816786	0.35637267	2.63416225
F	-1.24056200	-1.60698839	1.86678627
V	2.28943133	-0.02712023	0.07223467

1 21 1.0

2 3 1.0 4 1.0 21 1.0

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9 12 1.0 13 1.0 15 1.0

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11 18 1.0 19 1.0 20 1.0

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Title Card Required

0 1

N	2.13413143	-0.11761419	-1.48151973
N	2.86665160	-1.67643458	0.73908447
H	3.12951239	-1.87546724	1.70550095
H	3.04541129	-2.51765455	0.19258623
N	2.79627567	1.71265851	0.53700877
H	3.74077284	2.02840445	0.75330764
H	2.16474194	2.49943080	0.69504371
P	-0.12401185	-0.01604524	0.06432040
C	-0.91278237	-1.27220832	-1.12287714
C	-0.90496034	1.59456615	-0.57289499
C	-1.23181884	-0.29273770	1.58583945
F	-0.78479430	-0.84143817	-2.37834685
F	-0.30737764	-2.45591120	-0.99952560
F	-0.18189260	2.12035963	-1.55600713
F	-2.21951363	-1.44580556	-0.86672186



F	-2.15505155	1.41307219	-1.01833760
F	-0.94507014	2.46697547	0.44985661
F	-2.49507702	0.11847880	1.44648810
F	-0.69816786	0.35637267	2.63416225
F	-1.24056200	-1.60698839	1.86678627
V	2.28943133	-0.02712023	0.07223467

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 2 3 1.0 4 1.0 21 1.0  
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 5 6 1.0 7 1.0 21 1.0  
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 8 9 1.0 10 1.0 11 1.0 21 1.0  
 9 12 1.0 13 1.0 15 1.0  
 10 14 1.0 16 1.0 17 1.0  
 11 18 1.0 19 1.0 20 1.0  
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 \$END

### NV(NH<sub>2</sub>)<sub>2</sub>(PCy<sub>3</sub>) – Ground State

%Mem=4GB

%Nprocs=4

%chk=M\_PCy3\_freq.chk

# opt=calcall freq m06l/cc-pvdz pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

V	0.42670795	-0.87775000	2.42116364
P	-0.05242881	-0.06821327	0.10223747
C	-1.60667637	-0.89506578	-0.49300223
C	-2.76317688	-0.68534565	0.48761757
C	-2.03894486	-0.56057799	-1.92049890
H	-1.33685050	-1.96562750	-0.43668865
C	-3.97899816	-1.50492678	0.07201991

H	-3.03682846	0.38650539	0.51778902
H	-2.43999476	-0.95646352	1.50340926
C	-3.24842593	-1.39557809	-2.32924732
H	-2.31148369	0.50967864	-1.97671712
H	-1.21184140	-0.71032971	-2.63403787
C	-4.40509071	-1.20190087	-1.35799239
H	-4.81041291	-1.32722724	0.77109051
H	-3.72972510	-2.57711218	0.16128038
H	-3.55375347	-1.14359712	-3.35664337
H	-2.95899575	-2.46170073	-2.34769967
H	-5.26238661	-1.82809001	-1.64939974
H	-4.75686175	-0.15565413	-1.42027865
C	-0.33751881	1.76757819	-0.10937866
C	0.39023625	2.56482437	0.97995687
C	-0.03649747	2.34533959	-1.49530509
H	-1.42414275	1.87862884	0.07728558
C	0.05466149	4.04900473	0.90358219
H	1.48192820	2.42618131	0.86787389
H	0.13073210	2.15884607	1.97161987
C	-0.38873064	3.82785791	-1.55779885
H	1.03851694	2.22576004	-1.71804080
H	-0.57094381	1.79019548	-2.28069309
C	0.34166998	4.61671219	-0.47971418
H	0.60816334	4.60432500	1.67618722
H	-1.01661174	4.18599632	1.13745845
H	-0.15884794	4.22844581	-2.55703326
H	-1.47917152	3.94752688	-1.42369603
H	0.06727561	5.68165452	-0.52572785
H	1.42906362	4.57298256	-0.67306570
C	1.25465323	-0.54376351	-1.13607390
C	2.61368206	0.06133108	-0.76794012
C	1.36357123	-2.06770361	-1.25552186
H	0.94029591	-0.13354997	-2.11534443
C	3.69238413	-0.34576323	-1.76412660
H	2.88670196	-0.28487956	0.24476983
H	2.54974771	1.15980766	-0.70748690
C	2.45403646	-2.47060938	-2.24078747
H	1.57608816	-2.48924528	-0.25649380
H	0.40191252	-2.50358863	-1.56724392
C	3.79817438	-1.86026054	-1.87190870
H	4.65830726	0.09361289	-1.47077744
H	3.45422424	0.07610139	-2.75815864
H	2.52375614	-3.56784433	-2.29108972

H	2.17020021	-2.13604949	-3.25574049
H	4.56887933	-2.14540629	-2.60445467
H	4.12871718	-2.27012819	-0.90071035
N	-0.80895953	-0.04659398	3.57629924
H	-1.62827700	-0.47812967	4.00013814
H	-0.65506978	0.84252684	4.05367475
N	2.28677974	-0.88264688	2.71297978
H	2.82185919	-0.08801492	3.06605287
H	2.89658635	-1.69753257	2.74264951
N	-0.04534365	-2.33419790	2.12962602

1 2 1.0 54 1.0 57 1.0 60 1.0

2 3 1.0 20 1.0 37 1.0

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 57 58 1.0 59 1.0  
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 \$END

### NV(NH<sub>2</sub>)<sub>2</sub>(PCy<sub>3</sub>) – Transition State

%Mem=4GB  
 %Nprocs=4  
 %chk=M\_PCy3\_QST3.chk  
 # opt=(calcall,qst3) freq m06l/cc-pvdz pop=(nbo6,savenbos)  
 geom=connectivity  
 Title Card Required  
 0 1  

V	0.42670795	-0.87775000	2.42116364
P	-0.05242881	-0.06821327	0.10223747
C	-1.60667637	-0.89506578	-0.49300223
C	-2.76317688	-0.68534565	0.48761757
C	-2.03894486	-0.56057799	-1.92049890
H	-1.33685050	-1.96562750	-0.43668865

C	-3.97899816	-1.50492678	0.07201991
H	-3.03682846	0.38650539	0.51778902
H	-2.43999476	-0.95646352	1.50340926
C	-3.24842593	-1.39557809	-2.32924732
H	-2.31148369	0.50967864	-1.97671712
H	-1.21184140	-0.71032971	-2.63403787
C	-4.40509071	-1.20190087	-1.35799239
H	-4.81041291	-1.32722724	0.77109051
H	-3.72972510	-2.57711218	0.16128038
H	-3.55375347	-1.14359712	-3.35664337
H	-2.95899575	-2.46170073	-2.34769967
H	-5.26238661	-1.82809001	-1.64939974
H	-4.75686175	-0.15565413	-1.42027865
C	-0.33751881	1.76757819	-0.10937866
C	0.39023625	2.56482437	0.97995687
C	-0.03649747	2.34533959	-1.49530509
H	-1.42414275	1.87862884	0.07728558
C	0.05466149	4.04900473	0.90358219
H	1.48192820	2.42618131	0.86787389
H	0.13073210	2.15884607	1.97161987
C	-0.38873064	3.82785791	-1.55779885
H	1.03851694	2.22576004	-1.71804080
H	-0.57094381	1.79019548	-2.28069309
C	0.34166998	4.61671219	-0.47971418
H	0.60816334	4.60432500	1.67618722
H	-1.01661174	4.18599632	1.13745845
H	-0.15884794	4.22844581	-2.55703326
H	-1.47917152	3.94752688	-1.42369603
H	0.06727561	5.68165452	-0.52572785
H	1.42906362	4.57298256	-0.67306570
C	1.25465323	-0.54376351	-1.13607390
C	2.61368206	0.06133108	-0.76794012
C	1.36357123	-2.06770361	-1.25552186
H	0.94029591	-0.13354997	-2.11534443
C	3.69238413	-0.34576323	-1.76412660
H	2.88670196	-0.28487956	0.24476983
H	2.54974771	1.15980766	-0.70748690
C	2.45403646	-2.47060938	-2.24078747
H	1.57608816	-2.48924528	-0.25649380
H	0.40191252	-2.50358863	-1.56724392
C	3.79817438	-1.86026054	-1.87190870
H	4.65830726	0.09361289	-1.47077744
H	3.45422424	0.07610139	-2.75815864

H	2.52375614	-3.56784433	-2.29108972
H	2.17020021	-2.13604949	-3.25574049
H	4.56887933	-2.14540629	-2.60445467
H	4.12871718	-2.27012819	-0.90071035
N	-0.80895953	-0.04659398	3.57629924
H	-1.62827700	-0.47812967	4.00013814
H	-0.65506978	0.84252684	4.05367475
N	2.28677974	-0.88264688	2.71297978
H	2.82185919	-0.08801492	3.06605287
H	2.89658635	-1.69753257	2.74264951
N	-0.04534365	-2.33419790	2.12962602

1 2 1.0 54 1.0 57 1.0 60 1.0

2 3 1.0 20 1.0 37 1.0

3 4 1.0 5 1.0 6 1.0

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 47 52 1.0 53 1.0  
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 57 58 1.0 59 1.0  
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# Title Card Required

0 1

V	0.42670795	-0.87775000	2.42116364
P	-0.05242881	-0.06821327	0.10223747
C	-1.60667637	-0.89506578	-0.49300223
C	-2.76317688	-0.68534565	0.48761757
C	-2.03894486	-0.56057799	-1.92049890
H	-1.33685050	-1.96562751	-0.43668865
C	-3.97899816	-1.50492678	0.07201991
H	-3.03682846	0.38650539	0.51778902
H	-2.43999476	-0.95646352	1.50340926
C	-3.24842593	-1.39557809	-2.32924732
H	-2.31148369	0.50967864	-1.97671712
H	-1.21184140	-0.71032971	-2.63403787
C	-4.40509071	-1.20190087	-1.35799239

H	-4.81041291	-1.32722724	0.77109051
H	-3.72972510	-2.57711218	0.16128038
H	-3.55375347	-1.14359712	-3.35664337
H	-2.95899575	-2.46170073	-2.34769967
H	-5.26238661	-1.82809001	-1.64939974
H	-4.75686175	-0.15565413	-1.42027865
C	-0.33751881	1.76757819	-0.10937866
C	0.39023625	2.56482437	0.97995687
C	-0.03649747	2.34533959	-1.49530509
H	-1.42414275	1.87862884	0.07728558
C	0.05466149	4.04900473	0.90358219
H	1.48192820	2.42618131	0.86787389
H	0.13073210	2.15884607	1.97161987
C	-0.38873064	3.82785791	-1.55779885
H	1.03851694	2.22576004	-1.71804080
H	-0.57094381	1.79019548	-2.28069309
C	0.34166998	4.61671219	-0.47971418
H	0.60816334	4.60432500	1.67618722
H	-1.01661174	4.18599632	1.13745845
H	-0.15884794	4.22844581	-2.55703326
H	-1.47917152	3.94752688	-1.42369603
H	0.06727561	5.68165452	-0.52572785
H	1.42906362	4.57298256	-0.67306570
C	1.25465323	-0.54376351	-1.13607390
C	2.61368206	0.06133108	-0.76794012
C	1.36357123	-2.06770361	-1.25552186
H	0.94029591	-0.13354997	-2.11534443
C	3.69238413	-0.34576323	-1.76412660
H	2.88670196	-0.28487956	0.24476983
H	2.54974771	1.15980766	-0.70748690
C	2.45403646	-2.47060938	-2.24078747
H	1.57608816	-2.48924528	-0.25649380
H	0.40191252	-2.50358863	-1.56724392
C	3.79817438	-1.86026054	-1.87190870
H	4.65830726	0.09361289	-1.47077744
H	3.45422424	0.07610139	-2.75815864
H	2.52375614	-3.56784433	-2.29108972
H	2.17020021	-2.13604949	-3.25574049
H	4.56887933	-2.14540629	-2.60445467
H	4.12871718	-2.27012819	-0.90071035
N	-0.80895953	-0.04659398	3.57629924
H	-0.65281511	0.84097641	4.05062117
H	-1.63053167	-0.47657923	4.00319172



N	2.28677974	-0.88264688	2.71297978
H	2.82185919	-0.08801492	3.06605287
H	2.89658635	-1.69753257	2.74264951
N	-0.04534365	-2.33419790	2.12962602

1 2 1.0 54 1.0 57 1.0 60 1.0  
 2 3 1.0 20 1.0 37 1.0  
 3 4 1.0 5 1.0 6 1.0  
 4 7 1.0 8 1.0 9 1.0  
 5 10 1.0 11 1.0 12 1.0  
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 7 13 1.0 14 1.0 15 1.0  
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 38 41 1.0 42 1.0 43 1.0  
 39 44 1.0 45 1.0 46 1.0

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 54 55 1.0 56 1.0  
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 57 58 1.0 59 1.0  
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Title Card Required

0 1

V	0.42670795	-0.87775000	2.42116364
P	-0.05242881	-0.06821327	0.10223747
C	-1.60667637	-0.89506578	-0.49300223
C	-2.76317688	-0.68534565	0.48761757
C	-2.03894486	-0.56057799	-1.92049890
H	-1.33685050	-1.96562750	-0.43668865
C	-3.97899816	-1.50492678	0.07201991
H	-3.03682846	0.38650539	0.51778902
H	-2.43999476	-0.95646352	1.50340926
C	-3.24842593	-1.39557809	-2.32924732
H	-2.31148369	0.50967864	-1.97671712
H	-1.21184140	-0.71032971	-2.63403787
C	-4.40509071	-1.20190087	-1.35799239
H	-4.81041291	-1.32722724	0.77109051
H	-3.72972510	-2.57711218	0.16128038
H	-3.55375347	-1.14359712	-3.35664337
H	-2.95899575	-2.46170073	-2.34769967
H	-5.26238661	-1.82809001	-1.64939974
H	-4.75686175	-0.15565413	-1.42027865
C	-0.33751881	1.76757819	-0.10937866

C	0.39023625	2.56482437	0.97995687
C	-0.03649747	2.34533959	-1.49530509
H	-1.42414275	1.87862884	0.07728558
C	0.05466149	4.04900473	0.90358219
H	1.48192820	2.42618131	0.86787389
H	0.13073210	2.15884607	1.97161987
C	-0.38873064	3.82785791	-1.55779885
H	1.03851694	2.22576004	-1.71804080
H	-0.57094381	1.79019548	-2.28069309
C	0.34166998	4.61671219	-0.47971418
H	0.60816334	4.60432500	1.67618722
H	-1.01661174	4.18599632	1.13745845
H	-0.15884794	4.22844581	-2.55703326
H	-1.47917152	3.94752688	-1.42369603
H	0.06727561	5.68165452	-0.52572785
H	1.42906362	4.57298256	-0.67306570
C	1.25465323	-0.54376351	-1.13607390
C	2.61368206	0.06133108	-0.76794012
C	1.36357123	-2.06770361	-1.25552186
H	0.94029591	-0.13354997	-2.11534443
C	3.69238413	-0.34576323	-1.76412660
H	2.88670196	-0.28487956	0.24476983
H	2.54974771	1.15980766	-0.70748690
C	2.45403646	-2.47060938	-2.24078747
H	1.57608816	-2.48924528	-0.25649380
H	0.40191252	-2.50358863	-1.56724392
C	3.79817438	-1.86026054	-1.87190870
H	4.65830726	0.09361289	-1.47077744
H	3.45422424	0.07610139	-2.75815864
H	2.52375614	-3.56784433	-2.29108972
H	2.17020021	-2.13604949	-3.25574049
H	4.56887933	-2.14540629	-2.60445467
H	4.12871718	-2.27012819	-0.90071035
N	-0.80895953	-0.04659398	3.57629924
H	-1.72810555	0.31245034	3.32450299
H	-0.76406402	-0.07296421	4.59580612
N	2.28677974	-0.88264688	2.71297978
H	2.82185919	-0.08801492	3.06605287
H	2.89658635	-1.69753257	2.74264951
N	-0.04534365	-2.33419790	2.12962602
1 2 1.0 54 1.0 57 1.0 60 1.0			
2 3 1.0 20 1.0 37 1.0			
3 4 1.0 5 1.0 6 1.0			

4 7 1.0 8 1.0 9 1.0  
5 10 1.0 11 1.0 12 1.0  
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21 24 1.0 25 1.0 26 1.0  
22 27 1.0 28 1.0 29 1.0  
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37 38 1.0 39 1.0 40 1.0  
38 41 1.0 42 1.0 43 1.0  
39 44 1.0 45 1.0 46 1.0  
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44 47 1.0 50 1.0 51 1.0  
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54 55 1.0 56 1.0
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57 58 1.0 59 1.0
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$END

```

# **NV(NH<sub>2</sub>)<sub>2</sub>(P(OCH<sub>2</sub>CH<sub>2</sub>)<sub>3</sub>CH) – Ground State**

%chk=VPpaulh\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

```

0 1
V      -2.14426531  0.00000400 -0.05481473
N      -2.70950552  1.68404059  0.54282772
H      -2.93336726  2.48927671 -0.03906952
H      -2.93160979  1.93070382  1.50823365
N      -2.70947535 -1.68405199  0.54279968
H      -2.93331577 -2.48927915 -0.03911853
H      -2.93157194 -1.93074630  1.50819908
N      -2.07628326  0.00001506 -1.61026976
P      0.30294750 -0.00001295  0.05559132
O      1.02606770 -1.28753941 -0.69049556
O      1.02602942  1.28704679 -0.69133628
O      1.08874961  0.00044288  1.52368710
C      2.46776584 -1.24629380 -0.71344833
C      2.46782123  1.24760504 -0.71120468
C      2.52919054 -0.00126721  1.44602909
C      2.98891974  0.00001151 -0.00691196
H      2.78496094 -1.26730873 -1.76788587
H      2.83577429 -2.16289356 -0.22608725
H      2.78700402  1.27169948 -1.76495193
H      2.83396136  2.16333327 -0.22075187

```

H	2.89430912	-0.89404272	1.97835650
H	2.89625198	0.88938140	1.98053109
H	4.08938364	0.00001726	-0.03971668

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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9 10 1.0 11 1.0 12 1.0

10 13 1.0

11 14 1.0

12 15 1.0

13 16 1.0 17 1.0 18 1.0

14 16 1.0 19 1.0 20 1.0

15 16 1.0 21 1.0 22 1.0

16 23 1.0

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## NV(NH<sub>2</sub>)<sub>2</sub>(P(OCH<sub>2</sub>CH<sub>2</sub>)<sub>3</sub>CH) – Transition State

%chk=VPpaulh\_TS\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	-2.14426531	0.00000400	-0.05481473
---	-------------	------------	-------------

N	-2.70950552	1.68404059	0.54282772
---	-------------	------------	------------

H	-2.93336726	2.48927671	-0.03906952
---	-------------	------------	-------------

H	-2.93160979	1.93070382	1.50823365
---	-------------	------------	------------

N	-2.70947535	-1.68405199	0.54279968
---	-------------	-------------	------------

H	-2.93331577	-2.48927915	-0.03911853
---	-------------	-------------	-------------

H	-2.93157194	-1.93074630	1.50819908
---	-------------	-------------	------------

N	-2.07628326	0.00001506	-1.61026976
---	-------------	------------	-------------

P	0.30294750	-0.00001295	0.05559132
O	1.02606770	-1.28753941	-0.69049556
O	1.02602942	1.28704679	-0.69133628
O	1.08874961	0.00044288	1.52368710
C	2.46776584	-1.24629380	-0.71344833
C	2.46782123	1.24760504	-0.71120468
C	2.52919054	-0.00126721	1.44602909
C	2.98891974	0.00001151	-0.00691196
H	2.78496094	-1.26730873	-1.76788587
H	2.83577429	-2.16289356	-0.22608725
H	2.78700402	1.27169948	-1.76495193
H	2.83396136	2.16333327	-0.22075187
H	2.89430912	-0.89404272	1.97835650
H	2.89625198	0.88938140	1.98053109
H	4.08938364	0.00001726	-0.03971668

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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9 10 1.0 11 1.0 12 1.0

10 13 1.0

11 14 1.0

12 15 1.0

13 16 1.0 17 1.0 18 1.0

14 16 1.0 19 1.0 20 1.0

15 16 1.0 21 1.0 22 1.0

16 23 1.0

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Title Card Required

0 1

V	-2.14426531	0.00000400	-0.05481473
N	-2.80776107	1.97677621	0.64671575
H	-2.27488201	2.84370312	0.60669901
H	-3.76017359	2.34026296	0.59222314
N	-2.70947535	-1.68405199	0.54279968
H	-2.93331577	-2.48927915	-0.03911853
H	-2.93157194	-1.93074630	1.50819908
N	-2.07628326	0.00001506	-1.61026976
P	0.30294750	-0.00001295	0.05559132
O	1.02606770	-1.28753941	-0.69049556
O	1.02602942	1.28704679	-0.69133628
O	1.08874961	0.00044288	1.52368710
C	2.46776584	-1.24629380	-0.71344833
C	2.46782123	1.24760504	-0.71120468
C	2.52919054	-0.00126721	1.44602909
C	2.98891974	0.00001151	-0.00691196
H	2.78496094	-1.26730873	-1.76788587
H	2.83577429	-2.16289356	-0.22608725
H	2.78700402	1.27169948	-1.76495193
H	2.83396136	2.16333327	-0.22075187
H	2.89430912	-0.89404272	1.97835650
H	2.89625198	0.88938140	1.98053109
H	4.08938364	0.00001726	-0.03971668

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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5 6 1.0 7 1.0

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9 10 1.0 11 1.0 12 1.0

10 13 1.0

11 14 1.0

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13 16 1.0 17 1.0 18 1.0

14 16 1.0 19 1.0 20 1.0

15 16 1.0 21 1.0 22 1.0

16 23 1.0

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# Title Card Required

0 1

V	-2.14426531	0.00000400	-0.05481473
N	-2.70950552	1.68404059	0.54282772
H	-2.93005677	1.92704072	1.50689814
H	-2.93492027	2.49293980	-0.03773400
N	-2.70947535	-1.68405199	0.54279968
H	-2.93331577	-2.48927915	-0.03911853
H	-2.93157194	-1.93074630	1.50819908
N	-2.07628326	0.00001506	-1.61026976
P	0.30294750	-0.00001295	0.05559132
O	1.02606770	-1.28753941	-0.69049556
O	1.02602942	1.28704679	-0.69133628
O	1.08874961	0.00044288	1.52368710
C	2.46776584	-1.24629380	-0.71344833
C	2.46782123	1.24760504	-0.71120468
C	2.52919054	-0.00126721	1.44602909
C	2.98891974	0.00001151	-0.00691196
H	2.78496094	-1.26730873	-1.76788587
H	2.83577429	-2.16289356	-0.22608725
H	2.78700402	1.27169948	-1.76495193
H	2.83396136	2.16333327	-0.22075187
H	2.89430912	-0.89404272	1.97835650
H	2.89625198	0.88938140	1.98053109
H	4.08938364	0.00001726	-0.03971668

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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5 6 1.0 7 1.0

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9 10 1.0 11 1.0 12 1.0

10 13 1.0

11 14 1.0

12 15 1.0  
 13 16 1.0 17 1.0 18 1.0  
 14 16 1.0 19 1.0 20 1.0  
 15 16 1.0 21 1.0 22 1.0  
 16 23 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(PH<sub>2</sub>Me) – Ground State

%chk=VPH2Me\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -0.83535292 0.08628986 0.06980373  
 N -2.08098047 -1.29904916 -0.18813486  
 H -2.47469735 -1.89587021 0.53107465  
 H -2.58263257 -1.47947226 -1.05416953  
 N -0.96672505 1.83438789 -0.61968872  
 H -0.85447947 2.69571417 -0.09624845  
 H -1.31990281 2.07363992 -1.54292976  
 N -0.45828504 0.16940199 1.58322573  
 P 1.46992589 -0.67444813 -0.43920782  
 H 2.01503326 -0.88918426 -1.73722955  
 H 1.80500728 -1.93555150 0.11564670  
 C 2.71457663 0.43467111 0.31712787  
 H 3.73824162 0.06856342 0.19029121  
 H 2.62062797 1.42769697 -0.13517331  
 H 2.47150524 0.52530707 1.38078729

1 2 1.0 5 1.0 8 3.0 9 1.0  
 2 3 1.0 4 1.0  
 3  
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 5 6 1.0 7 1.0  
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 9 10 1.0 11 1.0 12 1.0  
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 12 13 1.0 14 1.0 15 1.0  
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 14  
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# **NV(NH<sub>2</sub>)<sub>2</sub>(PH<sub>2</sub>Me) – Transition State 1**

%chk=VPH2Me\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -0.83549522 0.08632010 0.06978186  
 N -2.07990503 -1.30014286 -0.18803636  
 H -2.47183754 -1.89805996 0.53124392  
 H -2.58198872 -1.48113338 -1.05369384  
 N -0.96858985 1.83447962 -0.61914515  
 H -0.85628931 2.69579760 -0.09570168  
 H -1.32238834 2.07371914 -1.54215381  
 N -0.45763471 0.16917974 1.58304415  
 P 1.46986779 -0.67377826 -0.43924204  
 H 2.01527077 -0.88991328 -1.73692308  
 H 1.80383923 -1.93470519 0.11669289  
 C 2.71526070 0.43486649 0.31657069  
 H 3.73845063 0.06675948 0.19169569  
 H 2.62364272 1.42719281 -0.13773989  
 H 2.47101661 0.52784000 1.37976491

1 2 1.0 5 1.0 8 3.0 9 1.0  
 2 3 1.0 4 1.0  
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 5 6 1.0 7 1.0  
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 7  
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 9 10 1.0 11 1.0 12 1.0  
 10  
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12 13 1.0 14 1.0 15 1.0  
13  
14  
15

Title Card Required

0 1  
V -0.83549522 0.08632010 0.06978186  
N -2.07990503 -1.30014286 -0.18803636  
H -2.57840086 -1.47800747 -1.05310640  
H -2.47542539 -1.90118586 0.53065648  
N -0.96858985 1.83447962 -0.61914515  
H -0.85628931 2.69579760 -0.09570168  
H -1.32238834 2.07371914 -1.54215381  
N -0.45763471 0.16917974 1.58304415  
P 1.46986779 -0.67377826 -0.43924204  
H 2.01527077 -0.88991328 -1.73692308  
H 1.80383923 -1.93470519 0.11669289  
C 2.71526070 0.43486649 0.31657069  
H 3.73845063 0.06675948 0.19169569  
H 2.62364272 1.42719281 -0.13773989  
H 2.47101661 0.52784000 1.37976491

1 2 1.0 5 1.0 8 3.0 9 1.0  
2 3 1.0 4 1.0  
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5 6 1.0 7 1.0  
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9 10 1.0 11 1.0 12 1.0  
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12 13 1.0 14 1.0 15 1.0  
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Title Card Required

0 1

V	-0.81747315	0.02939450	0.06442259
N	-2.41967380	-1.00176799	-0.27863597
H	-3.24506075	-0.78200245	0.27915353
H	-2.30812704	-2.00786626	-0.13232453
N	-0.78986086	1.76238865	-0.63474888
H	-0.56402122	2.62047021	-0.14561371
H	-1.23986905	1.99095535	-1.51817209
N	-0.39493469	0.18322875	1.56899011
P	1.50130035	-0.73196032	-0.41381578
H	2.05451293	-0.98343613	-1.70137959
H	1.87592373	-1.95844745	0.19460777
C	2.69869511	0.45116359	0.30106844
H	3.73429571	0.11400429	0.19277908
H	2.57108716	1.41794068	-0.19700516
H	2.44275063	0.57778576	1.35782436

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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## NV(NH<sub>2</sub>)<sub>2</sub>(PH<sub>2</sub>Me) – Transition State 2

%chk=VPH2Me\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1

V	-0.83549522	0.08632010	0.06978186
N	-2.07990503	-1.30014286	-0.18803636
H	-2.47183754	-1.89805996	0.53124392
H	-2.58198872	-1.48113338	-1.05369384

N	-0.96858985	1.83447962	-0.61914515
H	-0.85628931	2.69579760	-0.09570168
H	-1.32238834	2.07371914	-1.54215381
N	-0.45763471	0.16917974	1.58304415
P	1.46986779	-0.67377826	-0.43924204
H	2.01527077	-0.88991328	-1.73692308
H	1.80383923	-1.93470519	0.11669289
C	2.71526070	0.43486649	0.31657069
H	3.73845063	0.06675948	0.19169569
H	2.62364272	1.42719281	-0.13773989
H	2.47101661	0.52784000	1.37976491

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2 3 1.0 4 1.0

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12 13 1.0 14 1.0 15 1.0

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Title Card Required

0 1

V	-0.83549522	0.08632010	0.06978186
N	-2.07990503	-1.30014286	-0.18803636
H	-2.47183754	-1.89805996	0.53124392
H	-2.58198872	-1.48113338	-1.05369384
N	-0.96858985	1.83447962	-0.61914515
H	-1.32139464	2.06919065	-1.54050971
H	-0.85728301	2.70032609	-0.09734578
N	-0.45763471	0.16917974	1.58304415
P	1.46986779	-0.67377826	-0.43924204
H	2.01527077	-0.88991328	-1.73692308
H	1.80383923	-1.93470519	0.11669289
C	2.71526070	0.43486649	0.31657069

H	3.73845063	0.06675948	0.19169569
H	2.62364272	1.42719281	-0.13773989
H	2.47101661	0.52784000	1.37976491

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2 3 1.0 4 1.0

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12 13 1.0 14 1.0 15 1.0

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Title Card Required

0 1

V	-0.81175998	0.06036192	0.05672466
N	-1.73181872	-1.55531210	-0.08747427
H	-1.88576270	-2.24582196	0.63768807
H	-2.34920325	-1.75037379	-0.87231946
N	-1.71422024	1.62314567	-0.64515921
H	-2.46275019	2.02172279	-0.07787106
H	-1.10221844	2.42590288	-0.80931987
N	-0.32603823	0.14629980	1.54929481
P	1.55167580	-0.47632422	-0.50468546
H	2.12865907	-0.63848311	-1.79721005
H	1.87301923	-1.75386421	0.01383188
C	2.76854498	0.61125931	0.32489697
H	3.79462585	0.24602457	0.21712899
H	2.70105584	1.62062296	-0.09512498
H	2.49118776	0.66431964	1.38280022

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2 3 1.0 4 1.0

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12 13 1.0 14 1.0 15 1.0  
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# NV(NH<sub>2</sub>)<sub>2</sub>(PHMe<sub>2</sub>) – Ground State

%chk=VPHMe2\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
V -1.09914214 -0.06545011 -0.00638243  
N -2.06953847 1.50473670 -0.38128048  
H -2.57161418 1.71001959 -1.23811866  
H -2.30234860 2.22562381 0.29707018  
N -1.21488772 -1.09311273 1.57264559  
H -1.33266443 -2.09904914 1.62519077  
H -1.33771949 -0.71646790 2.50926595  
N -1.15156061 -1.01975077 -1.24092710  
P 1.32917290 0.30489387 -0.32690730  
H 1.65080142 0.93645891 -1.55629585  
C 2.19000889 -1.29946906 -0.49600824  
H 3.25483621 -1.17699208 -0.72577426  
H 2.08198284 -1.85490061 0.44262153  
H 1.69511840 -1.87438952 -1.28511048  
C 2.38759155 1.25032380 0.83856553  
H 2.32486868 0.78906918 1.83113353  
H 3.43683790 1.26228228 0.52095475  
H 2.02888196 2.28204913 0.92105817

1 2 1.0 5 1.0 8 3.0 9 1.0  
2 3 1.0 4 1.0  
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5 6 1.0 7 1.0



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11 12 1.0 13 1.0 14 1.0  
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15 16 1.0 17 1.0 18 1.0  
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### V(NH<sub>2</sub>)<sub>2</sub>(PHMe<sub>2</sub>) – Transition State 1

%chk=VPHMe2\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
V -1.09913562 -0.06532000 -0.00649124  
N -2.07019123 1.50460273 -0.38071643  
H -2.57204739 1.71024734 -1.23759574  
H -2.30369424 2.22480546 0.29812039  
N -1.21554836 -1.09373946 1.57195883  
H -1.33261538 -2.09978445 1.62398463  
H -1.33926492 -0.71755030 2.50864299  
N -1.15053369 -1.01902719 -1.24155992  
P 1.32927942 0.30475858 -0.32652910  
H 1.65027482 0.93564903 -1.55643182  
C 2.18992657 -1.29971670 -0.49512910  
H 3.25469625 -1.17748567 -0.72518903  
H 2.08204963 -1.85475615 0.44373706  
H 1.69475857 -1.87486575 -1.28387160  
C 2.38812430 1.25081550 0.83798538  
H 2.32656394 0.78947526 1.83057296  
H 3.43707422 1.26354172 0.51950001  
H 2.02874013 2.28225958 0.92085014

1 2 1.0 5 1.0 8 3.0 9 1.0  
2 3 1.0 4 1.0  
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 9 10 1.0 11 1.0 15 1.0  
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 11 12 1.0 13 1.0 14 1.0  
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 15 16 1.0 17 1.0 18 1.0  
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# Title Card Required

0 1  
 V            -1.09913562   -0.06532000   -0.00649124  
 N            -2.07019123   1.50460273   -0.38071643  
 H            -2.30079137   2.22115062   0.29882323  
 H            -2.57495026   1.71390218   -1.23829857  
 N            -1.21554836   -1.09373946   1.57195883  
 H            -1.33261538   -2.09978445   1.62398463  
 H            -1.33926492   -0.71755030   2.50864299  
 N            -1.15053369   -1.01902719   -1.24155992  
 P            1.32927942   0.30475858   -0.32652910  
 H            1.65027482   0.93564903   -1.55643182  
 C            2.18992657   -1.29971670   -0.49512910  
 H            3.25469625   -1.17748567   -0.72518903  
 H            2.08204963   -1.85475615   0.44373706  
 H            1.69475857   -1.87486575   -1.28387160  
 C            2.38812430   1.25081550   0.83798538  
 H            2.32656394   0.78947526   1.83057296  
 H            3.43707422   1.26354172   0.51950001  
 H            2.02874013   2.28225958   0.92085014

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11 12 1.0 13 1.0 14 1.0  
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15 16 1.0 17 1.0 18 1.0  
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# Title Card Required

0 1  
V -1.07775111 -0.05844230 -0.03836310  
N -2.40987494 1.31623726 -0.35177994  
H -2.22895258 1.89055051 -1.17850797  
H -3.37143139 1.00836195 -0.49849643  
N -1.01476889 -0.79863068 1.68247780  
H -1.00154806 -1.78211565 1.92617646  
H -1.24553812 -0.25623682 2.51168468  
N -1.07808970 -1.27683126 -1.02622265  
P 1.35382876 0.30262908 -0.41029564  
H 1.72715539 0.75755395 -1.70369346  
C 2.20519450 -1.31075596 -0.31942169  
H 3.27861341 -1.22265485 -0.52299301  
H 2.05603342 -1.72250210 0.68502806  
H 1.73243335 -1.99081877 -1.03468945  
C 2.35923927 1.40260474 0.65949108  
H 2.24317155 1.07847062 1.70024580  
H 3.42239619 1.37257322 0.39429462  
H 2.00104296 2.43503472 0.58599376

1 2 1.0 5 1.0 8 3.0 9 1.0  
2 3 1.0 4 1.0  
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 9 10 1.0 11 1.0 15 1.0  
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 11 12 1.0 13 1.0 14 1.0  
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 15 16 1.0 17 1.0 18 1.0  
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### V(NH<sub>2</sub>)<sub>2</sub>(PHMe<sub>2</sub>) – Transition State 2

%chk=VPHMe2\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -1.09913562 -0.06532000 -0.00649124  
 N -2.07019123 1.50460273 -0.38071643  
 H -2.57204739 1.71024734 -1.23759574  
 H -2.30369424 2.22480546 0.29812039  
 N -1.21554836 -1.09373946 1.57195883  
 H -1.33261538 -2.09978445 1.62398463  
 H -1.33926492 -0.71755030 2.50864299  
 N -1.15053369 -1.01902719 -1.24155992  
 P 1.32927942 0.30475858 -0.32652910  
 H 1.65027482 0.93564903 -1.55643182  
 C 2.18992657 -1.29971670 -0.49512910  
 H 3.25469625 -1.17748567 -0.72518903  
 H 2.08204963 -1.85475615 0.44373706  
 H 1.69475857 -1.87486575 -1.28387160  
 C 2.38812430 1.25081550 0.83798538  
 H 2.32656394 0.78947526 1.83057296  
 H 3.43707422 1.26354172 0.51950001  
 H 2.02874013 2.28225958 0.92085014

1 2 1.0 5 1.0 8 3.0 9 1.0  
 2 3 1.0 4 1.0  
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 5 6 1.0 7 1.0

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9 10 1.0 11 1.0 15 1.0  
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11 12 1.0 13 1.0 14 1.0  
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15 16 1.0 17 1.0 18 1.0  
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# Title Card Required

0 1  
V -1.09913562 -0.06532000 -0.00649124  
N -2.07019123 1.50460273 -0.38071643  
H -2.57204739 1.71024734 -1.23759574  
H -2.30369424 2.22480546 0.29812039  
N -1.21554836 -1.09373946 1.57195883  
H -1.33831281 -0.71505971 2.50473341  
H -1.33356749 -2.10227504 1.62789421  
N -1.15053369 -1.01902719 -1.24155992  
P 1.32927942 0.30475858 -0.32652910  
H 1.65027482 0.93564903 -1.55643182  
C 2.18992657 -1.29971670 -0.49512910  
H 3.25469625 -1.17748567 -0.72518903  
H 2.08204963 -1.85475615 0.44373706  
H 1.69475857 -1.87486575 -1.28387160  
C 2.38812430 1.25081550 0.83798538  
H 2.32656394 0.78947526 1.83057296  
H 3.43707422 1.26354172 0.51950001  
H 2.02874013 2.28225958 0.92085014

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 11 12 1.0 13 1.0 14 1.0  
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 15 16 1.0 17 1.0 18 1.0  
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# Title Card Required

0 1

V	1.08294937	0.05940123	-0.02356619
N	1.81944359	-1.57954006	-0.53763793
H	2.12618939	-1.85294949	-1.46380149
H	2.18688030	-2.24112453	0.14233396
N	1.80216827	0.89327431	1.57454048
H	2.69143405	1.38462316	1.47865979
H	1.19572766	1.60675543	1.98587616
N	1.03293855	0.94703585	-1.31831935
P	-1.37726080	-0.22683634	-0.22023711
H	-1.65232352	-0.87437009	-1.44967408
C	-2.24566628	1.36963175	-0.43223032
H	-3.30116007	1.23103736	-0.69282203
H	-2.18373518	1.94441599	0.49918084
H	-1.73386397	1.93668270	-1.21632293
C	-2.44994099	-1.17251613	0.93103794
H	-2.41734794	-0.70861277	1.92362821
H	-3.49102160	-1.20001687	0.58856924
H	-2.07791193	-2.19820835	1.02702333

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 9 10 1.0 11 1.0 15 1.0

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 15 16 1.0 17 1.0 18 1.0  
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# **NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Et) – Ground State**

%chk=VPM<sub>2</sub>Et\_GE\_M06L.chk

# opt=calcall freq m06l/cc-pvdz geom=connectivity

Title Card Required

```

0 1
V      -1.54837308  -0.17137709  -0.08764547
N      -2.50389828   1.43979625   0.14144619
H      -2.85269835   2.04099074  -0.59695862
H      -2.89977923   1.76492075   1.01984243
N      -1.90472726  -1.81518611   0.76818029
H      -1.97571316  -2.72234957   0.32056150
H      -2.22160919  -1.91718446   1.72901135
N      -1.31174848  -0.42167488  -1.61266558
P       0.85161968   0.32550619   0.19958175
C       1.34427846   1.69920002  -0.90197113
H       0.79026899   2.60197420  -0.62195030
H       2.41976000   1.90892959  -0.84671842
H       1.06426552   1.43667567  -1.92796642
C       1.85185797  -1.10998515  -0.37520099
H       1.56683547  -1.95683521   0.26448213
H       1.45476443  -1.34540744  -1.37183654
C       1.61055360   0.79304822   1.80425260
H       1.09374515   1.66889400   2.21268534
H       1.50690864  -0.02895752   2.52215693
H       2.67447758   1.03820208   1.69518129
C       3.35754328  -0.91877129  -0.39839320
H       3.76494677  -0.72578045   0.60221465
H       3.85420456  -1.81940370  -0.77994782
H       3.65512681  -0.08708617  -1.04948793

```

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 14 15 1.0 16 1.0 21 1.0  
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 17 18 1.0 19 1.0 20 1.0  
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 21 22 1.0 23 1.0 24 1.0  
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### NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Et) – Transition State 1

%chk=VPMc2Et\_TS1\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -1.54848710 -0.17151140 -0.08770648  
 N -2.50353134 1.43999868 0.14123269  
 H -2.85142835 2.04160425 -0.59726696  
 H -2.89920924 1.76564486 1.01952450  
 N -1.90386612 -1.81545759 0.76830634  
 H -1.97363454 -2.72279646 0.32084656  
 H -2.22045216 -1.91776179 1.72920207  
 N -1.31156211 -0.42188865 -1.61266348  
 P 0.85139677 0.32544989 0.19965736  
 C 1.34401815 1.69882741 -0.90230207  
 H 0.78987802 2.60161651 -0.62257979  
 H 2.41946892 1.90872599 -0.84706743



H	1.06408839	1.43595355	-1.92823133
C	1.85187588	-1.11019286	-0.37436116
H	1.56760559	-1.95650244	0.26638160
H	1.45421777	-1.34682989	-1.37048797
C	1.60993192	0.79378197	1.80428023
H	1.09337249	1.67021685	2.21177854
H	1.50557782	-0.02758793	2.52280358
H	2.67402197	1.03835992	1.69551511
C	3.35743550	-0.91836445	-0.39876527
H	3.76539845	-0.72373886	0.60129268
H	3.85429079	-1.81929183	-0.77933282
H	3.65420400	-0.08747847	-1.05122894

1 2 1.0 5 1.0 8 3.0 9 1.0

2 3 1.0 4 1.0

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Title Card Required

0 1

V	-1.54848710	-0.17151140	-0.08770648
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N	-2.50353134	1.43999868	0.14123269
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H	-2.89627094	1.76198074	1.01897210
H	-2.85436665	2.04526836	-0.59671456
N	-1.90386612	-1.81545759	0.76830634
H	-1.97363454	-2.72279646	0.32084656
H	-2.22045216	-1.91776179	1.72920207
N	-1.31156211	-0.42188865	-1.61266348
P	0.85139677	0.32544989	0.19965736
C	1.34401815	1.69882741	-0.90230207
H	0.78987802	2.60161651	-0.62257979
H	2.41946892	1.90872599	-0.84706743
H	1.06408839	1.43595355	-1.92823133
C	1.85187588	-1.11019286	-0.37436116
H	1.56760559	-1.95650244	0.26638160
H	1.45421777	-1.34682989	-1.37048797
C	1.60993192	0.79378197	1.80428023
H	1.09337249	1.67021685	2.21177854
H	1.50557782	-0.02758793	2.52280358
H	2.67402197	1.03835992	1.69551511
C	3.35743550	-0.91836445	-0.39876527
H	3.76539845	-0.72373886	0.60129268
H	3.85429079	-1.81929183	-0.77933282
H	3.65420400	-0.08747847	-1.05122894

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Title Card Required

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V	-1.53234226	-0.14466434	-0.09132879
N	-2.84405707	1.24733908	0.24550720
H	-2.52647072	2.18722653	-0.00344804
H	-3.73415578	1.17466004	-0.24819219
N	-1.74558849	-1.78108599	0.79573259
H	-1.70484193	-2.70907320	0.39073304
H	-2.17911251	-1.84218928	1.71405275
N	-1.23983221	-0.49087671	-1.59624305
P	0.86969463	0.37993513	0.18498250
C	1.39876831	1.71339531	-0.95111740
H	0.88964295	2.64875841	-0.69185479
H	2.48149107	1.88381926	-0.90550094
H	1.10618499	1.43758955	-1.97012891
C	1.82716598	-1.09578063	-0.35554066
H	1.50285418	-1.92055921	0.29369344
H	1.43309091	-1.33116879	-1.35308428
C	1.63191233	0.86201978	1.78233921
H	1.13721195	1.75740162	2.17503048
H	1.50032038	0.05558504	2.51306708
H	2.70272971	1.07496945	1.67402421
C	3.33814989	-0.95286432	-0.35726053
H	3.73737874	-0.76449160	0.64735830
H	3.80870915	-1.87363776	-0.72313936
H	3.67378473	-0.13889248	-1.01228696

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### NV(NH<sub>2</sub>)<sub>2</sub>(PMe<sub>2</sub>Et) – Transition State 2

%chk=VPM<sub>2</sub>Et\_TS2\_M06L.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz geom=connectivity

Title Card Required

0 1  
 V -1.54848710 -0.17151140 -0.08770648  
 N -2.50353134 1.43999868 0.14123269  
 H -2.85142835 2.04160425 -0.59726696  
 H -2.89920924 1.76564486 1.01952450  
 N -1.90386612 -1.81545759 0.76830634  
 H -1.97363454 -2.72279646 0.32084656  
 H -2.22045216 -1.91776179 1.72920207  
 N -1.31156211 -0.42188865 -1.61266348  
 P 0.85139677 0.32544989 0.19965736  
 C 1.34401815 1.69882741 -0.90230207  
 H 0.78987802 2.60161651 -0.62257979  
 H 2.41946892 1.90872599 -0.84706743  
 H 1.06408839 1.43595355 -1.92823133  
 C 1.85187588 -1.11019286 -0.37436116  
 H 1.56760559 -1.95650244 0.26638160  
 H 1.45421777 -1.34682989 -1.37048797  
 C 1.60993192 0.79378197 1.80428023  
 H 1.09337249 1.67021685 2.21177854  
 H 1.50557782 -0.02758793 2.52280358  
 H 2.67402197 1.03835992 1.69551511  
 C 3.35743550 -0.91836445 -0.39876527

H	3.76539845	-0.72373886	0.60129268
H	3.85429079	-1.81929183	-0.77933282
H	3.65420400	-0.08747847	-1.05122894

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Title Card Required

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V	-1.54848710	-0.17151140	-0.08770648
N	-2.50353134	1.43999868	0.14123269
H	-2.85142835	2.04160425	-0.59726696
H	-2.89920924	1.76564486	1.01952450
N	-1.90386612	-1.81545759	0.76830634
H	-2.21892490	-1.91377066	1.72717246
H	-1.97516180	-2.72678759	0.32287617
N	-1.31156211	-0.42188865	-1.61266348
P	0.85139677	0.32544989	0.19965736
C	1.34401815	1.69882741	-0.90230207
H	0.78987802	2.60161651	-0.62257979

H	2.41946892	1.90872599	-0.84706743
H	1.06408839	1.43595355	-1.92823133
C	1.85187588	-1.11019286	-0.37436116
H	1.56760559	-1.95650244	0.26638160
H	1.45421777	-1.34682989	-1.37048797
C	1.60993192	0.79378197	1.80428023
H	1.09337249	1.67021685	2.21177854
H	1.50557782	-0.02758793	2.52280358
H	2.67402197	1.03835992	1.69551511
C	3.35743550	-0.91836445	-0.39876527
H	3.76539845	-0.72373886	0.60129268
H	3.85429079	-1.81929183	-0.77933282
H	3.65420400	-0.08747847	-1.05122894

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Title Card Required

0 1

V	1.53224955	0.16453207	-0.09437890
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N	2.34516926	-1.51078898	0.11081452
H	2.58369183	-2.17132824	-0.61968169
H	2.84446036	-1.76548126	0.95984720
N	2.32631033	1.67866067	0.82680503
H	1.69330905	2.47476884	0.93601340
H	3.14813227	2.10461770	0.39732103
N	1.25584521	0.33949803	-1.63159856
P	-0.88319081	-0.27279811	0.22305142
C	-1.35839613	-1.67761213	-0.84305771
H	-0.79820384	-2.56628734	-0.53284896
H	-2.43261120	-1.89216222	-0.78382043
H	-1.07372269	-1.44005842	-1.87355192
C	-1.88371902	1.14447191	-0.39842141
H	-1.60752765	2.01752710	0.21035159
H	-1.48971092	1.34543698	-1.40382313
C	-1.63995208	-0.69884026	1.83897011
H	-1.11331966	-1.55753683	2.27029097
H	-1.54358865	0.14158778	2.53607281
H	-2.70127578	-0.95687241	1.73566735
C	-3.38930307	0.94915401	-0.41198104
H	-3.79417686	0.79201656	0.59567337
H	-3.88822505	1.83378448	-0.82611227
H	-3.68416044	0.09309203	-1.03166262

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## NV(NH<sub>2</sub>)<sub>2</sub>(P(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>) – Ground State

%mem=4GB

%nprocs=4

%chk=PC6F5\_freq.chk

# opt=calcfc freq m06l/cc-pvdz pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

N	1.62130964	-0.33405855	3.17986633
N	-0.90211008	0.21518128	4.25794976
H	-1.74883852	0.76818885	4.39905989
H	-0.85649248	-0.48006837	4.99981218
N	1.09588506	2.33621721	2.58853681
H	2.07961817	2.59922780	2.56141534
H	0.54623330	3.19583824	2.54845342
P	0.02418182	0.01319406	0.58743367
V	0.41209992	0.62548116	2.99147677
C	-0.71603494	-1.56485263	0.00201932
C	-1.87740156	-1.96950082	0.66883228
C	-0.25218162	-2.38970999	-1.02609620
C	-2.53426440	-3.15453489	0.36673986
C	-0.89046279	-3.58445590	-1.34266606
C	-2.03028221	-3.96822182	-0.64331942
C	1.69431889	0.12911299	-0.14032529
C	2.58506213	-0.91885052	0.10909416
C	2.21639410	1.29209045	-0.70584617
C	3.93042307	-0.83523963	-0.21597966
C	3.56270921	1.40076711	-1.03551904
C	4.42033304	0.33413928	-0.79097122
C	-1.04619377	1.21227077	-0.29310904
C	-1.83954713	2.08475845	0.45207787
C	-1.15464668	1.26788508	-1.68304865
C	-2.70146198	2.99125019	-0.15473395
C	-2.00277250	2.16505473	-2.31622672
C	-2.77862825	3.02814263	-1.54373888
F	-2.39933146	-1.18378794	1.61715339
F	-3.63775854	-3.50731084	1.02105440
F	-2.64541493	-5.10368610	-0.94944850



F	-0.42485344	-4.35622795	-2.32192365
F	0.81651404	-2.06148757	-1.75390702
F	-0.41061840	0.45078458	-2.43491773
F	-2.08420045	2.21236796	-3.64323766
F	-3.59643420	3.88743575	-2.13742445
F	-3.44962523	3.81412909	0.57545255
F	-1.80053541	2.06748680	1.79437024
F	1.44181368	2.36219030	-0.92964394
F	4.03297609	2.52305012	-1.57932748
F	5.70672582	0.43063015	-1.10776961
F	4.75044096	-1.85635469	0.01576891
F	2.13593324	-2.04690592	0.66138041

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\$END

### NV(NH<sub>2</sub>)<sub>2</sub>(P(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>) – Transition State

%Mem=4GB

%Nprocs=4

%chk=PC6F5\_QST3\_5.chk

# opt=(calcall,qst3) freq m06l/cc-pvdz pop=(nbo6,savenbos)

geom=connectivity

Title Card Required

0 1

N	1.62130964	-0.33405855	3.17986633
N	-0.90211008	0.21518128	4.25794976
H	-1.74883852	0.76818885	4.39905989
H	-0.85649248	-0.48006837	4.99981218
N	1.09588506	2.33621721	2.58853681
H	2.07961817	2.59922780	2.56141534
H	0.54623330	3.19583824	2.54845342
P	0.02418182	0.01319406	0.58743367
V	0.41209992	0.62548116	2.99147677
C	-0.71603494	-1.56485263	0.00201932
C	-1.87740156	-1.96950082	0.66883228
C	-0.25218162	-2.38970999	-1.02609620
C	-2.53426440	-3.15453489	0.36673986
C	-0.89046279	-3.58445590	-1.34266606
C	-2.03028221	-3.96822182	-0.64331942
C	1.69431889	0.12911299	-0.14032529
C	2.58506213	-0.91885052	0.10909416
C	2.21639410	1.29209045	-0.70584617
C	3.93042307	-0.83523963	-0.21597966
C	3.56270921	1.40076711	-1.03551904
C	4.42033304	0.33413928	-0.79097122
C	-1.04619377	1.21227077	-0.29310904

C	-1.83954713	2.08475845	0.45207787
C	-1.15464668	1.26788508	-1.68304865
C	-2.70146198	2.99125019	-0.15473395
C	-2.00277250	2.16505473	-2.31622672
C	-2.77862825	3.02814263	-1.54373888
F	-2.39933146	-1.18378794	1.61715339
F	-3.63775854	-3.50731084	1.02105440
F	-2.64541493	-5.10368610	-0.94944850
F	-0.42485344	-4.35622795	-2.32192365
F	0.81651404	-2.06148757	-1.75390702
F	-0.41061840	0.45078458	-2.43491773
F	-2.08420045	2.21236796	-3.64323766
F	-3.59643420	3.88743575	-2.13742445
F	-3.44962523	3.81412909	0.57545255
F	-1.80053541	2.06748680	1.79437024
F	1.44181368	2.36219030	-0.92964394
F	4.03297609	2.52305012	-1.57932748
F	5.70672582	0.43063015	-1.10776961
F	4.75044096	-1.85635469	0.01576891
F	2.13593324	-2.04690592	0.66138041

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# Title Card Required

0 1

N	1.62130964	-0.33405855	3.17986633
N	-0.90211008	0.21518128	4.25794976
H	-1.74883852	0.76818885	4.39905989
H	-0.85649248	-0.48006837	4.99981218
N	1.09588506	2.33621721	2.58853681
H	2.07961817	2.59922780	2.56141534
H	0.54623330	3.19583824	2.54845342
P	0.02418182	0.01319406	0.58743367
V	0.41209992	0.62548116	2.99147677
C	-0.71603494	-1.56485263	0.00201932
C	-1.87740156	-1.96950082	0.66883228
C	-0.25218162	-2.38970999	-1.02609620
C	-2.53426440	-3.15453489	0.36673986
C	-0.89046279	-3.58445590	-1.34266606
C	-2.03028221	-3.96822182	-0.64331942
C	1.69431889	0.12911299	-0.14032529
C	2.58506213	-0.91885052	0.10909416
C	2.21639410	1.29209045	-0.70584617
C	3.93042307	-0.83523963	-0.21597966
C	3.56270921	1.40076711	-1.03551904
C	4.42033304	0.33413928	-0.79097122
C	-1.04619377	1.21227077	-0.29310904

C	-1.83954713	2.08475845	0.45207787
C	-1.15464668	1.26788508	-1.68304865
C	-2.70146198	2.99125019	-0.15473395
C	-2.00277250	2.16505473	-2.31622672
C	-2.77862825	3.02814263	-1.54373888
F	-2.39933146	-1.18378794	1.61715339
F	-3.63775854	-3.50731084	1.02105440
F	-2.64541493	-5.10368610	-0.94944850
F	-0.42485344	-4.35622795	-2.32192365
F	0.81651404	-2.06148757	-1.75390702
F	-0.41061840	0.45078458	-2.43491773
F	-2.08420045	2.21236796	-3.64323766
F	-3.59643420	3.88743575	-2.13742445
F	-3.44962523	3.81412909	0.57545255
F	-1.80053541	2.06748680	1.79437024
F	1.44181368	2.36219030	-0.92964394
F	4.03297609	2.52305012	-1.57932748
F	5.70672582	0.43063015	-1.10776961
F	4.75044096	-1.85635469	0.01576891
F	2.13593324	-2.04690592	0.66138041

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Title Card Required

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N	-1.45848478	0.79053147	3.08880170
N	0.89347404	-0.08873310	4.21598428
H	1.53192780	-0.83487801	4.49845427
H	0.99964685	0.69523154	4.85518502
N	-1.26567639	-2.19376146	2.94854882
H	-1.95131234	-2.35625045	3.69433235
H	-1.80803715	-2.43433845	2.11213106
P	0.00548499	-0.00419432	0.55976394
V	-0.47447582	-0.42128296	3.00422107
C	0.80649796	1.52377403	-0.05373946
C	1.95803566	1.91994199	0.63428820
C	0.40601818	2.30520501	-1.14076608
C	2.66360731	3.06689914	0.29682023
C	1.09486103	3.46085455	-1.49268672
C	2.22178326	3.84270957	-0.77081548
C	-1.68458015	-0.06495037	-0.13128008
C	-2.51078972	1.05449878	0.01763001
C	-2.28313317	-1.24490949	-0.57578356
C	-3.86048763	1.01789986	-0.30094287
C	-3.63405948	-1.30645592	-0.89605997
C	-4.42340134	-0.16957622	-0.76017400
C	1.00004302	-1.28762550	-0.28471107

C	1.82274270	-2.10949608	0.48962438
C	1.01516515	-1.46822098	-1.66875904
C	2.61898358	-3.09236628	-0.08954668
C	1.79688112	-2.44347692	-2.26940178
C	2.60047668	-3.25675294	-1.47099113
F	2.41692729	1.16234654	1.63408111
F	3.75484325	3.41777706	0.97123229
F	2.88525532	4.93991455	-1.11136515
F	0.69119984	4.19636641	-2.52535719
F	-0.64724826	1.97001583	-1.88719991
F	0.24463119	-0.69739806	-2.44325180
F	1.79078502	-2.61100334	-3.58941250
F	3.35553328	-4.18980484	-2.03542311
F	3.39818360	-3.86540670	0.66032687
F	1.87811740	-1.96056714	1.81530836
F	-1.57333296	-2.37868614	-0.67631315
F	-4.17362542	-2.44676082	-1.32221367
F	-5.71398741	-0.21776676	-1.06658066
F	-4.61661920	2.10331795	-0.17012234
F	-1.99939751	2.20417615	0.45482200

1 9 1.0

2 3 1.0 4 1.0 9 1.0

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5 6 1.0 7 1.0 9 1.0

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8 9 1.0 10 1.0 16 1.0 22 1.0

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10 11 1.5 12 1.5

11 13 1.5 28 1.0

12 14 1.5 32 1.0

13 15 1.5 29 1.0

14 15 1.5 31 1.0

15 30 1.0

16 17 1.5 18 1.5

17 19 1.5 42 1.0

18 20 1.5 38 1.0

19 21 1.5 41 1.0

20 21 1.5 39 1.0

21 40 1.0

22 23 1.5 24 1.5

23 25 1.5 37 1.0

24 26 1.5 33 1.0  
 25 27 1.5 36 1.0  
 26 27 1.5 34 1.0  
 27 35 1.0  
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 \$END

## Input Files for Nickel Complexes

### Ni(PH<sub>3</sub>)(PMe<sub>3</sub>)

%chk=NiPH3PMe3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

```

0 1
Ni      -0.84892109  -0.00267661  -0.00181003
P       -2.95655581   0.00118219   0.00081516
H       -3.70604893   1.18689341   0.29231075
H       -3.71289809  -0.33741080  -1.16803539
H       -3.71030678  -0.84015386   0.88223415
P       1.30568974  -0.00012180  -0.00004818
C       2.15557777  -1.16851436   1.14625920
H       1.85932525  -2.19937936   0.91218681
H       3.25054495  -1.08441122   1.06932195
H       1.85317630  -0.95955370   2.18071521
C       2.15780830  -0.40491520  -1.58481170
H       1.85764370   0.31107031  -2.36101206
  
```



H	3.25262632	-0.37435988	-1.47355217
H	1.86083277	-1.40713421	-1.92036954
C	2.15049539	1.57861720	0.44197631
H	1.84894401	1.89131762	1.45019190
H	3.24581016	1.47197875	0.41269632
H	1.84984317	2.36905650	-0.25805469

```

1 2 1.0 6 1.0
2 3 1.0 4 1.0 5 1.0
3
4
5
6 7 1.0 11 1.0 15 1.0
7 8 1.0 9 1.0 10 1.0
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9
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11 12 1.0 13 1.0 14 1.0
12
13
14
15 16 1.0 17 1.0 18 1.0
16
17
18

```

**{HNi(PH<sub>3</sub>)(PMe<sub>3</sub>)}<sup>+</sup>**

%chk=NiHPH3PMe3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

```

1 1
Ni      -0.79984157  0.18058114 -0.00000706
H       -0.66366925 -1.24305149 -0.00004882
P       -3.01548927 -0.06502284  0.00000072
H       -3.89387388  1.05041301 -0.00002802
H       -3.56747582 -0.79480242 -1.08140527
H       -3.56745392 -0.79473862  1.08146158
P       1.38880318 -0.01735923 -0.00000044
C       2.04701636 -0.90334196  1.44688381
H       1.65191346 -1.92605702  1.47170621
H       3.14357962 -0.94338926  1.39613422

```

H	1.75211177	-0.39438738	2.37260563
C	2.04703210	-0.90360389	-1.44671740
H	1.75208873	-0.39484957	-2.37253700
H	3.14359788	-0.94359021	-1.39597650
H	1.65197593	-1.92634206	-1.47132595
C	2.25244221	1.59307297	-0.00014456
H	1.98756250	2.17423439	0.89188638
H	3.33894500	1.42521050	-0.00009846
H	1.98760913	2.17404661	-0.89231162

1 2 1.0 3 1.0 7 1.0  
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 3 4 1.0 5 1.0 6 1.0  
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 7 8 1.0 12 1.0 16 1.0  
 8 9 1.0 10 1.0 11 1.0  
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 12 13 1.0 14 1.0 15 1.0  
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 16 17 1.0 18 1.0 19 1.0  
 17  
 18  
 19

### Ni(PH<sub>3</sub>)(PEt<sub>3</sub>)

%chk=NiPH3PEt3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1			
Ni	1.61279783	0.01228279	0.00243650
P	-0.55453757	0.00498892	0.00169651
P	3.71496626	-0.00749234	-0.00151421
H	4.45729286	-0.88033958	0.85848930
H	4.46307651	-0.33295684	-1.18015796
H	4.48896971	1.15790539	0.31309133

C	-1.30368614	-1.56520096	0.67637028
H	-0.59908145	-1.90151523	1.45262439
H	-1.20715253	-2.30888235	-0.13216534
C	-1.32330999	1.36784699	1.01856422
H	-0.62400598	2.21359058	0.93029908
H	-1.23545895	1.03843250	2.06733784
C	-1.31088157	0.19784195	-1.69322377
H	-1.22877705	1.27119084	-1.93261615
H	-0.60199856	-0.29694973	-2.37497682
C	-2.71600432	-0.31851339	-1.95316316
H	-2.99689818	-0.16240574	-3.00538142
H	-2.79336431	-1.39874993	-1.76213157
H	-3.47627950	0.18130593	-1.33792157
C	-2.71452420	-1.54451276	1.24003054
H	-3.47019223	-1.26804308	0.49241548
H	-2.99037998	-2.53647736	1.62780308
H	-2.80617597	-0.84036840	2.07975074
C	-2.73444904	1.83560077	0.70474723
H	-3.02416194	2.66364450	1.36870593
H	-2.81782745	2.21225314	-0.32508137
H	-3.48522305	1.04362303	0.82900654

1 2 1.0 3 1.0  
 2 7 1.0 10 1.0 13 1.0  
 3 4 1.0 5 1.0 6 1.0  
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 7 8 1.0 9 1.0 20 1.0  
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 10 11 1.0 12 1.0 24 1.0  
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 13 14 1.0 15 1.0 16 1.0  
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 16 17 1.0 18 1.0 19 1.0  
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 20 21 1.0 22 1.0 23 1.0  
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 24 25 1.0 26 1.0 27 1.0  
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**{HNi(PH<sub>3</sub>)(PEt<sub>3</sub>)}<sup>+</sup>**

%chk=NiHPH3PEt3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

```

1 1
Ni      -1.54984129  0.17266440 -0.00959011
H       -1.37136281 -1.24720287  0.04772147
P        0.64124539  0.01547701 -0.00285238
P       -3.76555104 -0.08163481  0.00662586
H       -4.31207895 -0.76441053  1.12169829
H       -4.65727085  1.02249290 -0.04127650
H       -4.32151648 -0.86495395 -1.03519407
C        1.26399933 -0.59706768  1.62213590
H        0.51637681 -1.32672912  1.96785379
H        1.18291425  0.25574485  2.31555117
C        1.24935166 -1.11357005 -1.32686800
H        0.53993772 -1.00073000 -2.16120076
H        1.08356188 -2.13317526 -0.94210296
C        1.36829394  1.69205088 -0.30579323
H        1.27953723  1.86456071 -1.39078072
H        0.68530183  2.41795721  0.16455577
C        2.78739826  1.93213113  0.18672800
H        3.08862991  2.96153176 -0.04820744
H        2.86744065  1.81541283  1.27565031
H        3.51750842  1.26185995 -0.28336895
C        2.65261105 -1.21456940  1.65262195
H        3.43960234 -0.51451098  1.34601148
H        2.88806968 -1.54134226  2.67385082
H        2.71771503 -2.10318133  1.01052447
C        2.67406150 -0.91841845 -1.81634170
H        2.89789814 -1.65057416 -2.60309204
H        2.82295670  0.07659849 -2.25709133
H        3.42062498 -1.05492314 -1.02407953

```

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 3 8 1.0 11 1.0 14 1.0  
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 8 9 1.0 10 1.0 21 1.0  
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 11 12 1.0 13 1.0 25 1.0  
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 14 15 1.0 16 1.0 17 1.0  
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 25 26 1.0 27 1.0 28 1.0  
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# **Ni(PH<sub>3</sub>)(P<sup>i</sup>Pr<sub>3</sub>)**

%chk=NiPH3PiPr3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1  
 Ni        -1.53510130   0.05278341   -0.10979838  
 P        0.62792780   -0.09062099   -0.04914304  
 P        -3.63274340   0.22302747   -0.11879700  
 H        -4.48012151   -0.81474746   -0.62912024  
 H        -4.38008955   0.40127851   1.09126149  
 H        -4.29861771   1.27717210   -0.82610783  
 C        1.36701530   0.37658757   1.61675363

H	2.41619599	0.02604142	1.64114274
C	1.54430119	0.94768815	-1.32951671
H	1.40207488	0.33293752	-2.23687908
C	1.36764282	-1.77130583	-0.47900627
H	2.42279683	-1.58715404	-0.75148927
C	3.04370257	1.09979391	-1.10801497
H	3.51481396	1.56741633	-1.98655017
H	3.27635207	1.74125586	-0.24599146
H	3.55189418	0.13824146	-0.94672589
C	0.85541356	2.28240962	-1.58452839
H	0.94926929	2.96978413	-0.73165071
H	1.29727478	2.78727963	-2.45790119
H	-0.21989710	2.14419456	-1.77380884
C	1.32954400	1.88741760	1.82195689
H	1.64754366	2.13846687	2.84570021
H	1.97999883	2.44203906	1.13463447
H	0.30369479	2.27039844	1.69541799
C	0.57058798	-0.28065119	2.74114239
H	1.00197160	-0.01754218	3.71984212
H	-0.47085718	0.08012780	2.72354304
H	0.53213620	-1.37407874	2.67796765
C	1.34003887	-2.78100853	0.65701838
H	1.71468617	-3.75460530	0.30467434
H	1.96880973	-2.48240613	1.50666208
H	0.31528926	-2.94299579	1.02688064
C	0.63257337	-2.32431269	-1.69514125
H	0.62307831	-1.62670995	-2.54495880
H	1.10007807	-3.25910350	-2.04179301
H	-0.41822299	-2.54103496	-1.44527739

1 2 1.0 3 1.0

2 7 1.0 9 1.0 11 1.0

3 4 1.0 5 1.0 6 1.0

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7 8 1.0 21 1.0 25 1.0

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9 10 1.0 13 1.0 17 1.0

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**{HNi(PH<sub>3</sub>)(P<sup>i</sup>Pr<sub>3</sub>)}<sup>+</sup>**

%chk=NiHHPH3PiPr3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1			
Ni	-1.36000864	0.15611491	0.01060784
H	-1.17225838	1.21644928	-0.95658973
P	0.82239214	0.04207065	0.05432360
P	-3.53912887	0.46250906	-0.26630041
H	-4.02330860	0.34773413	-1.59371072
H	-4.53458492	-0.30723807	0.39396265
H	-4.03303637	1.75729972	0.03254976
C	1.86163702	1.44545165	0.69704369
H	2.67649021	0.93407628	1.24270109
C	1.53685699	-0.75640138	-1.46436364
H	2.60164210	-0.95548081	-1.24479704
C	0.77068809	-1.16718288	1.47836802

H	0.82566861	-0.49581834	2.35258987
C	1.41527217	0.15496652	-2.68217418
H	1.82056599	-0.36274170	-3.56253445
H	0.36025601	0.38372952	-2.89575924
H	1.95318211	1.10296575	-2.58634976
C	0.80775188	-2.06815878	-1.74303452
H	-0.26527406	-1.88813891	-1.92353637
H	1.21154666	-2.52844363	-2.65532089
H	0.89999348	-2.80914330	-0.94020666
C	1.88317436	-2.19221567	1.60608236
H	2.87212692	-1.71455807	1.62479448
H	1.77715686	-2.74804539	2.54877982
H	1.88467247	-2.93105852	0.79468423
C	-0.64667845	-1.74877291	1.44237707
H	-0.85683110	-2.32703639	0.52956201
H	-0.85890198	-2.41145167	2.29495707
H	-1.43207942	-0.95098790	1.57283888
C	1.02559798	2.25137087	1.68673447
H	0.55689654	1.63321986	2.46620939
H	1.65681338	2.99018804	2.19898809
H	0.22570881	2.79968837	1.16737190
C	2.47348481	2.34001937	-0.36831608
H	3.02185448	3.15786412	0.11927023
H	3.18995222	1.80975430	-1.00766519
H	1.70633186	2.80279956	-1.00645977

1 2 1.0 3 1.0 4 1.0

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3 8 1.0 10 1.0 12 1.0

4 5 1.0 6 1.0 7 1.0

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8 9 1.0 30 1.0 34 1.0

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10 11 1.0 14 1.0 18 1.0

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12 13 1.0 22 1.0 26 1.0

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 30 31 1.0 32 1.0 33 1.0  
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 34 35 1.0 36 1.0 37 1.0  
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# **Ni(PH<sub>3</sub>)(PMe<sub>2</sub>Ph)**

%Mem=4GB

%Nprocs=4

%chk=Me2Ph\_freq\_2.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-0.33937019	-0.20020565	-0.00212580
P	1.86062613	-0.19679140	-0.00425160
H	2.31263747	-0.79290463	1.11950761
H	2.31063024	-0.87126759	-1.08363946
H	2.30860786	1.07589320	-0.04992741
P	-2.53936652	-0.20361991	-0.00000000
C	-3.14603264	0.70285169	1.45693701
C	-3.37660099	0.02470629	2.65419575
C	-3.38036746	2.07550926	1.37664673
C	-3.84204216	0.71902124	3.77066921
H	-3.19249131	-1.05760939	2.71695081
C	-3.84501206	2.77036012	2.49365056
H	-3.19852697	2.61018237	0.43314913
C	-4.07599920	2.09235905	3.69052002
H	-4.02439944	0.18445543	4.71421663

H	-4.02929425	3.85271132	2.43016691
H	-4.44292666	2.63959960	4.57096784
C	-3.14874781	0.60296633	-1.51343089
H	-2.88125431	0.01251610	-2.36473328
H	-4.21357101	0.69580795	-1.46411556
H	-2.70968058	1.57477659	-1.60120778
C	-3.14331529	-1.91950234	0.05825250
H	-4.20894668	-1.91945533	0.15484307
H	-2.86689939	-2.42569908	-0.84300169
H	-2.70916840	-2.42214021	0.89716349

1 2 1.0 6 1.0

2 3 1.0 4 1.0 5 1.0

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6 7 1.0 18 1.0 22 1.0

7 8 1.5 9 1.5

8 10 1.5 11 1.0

9 12 1.5 13 1.0

10 14 1.5 15 1.0

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12 14 1.5 16 1.0

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\$END

**{HNi(PH<sub>3</sub>)(PMe<sub>2</sub>Ph)}<sup>+</sup>**

%mem=4GB

%Nprocs=4

%chk=Me2Ph\_prod\_freq.chk

# opt=calcall freq m06l/6-311++g(d,p) pop=(nbo6,savento)

geom=connectivity

Title Card Required

1 1

Ni	-0.79912534	0.17907769	-0.00001402
H	-0.66315642	-1.24273795	0.00006523
P	-3.00879522	-0.06629823	-0.00000302
H	-3.87213238	1.04566148	-0.00005994
H	-3.55717058	-0.78750739	-1.07286975
H	-3.55716876	-0.78739811	1.07293820
P	1.38402676	-0.01770582	0.00000411
C	2.24177554	1.59074957	-0.00013503
C	2.04866564	-0.90186835	-1.44530270
H	3.29999808	1.43243008	-0.00010509
H	1.98316274	2.15833644	0.86926969
H	3.11697932	-0.92413804	-1.38953594
H	1.67110594	-1.90298877	-1.45562672
C	2.04865576	-0.90161521	1.44547029
C	2.20908106	-0.23248158	2.65914048
C	2.39753525	-2.24798189	1.33998089
C	2.71891077	-0.90946277	3.76683714
H	1.93465853	0.82917088	2.74177293
C	2.90661027	-2.92557464	2.44818690
H	2.27099320	-2.77556409	0.38354315
C	3.06746907	-2.25654163	3.66147016
H	2.84597619	-0.38194555	4.72332889
H	3.18121543	-3.98723252	2.36482748
H	3.46937707	-2.79012373	4.53500118
H	1.74866070	-0.39828790	-2.34045842
H	1.98318703	2.15817149	-0.86965463

1 2 1.0 3 1.0 7 1.0

2

3 4 1.0 5 1.0 6 1.0

4

5

6

7 8 1.0 9 1.0 14 1.0

8 10 1.0 11 1.0 26 1.0

9 12 1.0 13 1.0 25 1.0

10

11

12

13

14 15 1.5 16 1.5

15 17 1.5 18 1.0

16 19 1.5 20 1.0  
 17 21 1.5 22 1.0  
 18  
 19 21 1.5 23 1.0  
 20  
 21 24 1.0  
 22  
 23  
 24  
 25  
 26  
 \$END

### **Ni(PH<sub>3</sub>)(PH<sub>3</sub>)**

%chk=NiPH3PH3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1  
 Ni -1.16689281 0.27815468 0.00000000  
 P 1.03310719 0.27815468 0.00000000  
 H 1.48310679 -0.31938499 1.12380902  
 H 1.48310679 -0.39632237 -1.07938921  
 H 1.48310743 1.55017145 -0.04441980  
 P -3.36689281 0.27815468 0.00000000  
 H -3.81689241 0.95053745 1.08069504  
 H -3.81689241 0.87787235 -1.12264824  
 H -3.81689305 -0.99394584 0.04195320

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
 3  
 4  
 5  
 6 7 1.0 8 1.0 9 1.0  
 7  
 8  
 9

### **{HNi(PH<sub>3</sub>)(PH<sub>3</sub>)}<sup>+</sup>**

%chk=NiHPH3PH3.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1

Ni	0.00000000	0.17976941	0.00000016
H	-0.00000000	-1.24681094	0.00000198
P	2.19022705	-0.08774547	-0.00000019
H	3.03796160	1.05006786	-0.00001241
H	2.72772967	-0.81361513	1.08902177
H	2.72772767	-0.81363702	-1.08900854
P	-2.19022705	-0.08774547	-0.00000002
H	-2.72772619	-0.81365767	1.08899521
H	-3.03796160	1.05006786	0.00003592
H	-2.72773115	-0.81359448	-1.08903510

1 2 1.0 3 1.0 7 1.0

2

3 4 1.0 5 1.0 6 1.0

4

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7 8 1.0 9 1.0 10 1.0

8

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### **Ni(PH<sub>3</sub>)(POMe<sub>3</sub>)**

%chk=NiPH3POMe35.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1

Ni	1.50854168	-0.19374518	0.00603685
P	3.61602278	0.12048100	-0.00322214
H	4.12419812	1.33967978	-0.51076309
H	4.36054666	0.14041039	1.20195066
H	4.52175495	-0.71368443	-0.70701489
P	-0.56895519	-0.05878467	0.00013784
O	-1.17406114	1.22738149	-0.83478443
O	-1.41120288	-1.31938034	-0.65134461
O	-1.28390548	0.11228185	1.47655516
C	-2.30582580	1.98385538	-0.42994500

H	-2.24829297	2.24976874	0.62935688
H	-2.30882258	2.89628697	-1.02704620
H	-3.24275161	1.44269287	-0.61262349
C	-2.61155586	-1.18161638	-1.39830488
H	-2.51546111	-0.40634585	-2.16374949
H	-2.79696828	-2.14055373	-1.88326406
H	-3.46717348	-0.94379381	-0.75405753
C	-2.54731554	-0.43562554	1.82449957
H	-2.62026693	-1.48565890	1.52711628
H	-2.63724590	-0.36509098	2.90896573
H	-3.37315864	0.12376434	1.36745497

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
 3  
 4  
 5  
 6 7 1.0 8 1.0 9 1.0  
 7 10 1.0  
 8 14 1.0  
 9 18 1.0  
 10 11 1.0 12 1.0 13 1.0  
 11  
 12  
 13  
 14 15 1.0 16 1.0 17 1.0  
 15  
 16  
 17  
 18 19 1.0 20 1.0 21 1.0  
 19  
 20  
 21

**{HNi(PH<sub>3</sub>)(POMe<sub>3</sub>)}<sup>+</sup>**

%chk=NiHHPH3POMe32.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1			
Ni	1.46665618	0.20380677	0.04354976
H	1.31922827	-1.17793382	-0.28514690

P	3.66533139	-0.10070375	-0.02773044
H	4.55710265	0.95738283	0.23040766
H	4.18186704	-1.06998565	0.84679670
H	4.18916886	-0.56592693	-1.24428745
P	-0.67872633	0.01917153	0.01061160
O	-1.37224584	1.36338740	0.55498910
O	-1.24404274	-0.23734542	-1.46348253
O	-1.19540162	-1.17480086	0.94306230
C	-2.58235253	1.94965478	0.03363238
H	-3.45315998	1.37389181	0.35696460
H	-2.63727660	2.95386319	0.44676382
H	-2.54609443	1.99959352	-1.05596573
C	-2.44343424	-1.16421599	1.66548875
H	-2.42216086	-2.03518220	2.31578011
H	-2.52720014	-0.25736265	2.26674260
H	-3.29023151	-1.24244609	0.97924711
C	-2.41487991	-1.01827812	-1.77761153
H	-2.41520448	-1.14076393	-2.85790847
H	-2.35990841	-1.99658415	-1.29677777
H	-3.32405763	-0.49504515	-1.47083558

1 2 1.0 3 1.0 7 1.0  
 2  
 3 4 1.0 5 1.0 6 1.0  
 4  
 5  
 6  
 7 8 1.0 9 1.0 10 1.0  
 8 11 1.0  
 9 19 1.0  
 10 15 1.0  
 11 12 1.0 13 1.0 14 1.0  
 12  
 13  
 14  
 15 16 1.0 17 1.0 18 1.0  
 16  
 17  
 18  
 19 20 1.0 21 1.0 22 1.0  
 20  
 21  
 22

# Ni(PH<sub>3</sub>)(POEt<sub>3</sub>)

%chk=NiPH3POEt35.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1

Ni	1.98714868	0.02001099	-0.15789677
P	4.10687746	-0.00126843	0.01498926
H	4.74337697	-0.98291238	0.81329031
H	4.96820466	-0.15101607	-1.10164426
H	4.79741126	1.10363132	0.57101253
P	-0.10058062	0.00851925	-0.05102771
O	-0.73301137	-1.02848819	1.06087495
O	-0.80007054	1.44201635	0.35914506
O	-0.91114855	-0.40026703	-1.42637773
C	-1.95582101	-1.75654968	0.90410245
H	-1.98371620	-2.21052831	-0.09391654
H	-2.81081221	-1.06804384	0.97717538
C	-1.96360089	1.57834647	1.18278453
H	-1.84736402	0.96049901	2.08142442
H	-2.84824766	1.21048896	0.64275355
C	-2.17390315	0.14478610	-1.82656413
H	-2.14239978	1.23729187	-1.73540764
H	-2.96752162	-0.21820817	-1.15709535
C	-2.01738917	-2.80188300	1.98638987
H	-2.93934096	-3.38248075	1.90444773
H	-1.17139672	-3.48704169	1.90899998
H	-1.98969616	-2.34146733	2.97616029
C	-2.43671787	-0.28240052	-3.24649562
H	-3.39337269	0.11499685	-3.59382315
H	-1.65132835	0.08233093	-3.91086174
H	-2.46885985	-1.37090999	-3.32715640
C	-2.11896090	3.03499398	1.53170150
H	-2.99775746	3.18460259	2.16347277
H	-1.24211480	3.39803658	2.07061835
H	-2.23747839	3.64181120	0.63158618

1 2 1.0 6 1.0

2 3 1.0 4 1.0 5 1.0

3

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6 7 1.0 8 1.0 9 1.0  
 7 10 1.0  
 8 13 1.0  
 9 16 1.0  
 10 11 1.0 12 1.0 19 1.0  
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 13 14 1.0 15 1.0 27 1.0  
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 16 17 1.0 18 1.0 23 1.0  
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 19 20 1.0 21 1.0 22 1.0  
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 23 24 1.0 25 1.0 26 1.0  
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 27 28 1.0 29 1.0 30 1.0  
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 29  
 30

**{HNi(PH<sub>3</sub>)(POEt<sub>3</sub>)}<sup>+</sup>**

%chk=NiHPH3POEt32.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1			
Ni	1.92615997	-0.20556726	-0.07323426
H	1.77450754	1.09852312	0.48975081
P	4.12837592	0.05746547	0.04102208
H	5.01604115	-0.93926940	-0.40723801
H	4.65380748	1.16525766	-0.64364714
H	4.66366565	0.29065766	1.31819947
P	-0.21828900	-0.01855240	-0.01514111
O	-0.88575925	-1.26722662	-0.77427716
O	-0.78780573	-0.00446281	1.47774408
O	-0.72889197	1.30784485	-0.74849544

C	-2.14194777	-1.91154837	-0.39730799
H	-2.95864176	-1.21005760	-0.60601875
H	-2.11761304	-2.10273467	0.68045414
C	-1.99476713	1.41936680	-1.46841624
H	-2.03573101	0.61359497	-2.20827626
H	-2.81557616	1.27566189	-0.75575941
C	-2.00399744	0.68293056	1.90533636
H	-1.94221463	1.72219302	1.56614215
H	-2.86224345	0.20850222	1.41440753
C	-2.27325360	-3.17388753	-1.19651172
H	-1.45505368	-3.86242747	-0.98149043
H	-3.21063218	-3.67228501	-0.94265635
H	-2.27951077	-2.96496505	-2.26711372
C	-2.04095389	2.77751413	-2.10363241
H	-1.21478569	2.91042628	-2.80307378
H	-2.97564249	2.89308198	-2.65527152
H	-1.98997198	3.56686286	-1.35237004
C	-2.08875686	0.57672735	3.39906857
H	-1.22565792	1.04444328	3.87417348
H	-2.98826804	1.08401478	3.75252289
H	-2.13854625	-0.46515427	3.71861829

1 2 1.0 3 1.0 7 1.0

2

3 4 1.0 5 1.0 6 1.0

4

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6

7 8 1.0 9 1.0 10 1.0

8 11 1.0

9 17 1.0

10 14 1.0

11 12 1.0 13 1.0 20 1.0

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14 15 1.0 16 1.0 24 1.0

15

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17 18 1.0 19 1.0 28 1.0

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20 21 1.0 22 1.0 23 1.0

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 24 25 1.0 26 1.0 27 1.0  
 25  
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 28 29 1.0 30 1.0 31 1.0  
 29  
 30  
 31

# **Ni(PH<sub>3</sub>)(PMePh<sub>2</sub>)**

%Mem=4GB

%Nprocs=4

%chk=MePh2\_freq\_2.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-0.13574661	-0.02262443	0.00000000
P	2.06425339	-0.02262443	0.00000000
H	2.51425299	-0.62016410	1.12380902
H	2.51425299	-0.69710148	-1.07938921
H	2.51425363	1.24939234	-0.04441980
P	-2.33574661	-0.02262443	0.00000000
C	-2.94241273	0.88384716	1.45693701
H	-2.58574411	1.89210401	1.42368597
H	-4.01241273	0.88384864	1.45693609
H	-2.58574753	0.40851419	2.34673952
C	-2.94241359	-1.73760438	0.05655914
C	-3.29933833	-2.39050064	-1.12361146
C	-3.05043232	-2.39927335	1.27970029
C	-3.76480600	-3.70454100	-1.08048902
H	-3.21479158	-1.86831786	-2.08767513
C	-3.51509092	-3.71404905	1.32291038
H	-2.76899469	-1.88489909	2.20993735
C	-3.87239734	-4.36669179	0.14311099
H	-4.04675099	-4.21901373	-2.01060801
H	-3.59976468	-4.23563347	2.28740728
H	-4.23937217	-5.40278398	0.17685702
C	-2.94241273	0.78588384	-1.51349615
C	-3.86998988	1.82432946	-1.42573081
C	-2.47997569	0.36745709	-2.76114160
C	-4.33547953	2.44369911	-2.58543869

H	-4.23495090	2.15346080	-0.44200433
C	-2.94476390	0.98757137	-3.92124508
H	-1.74876583	-0.45086581	-2.83048702
C	-3.87247623	2.02545670	-3.83360446
H	-5.06707943	3.26179954	-2.51637513
H	-2.57966473	0.65772390	-4.90479857
H	-4.23959769	2.51399715	-4.74785082

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
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 6 7 1.0 11 1.0 22 1.0  
 7 8 1.0 9 1.0 10 1.0  
 8  
 9  
 10  
 11 12 1.5 13 1.5  
 12 14 1.5 15 1.0  
 13 16 1.5 17 1.0  
 14 18 1.5 19 1.0  
 15  
 16 18 1.5 20 1.0  
 17  
 18 21 1.0  
 19  
 20  
 21  
 22 23 1.5 24 1.5  
 23 25 1.5 26 1.0  
 24 27 1.5 28 1.0  
 25 29 1.5 30 1.0  
 26  
 27 29 1.5 31 1.0  
 28  
 29 32 1.0  
 30  
 31  
 32  
 \$END

**{HNi(PH<sub>3</sub>)(PMePh<sub>2</sub>)}<sup>+</sup>**

%mem=4GB

%Nprocs=4

%chk=MePh2\_prod\_freq.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savento) geom=connectivity

Title Card Required

1 1

Ni	-0.79912534	0.17907769	-0.00001402
H	-0.66315642	-1.24273795	0.00006523
P	-3.00879522	-0.06629823	-0.00000302
H	-3.87213238	1.04566148	-0.00005994
H	-3.55717058	-0.78750739	-1.07286975
H	-3.55716876	-0.78739811	1.07293820
P	1.38402676	-0.01770582	0.00000411
C	2.04866564	-0.90186835	-1.44530270
H	3.11697932	-0.92413804	-1.38953594
H	1.67110594	-1.90298877	-1.45562672
C	2.04865576	-0.90161521	1.44547029
C	2.20908106	-0.23248158	2.65914048
C	2.39753525	-2.24798189	1.33998089
C	2.71891077	-0.90946277	3.76683714
H	1.93465853	0.82917088	2.74177293
C	2.90661027	-2.92557464	2.44818690
H	2.27099320	-2.77556409	0.38354315
C	3.06746907	-2.25654163	3.66147016
H	2.84597619	-0.38194555	4.72332889
H	3.18121543	-3.98723252	2.36482748
H	3.46937707	-2.79012373	4.53500118
H	1.74866070	-0.39828790	-2.34045842
C	2.24042420	1.58821554	-0.00013481
C	3.27740019	1.82564936	-0.90278503
C	1.86002096	2.58164021	0.90205637
C	3.93421829	3.05601992	-0.90271959
H	3.57757696	1.04197419	-1.61341076
C	2.51628154	3.81279078	0.90158911
H	1.04262424	2.39473705	1.61343449
C	3.55333319	4.05007082	-0.00049685
H	4.75200087	3.24301832	-1.61374684
H	2.21586043	4.59602052	1.61276599
H	4.07131823	5.02011608	-0.00067126

1 2 1.0 3 1.0 7 1.0

2

3 4 1.0 5 1.0 6 1.0

4

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6  
 7 8 1.0 11 1.0 23 1.0  
 8 9 1.0 10 1.0 22 1.0  
 9  
 10  
 11 12 1.5 13 1.5  
 12 14 1.5 15 1.0  
 13 16 1.5 17 1.0  
 14 18 1.5 19 1.0  
 15  
 16 18 1.5 20 1.0  
 17  
 18 21 1.0  
 19  
 20  
 21  
 22  
 23 24 1.5 25 1.5  
 24 26 1.5 27 1.0  
 25 28 1.5 29 1.0  
 26 30 1.5 31 1.0  
 27  
 28 30 1.5 32 1.0  
 29  
 30 33 1.0  
 31  
 32  
 33  
 \$END

# **Ni(PH<sub>3</sub>)(PF<sub>3</sub>)**

%Mem=4GB

%Nprocs=4

%chk=PF3\_freq\_3.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-0.76923077	-0.27149321	0.00000000
P	1.43076923	-0.27149321	0.00000000
P	-2.96923077	-0.27149321	0.00000000
H	-3.41923037	0.40088957	1.08069504
H	-3.41923037	0.32822447	-1.12264824
H	-3.41923101	-1.54359372	0.04195320

```

F          1.97410285  1.26434926 -0.05363280
F          1.97410208 -0.99296703  1.35689533
F          1.97410208 -1.08586179 -1.30326253
1 2 1.0 3 1.0
2 7 1.0 8 1.0 9 1.0
3 4 1.0 5 1.0 6 1.0
4
5
6
7
8
9
$END

```

**{HNi(PH<sub>3</sub>)(PF<sub>3</sub>)}<sup>+</sup>**

```

%mem=4GB
%Nprocs=4
%chk=PF3_prod_freq.chk
# opt freq m06l/6-311++g(d,p) pop=(nbo,savenbos) geom=connectivity
Title Card Required
1 1
Ni          -0.79912534  0.17907769 -0.00001402
H           -0.66315642 -1.24273795  0.00006523
P           -3.00879522 -0.06629823 -0.00000302
H           -3.87213238  1.04566148 -0.00005994
H           -3.55717058 -0.78750739 -1.07286975
H           -3.55716876 -0.78739811  1.07293820
P           1.38402676 -0.01770582  0.00000411
F           1.97928026 -0.80956567 -1.29441903
F           2.15102007  1.42056440 -0.00012031
F           1.97927141 -0.80933896  1.29456998
1 2 1.0 3 1.0 7 1.0
2
3 4 1.0 5 1.0 6 1.0
4
5
6
7 8 1.0 9 1.0 10 1.0
8
9
10
$END

```

# Ni(PH<sub>3</sub>)(PCF<sub>3</sub>)<sub>3</sub>

%Mem=4GB

%Nprocs=4

%chk=CF3\_freq\_3.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-0.38461538	0.49773755	0.00000000
P	1.81538462	0.49773755	0.00000000
H	2.26538421	-0.09980212	1.12380902
H	2.26538421	-0.17673950	-1.07938921
H	2.26538485	1.76975432	-0.04441980
P	-2.58461538	0.49773755	0.00000000
C	-3.19128151	1.40420915	1.45693701
C	-3.19128151	1.30624582	-1.51349615
C	-3.19128237	-1.21724240	0.05655914
F	-4.54128237	-1.21724144	0.05656772
F	-2.74127499	-1.81696261	1.17920290
F	-2.74128978	-1.88962315	-1.02414008
F	-4.54128147	1.30597652	-1.51364002
F	-2.74103156	0.63403890	-2.59419630
F	-2.74153088	2.57843953	-1.55529986
F	-2.74128335	0.80448998	2.57958504
F	-2.74127905	2.67630890	1.41498477
F	-4.54128151	1.40421101	1.45693585

1 2 1.0 6 1.0

2 3 1.0 4 1.0 5 1.0

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6 7 1.0 8 1.0 9 1.0

7 16 1.0 17 1.0 18 1.0

8 13 1.0 14 1.0 15 1.0

9 10 1.0 11 1.0 12 1.0

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\$END

**{HNi(PH<sub>3</sub>)(PCF<sub>3</sub>)<sub>3</sub>}<sup>+</sup>**

%mem=4GB

%Nprocs=4

%chk=CF3\_prod\_freq\_3.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

1 1

Ni	-0.38461538	0.49773755	0.00000000
P	1.81538462	0.49773755	0.00000000
H	2.26538421	-0.09980212	1.12380902
H	2.26538421	-0.17673950	-1.07938921
H	2.26538485	1.76975432	-0.04441980
P	-2.58461538	0.49773755	0.00000000
C	-3.19128151	1.40420915	1.45693701
C	-3.19128151	1.30624582	-1.51349615
C	-3.19128237	-1.21724240	0.05655914
F	-4.54128237	-1.21724144	0.05656772
F	-2.74127499	-1.81696261	1.17920290
F	-2.74128978	-1.88962315	-1.02414008
F	-4.54128147	1.30597652	-1.51364002
F	-2.74103156	0.63403890	-2.59419630
F	-2.74153088	2.57843953	-1.55529986
F	-2.74128335	0.80448998	2.57958504
F	-2.74127905	2.67630890	1.41498477
F	-4.54128151	1.40421101	1.45693585
H	-0.38461538	1.52304238	1.02530483

1 2 1.0 6 1.0 19 1.0

2 3 1.0 4 1.0 5 1.0

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6 7 1.0 8 1.0 9 1.0

7 16 1.0 17 1.0 18 1.0

8 13 1.0 14 1.0 15 1.0

9 10 1.0 11 1.0 12 1.0

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\$END

## Ni(PH<sub>3</sub>)(PCy<sub>3</sub>)

%Mem=4GB

%Nprocs=4

%chk=Cy\_freq\_3.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-1.32864455	-1.12484463	-1.47036626
P	-2.63451309	-2.17282851	-2.73024327
H	-3.99215039	-2.38999265	-2.37155318
H	-2.92905426	-1.74275606	-4.05307713
H	-2.38968196	-3.52354640	-3.09717990
P	-0.00364703	-0.14044388	-0.06321026
C	1.39984352	-1.21416246	0.52934734
C	2.14736124	-1.83377197	-0.65493879
C	2.38211409	-0.56744800	1.50619397
H	0.88912110	-2.03921516	1.04805237
C	3.19889402	-2.83254199	-0.18135280
H	2.63981551	-1.03885699	-1.23454917
H	1.42903921	-2.30688937	-1.33571170
C	3.42183699	-1.57625678	1.98710239
H	2.89948932	0.26045916	1.00031897
H	1.85320810	-0.12728393	2.36018274
C	4.16631373	-2.19972659	0.81243580
H	3.74231511	-3.24507867	-1.03782370
H	2.69264001	-3.68183522	0.29818468
H	4.12358655	-1.09853621	2.67917586
H	2.91599203	-2.36685212	2.55926478
H	4.89227582	-2.93898615	1.16658171
H	4.74835630	-1.41903583	0.30247119
C	0.86623789	1.39247606	-0.70848188
C	0.12539644	1.96551439	-1.92276858
C	1.16157419	2.50266655	0.30471308
H	1.83357447	1.00695618	-1.07035802
C	0.90411838	3.10808660	-2.56439118
H	-0.86345031	2.32534314	-1.60240095
H	-0.07390462	1.16354653	-2.64434662

C	1.95498662	3.63490962	-0.34217357
H	0.21476800	2.90759949	0.68790600
H	1.69908008	2.11233699	1.17427761
C	1.22445633	4.20257890	-1.55317105
H	0.34660329	3.51823834	-3.41293525
H	1.84305604	2.71269449	-2.97737119
H	2.15495978	4.42283181	0.39195620
H	2.93643745	3.25146778	-0.65598655
H	1.81438274	4.99852184	-2.01953118
H	0.28757064	4.67044163	-1.21929369
C	-0.83236986	0.41183974	1.51255497
C	-2.08271452	1.23085282	1.16990061
C	-1.20833002	-0.78243603	2.39399594
H	-0.13646995	1.05024046	2.07700293
C	-2.82973017	1.67446423	2.42245503
H	-2.73778355	0.60814948	0.54138671
H	-1.81824729	2.09815317	0.55367169
C	-1.96742496	-0.34244149	3.64197922
H	-1.82603092	-1.47622307	1.80382201
H	-0.31328700	-1.34133037	2.68787012
C	-3.20113903	0.47905200	3.29104335
H	-3.72331904	2.24408218	2.14633851
H	-2.19467152	2.36105832	3.00085440
H	-2.24322109	-1.21715524	4.24045365
H	-1.29990034	0.26169345	4.27301545
H	-3.71588230	0.80701183	4.20013079
H	-3.91331709	-0.15445083	2.74459517

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2 3 1.0 4 1.0 5 1.0

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6 7 1.0 24 1.0 41 1.0

7 8 1.0 9 1.0 10 1.0

8 11 1.0 12 1.0 13 1.0

9 14 1.0 15 1.0 16 1.0

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25 28 1.0 29 1.0 30 1.0  
26 31 1.0 32 1.0 33 1.0  
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28 34 1.0 35 1.0 36 1.0  
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31 34 1.0 37 1.0 38 1.0  
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41 42 1.0 43 1.0 44 1.0  
42 45 1.0 46 1.0 47 1.0  
43 48 1.0 49 1.0 50 1.0  
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45 51 1.0 52 1.0 53 1.0  
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48 51 1.0 54 1.0 55 1.0  
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51 56 1.0 57 1.0  
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\$END

**{HNi(PH<sub>3</sub>)(PCy<sub>3</sub>)}<sup>+</sup>**

%Mem=4GB

%Nprocs=4

%chk=Cy\_prod\_freq\_3.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

1 1

Ni	-0.29412132	-0.58474875	-0.00200504
H	-0.29641756	0.86524822	-0.00012957
P	1.90587500	-0.58126221	-0.00401009
H	2.35789171	-1.85333954	-0.00359829
H	2.35386146	0.05513308	-1.10710083
H	2.35586902	0.05655933	1.09743854
P	-2.49411765	-0.58823529	0.00000000
C	-3.10078463	0.26670796	1.48775913
C	-3.94259896	1.45898170	1.08081822
C	-3.89566373	-0.70097586	2.34116314
H	-2.20487901	0.62121734	2.06208095
C	-4.53751749	2.15276473	2.28924001
H	-4.76868225	1.11767096	0.40298545
H	-3.31191148	2.18451956	0.50422453
C	-4.48990279	-0.00733619	3.55002558
H	-4.71945948	-1.15024103	1.72645326
H	-3.23107679	-1.53851872	2.67774546
C	-5.33081135	1.18579461	3.14412807
H	-5.20318851	2.98928008	1.95217980
H	-3.71396247	2.60376504	2.90302703
H	-5.12095582	-0.73269534	4.12636929
H	-3.66331125	0.33287212	4.22787136
H	-5.70214878	1.71289703	4.06111630
H	-6.22840260	0.83208848	2.57179264
C	-3.10349894	0.27080749	-1.48428432
C	-2.26898138	-0.13213140	-2.68302934
C	-4.56687906	-0.06001940	-1.69786183
H	-2.99249586	1.37262829	-1.30585056
C	-2.79418489	0.49655985	-3.95757034
H	-2.28050847	-1.24907048	-2.78636421
H	-1.20456182	0.18018208	-2.52146368
C	-5.09227986	0.56936305	-2.97200318
H	-4.69336066	-1.17330895	-1.75204354
H	-5.16613530	0.30515272	-0.82380075
C	-4.25762759	0.16801583	-4.17105161
H	-2.19561387	0.12998027	-4.83153692

H	-2.66597734	1.60971258	-3.90434922
H	-6.15651601	0.25670577	-3.13384491
H	-5.08135685	1.68625795	-2.86761619
H	-4.63236514	0.69928815	-5.08424235
H	-4.36992791	-0.93336918	-4.35184323
C	-3.09806556	-2.30510558	-0.00181602
C	-2.59501662	-3.01929139	-1.23981819
C	-2.63950279	-3.00627274	1.26096977
H	-4.21896747	-2.26842184	-0.02187942
C	-3.00581146	-4.47764409	-1.24090791
H	-1.47637839	-2.94731494	-1.28261745
H	-3.00024196	-2.51456299	-2.15506342
C	-3.05102130	-4.46444159	1.26022488
H	-1.52311376	-2.93377071	1.34322471
H	-3.07747377	-2.49291572	2.15600468
C	-2.54951334	-5.17909598	0.02200034
H	-2.56641450	-4.99096069	-2.13529138
H	-4.12205533	-4.55034450	-1.32512751
H	-2.64543146	-4.96929947	2.17519007
H	-4.16971691	-4.53568159	1.30398757
H	-2.92382110	-6.23573593	0.02075206
H	-1.42862987	-5.21849047	0.04235320

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3 4 1.0 5 1.0 6 1.0

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7 8 1.0 25 1.0 42 1.0

8 9 1.0 10 1.0 11 1.0

9 12 1.0 13 1.0 14 1.0

10 15 1.0 16 1.0 17 1.0

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12 18 1.0 19 1.0 20 1.0

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15 18 1.0 21 1.0 22 1.0

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 25 26 1.0 27 1.0 28 1.0  
 26 29 1.0 30 1.0 31 1.0  
 27 32 1.0 33 1.0 34 1.0  
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 29 35 1.0 36 1.0 37 1.0  
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 32 35 1.0 38 1.0 39 1.0  
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 35 40 1.0 41 1.0  
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 42 43 1.0 44 1.0 45 1.0  
 43 46 1.0 47 1.0 48 1.0  
 44 49 1.0 50 1.0 51 1.0  
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 46 52 1.0 53 1.0 54 1.0  
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 49 52 1.0 55 1.0 56 1.0  
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 52 57 1.0 58 1.0  
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 \$END

**Ni(PH<sub>3</sub>)(POCH<sub>2</sub>)CH**

%chk=NiPH3P3O2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

# Title Card Required

0 1

Ni	-1.70983207	-0.36056638	-0.00096443
P	-3.72891446	0.32476127	0.00085672
H	-4.69351662	-0.07249178	-0.96046115
H	-4.58630540	0.16387182	1.11811908
H	-3.93976380	1.71458824	-0.14856800
P	0.34369391	-0.15592346	-0.00135475
O	0.90430944	1.38999417	-0.20523969
O	1.20863450	-0.57584171	1.35060347
O	1.26569367	-0.92209468	-1.14867201
C	2.30178210	1.59362242	0.05942791
C	2.63839201	-0.57612948	1.21170156
C	2.62630600	-0.47707756	-1.26704002
C	3.04143531	0.26101680	0.00189026
H	2.41286250	2.06720800	1.04363369
H	2.67022739	2.28945515	-0.70089821
H	3.04882644	-0.16321548	2.13865302
H	2.98671284	-1.61245231	1.11172097
H	2.71498651	0.16964470	-2.14978438
H	3.24007317	-1.36851562	-1.43082865
H	4.12290958	0.43014330	0.00347560

1 2 1.0 6 1.0

2 3 1.0 4 1.0 5 1.0

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6 7 1.0 8 1.0 9 1.0

7 10 1.0

8 11 1.0

9 12 1.0

10 13 1.0 14 1.0 15 1.0

11 13 1.0 16 1.0 17 1.0

12 13 1.0 18 1.0 19 1.0

13 20 1.0

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%chk=NiHPH3P3O2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1

Ni	-1.69355203	-0.23355323	0.00163222
H	-1.53578285	1.18390171	-0.00283943
P	-3.87361222	0.16555192	-0.00115754
H	-4.79264271	-0.90025954	0.00270775
H	-4.36368757	0.92317640	1.07365941
H	-4.36227866	0.91407361	-1.08300147
P	0.45376729	-0.06849800	0.00080892
O	1.07696766	0.65461043	1.29676287
O	1.24573691	-1.47178822	-0.06867573
O	1.06607758	0.77132115	-1.22874869
C	2.52727828	0.84066123	1.23161434
C	2.70068631	-1.34642230	0.03494655
C	2.52888811	0.77891483	-1.26843761
C	3.08597062	0.13095751	-0.00104236
H	2.93400074	0.43296253	2.15904756
H	2.71237234	1.91743788	1.20339502
H	3.00264851	-1.82838071	0.96821767
H	3.11933634	-1.90222987	-0.80635128
H	2.82794885	1.82491866	-1.35963910
H	2.83190776	0.24128506	-2.17043040
H	4.17611113	0.21898135	-0.00243179

1 2 1.0 3 1.0 7 1.0

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3 4 1.0 5 1.0 6 1.0

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7 8 1.0 9 1.0 10 1.0

8 11 1.0

9 12 1.0

10 13 1.0

11 14 1.0 15 1.0 16 1.0

12 14 1.0 17 1.0 18 1.0

13 14 1.0 19 1.0 20 1.0  
 14 21 1.0  
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# **Ni(PH<sub>3</sub>)(PH<sub>2</sub>Me)**

%chk=NiPH3PH2Me2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1  
 Ni 0.38065982 -0.19243310 0.00024543  
 P 2.44478887 0.24788404 -0.00015102  
 H 2.89277879 1.59288551 -0.00748593  
 H 3.29899163 -0.17263097 1.05146124  
 H 3.30110682 -0.18485476 -1.04510515  
 P -1.72647837 -0.46939788 -0.00017384  
 H -2.33001986 -1.21024365 -1.04845638  
 H -2.33062203 -1.21091959 1.04728873  
 C -2.84688118 0.99589533 0.00001595  
 H -2.64185199 1.60531660 -0.88050955  
 H -3.90009864 0.71106820 -0.00022296  
 H -2.64213017 1.60484104 0.88093518

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
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 6 7 1.0 8 1.0 9 1.0  
 7  
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 9 10 1.0 11 1.0 12 1.0  
 10  
 11  
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**{HNi(PH<sub>3</sub>)(PH<sub>2</sub>Me)}<sup>+</sup>**

%chk=NiHPH3PH2Me2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1

Ni	0.36112889	0.06156283	0.00000887
H	0.50368782	-1.35654065	0.00001616
P	2.57124945	0.11072368	-0.00000670
H	3.25367054	1.34169317	-0.00001946
H	3.20593040	-0.52680217	1.07754107
H	3.20591529	-0.52681517	-1.07755591
P	-1.76009515	-0.50190381	-0.00000441
H	-2.10829749	-1.33561051	1.07512916
H	-2.10825239	-1.33560298	-1.07515903
C	-3.04930012	0.78773911	-0.00000605
H	-2.94868557	1.41462680	-0.88568445
H	-4.03809746	0.32828476	-0.00027044
H	-2.94899376	1.41427474	0.88595754

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**Ni(PH<sub>3</sub>)(PHMe<sub>2</sub>)**

%chk=NiPH3PHMe22.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1

Ni	-0.64046841	0.00059512	-0.15547389
----	-------------	------------	-------------

P	-2.72118106	-0.00022157	0.17734486
H	-3.34870132	-1.05034234	0.89577610
H	-3.34858622	1.04709826	0.89994810
H	-3.65633431	0.00191393	-0.89092466
P	1.48736521	0.00012584	-0.33643386
H	2.05139841	0.00014650	-1.63966618
C	2.42451455	-1.42153469	0.36415326
H	3.50044075	-1.32179616	0.20040836
H	2.23448915	-1.48310442	1.43702624
H	2.07937022	-2.35174427	-0.08839909
C	2.42656629	1.42007661	0.36485565
H	2.23486904	1.48287442	1.43735582
H	3.50252854	1.31770461	0.20298827
H	2.08439378	2.35077073	-0.08896263

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
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 6 7 1.0 8 1.0 12 1.0  
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 8 9 1.0 10 1.0 11 1.0  
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 12 13 1.0 14 1.0 15 1.0  
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**{HNi(PH<sub>3</sub>)(PHMe<sub>2</sub>)}<sup>+</sup>**

%chk=NiHPH3PHMe22.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1			
Ni	-0.61620727	-0.00006425	-0.27479109
H	-0.34963329	0.00040151	1.12798983
P	1.57596157	-0.00001369	-0.32378138
H	2.06226244	-0.00005669	-1.64960307
P	-2.77630444	0.00001621	0.23062587

H	-3.23476041	1.07561467	1.00808806
H	-3.75279911	-0.00026277	-0.78300506
H	-3.23469364	-1.07521956	1.00862889
C	2.37763196	-1.45258004	0.41327618
H	3.46041682	-1.39276058	0.29173652
H	2.14151548	-1.49762193	1.47715510
H	2.01742198	-2.36687892	-0.05828288
C	2.37745392	1.45271546	0.41315005
H	3.46017108	1.39352713	0.29072299
H	2.01636343	2.36700857	-0.05774409
H	2.14216657	1.49719721	1.47723936

1 2 1.0 3 1.0 5 1.0  
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 3 4 1.0 9 1.0 13 1.0  
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 5 6 1.0 7 1.0 8 1.0  
 6  
 7  
 8  
 9 10 1.0 11 1.0 12 1.0  
 10  
 11  
 12  
 13 14 1.0 15 1.0 16 1.0  
 14  
 15  
 16

# **Ni(PH<sub>3</sub>)(PMe<sub>2</sub>Et)**

%chk=NiPH3PMe2Et2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

0 1			
Ni	1.16755464	-0.01059712	0.00058443
P	3.25123886	0.25986794	-0.00042884
H	4.05866868	-0.16490628	1.08788559
H	4.07669211	-0.31822024	-1.00115675
H	3.83228798	1.55244016	-0.09020776
P	-0.96786985	-0.26582623	-0.00000178
C	-1.96530166	1.29662860	0.00515486

H	-1.62218849	1.87184231	-0.86131693
H	-1.62731261	1.86219202	0.87998079
C	-1.69629350	-1.18622357	-1.41695776
H	-1.21268367	-2.16106941	-1.49856532
H	-2.77319593	-1.33997287	-1.30312800
H	-1.50944114	-0.64390351	-2.34586564
C	-1.69577099	-1.19467693	1.41171162
H	-1.50549489	-0.65980622	2.34421470
H	-2.77329409	-1.34491414	1.29908543
H	-1.21451882	-2.17135966	1.48496044
C	-3.47990956	1.16526513	-0.00013033
H	-3.84896029	0.62681670	0.87645858
H	-3.95510804	2.14983711	0.00652692
H	-3.84386165	0.64115836	-0.88744715

1 2 1.0 6 1.0  
 2 3 1.0 4 1.0 5 1.0  
 3  
 4  
 5  
 6 7 1.0 10 1.0 14 1.0  
 7 8 1.0 9 1.0 18 1.0  
 8  
 9  
 10 11 1.0 12 1.0 13 1.0  
 11  
 12  
 13  
 14 15 1.0 16 1.0 17 1.0  
 15  
 16  
 17  
 18 19 1.0 20 1.0 21 1.0  
 19  
 20  
 21

**{HNi(PH<sub>3</sub>)(PMe<sub>2</sub>Et)}<sup>+</sup>**

%chk=NiHPH3PMe2Et2.chk

# opt=calcall freq m06l/6-311++g(d,p) geom=connectivity

Title Card Required

1 1

Ni	1.10538920	-0.16813288	-0.00000504
H	1.12578404	1.26010513	0.00009659
P	3.32891921	-0.18362480	-0.00000378
H	4.05768693	-1.38836712	-0.00008117
H	3.95975512	0.46862700	-1.07253665
H	3.95975861	0.46848918	1.07261056
P	-1.04213364	0.27021551	0.00001728
C	-1.59770229	1.22900901	1.43940104
H	-1.05768270	2.17546019	1.48375510
H	-2.66685620	1.44005656	1.36952834
H	-1.40464206	0.67956220	2.36192658
C	-1.59768375	1.22925616	-1.43920869
H	-1.40460827	0.67996879	-2.36182592
H	-2.66683898	1.44028968	-1.36931544
H	-1.05766568	2.17571622	-1.48339141
C	-2.04626800	-1.27145000	-0.00012273
H	-1.73503614	-1.85121545	0.87543844
H	-1.73503822	-1.85105232	-0.87579275
C	-3.55451447	-1.05858045	-0.00010048
H	-3.89399789	-0.51672559	-0.88474432
H	-4.06229374	-2.02456876	-0.00019165
H	-3.89399476	-0.51689389	0.88464749

1 2 1.0 3 1.0 7 1.0

2

3 4 1.0 5 1.0 6 1.0

4

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7 8 1.0 12 1.0 16 1.0

8 9 1.0 10 1.0 11 1.0

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12 13 1.0 14 1.0 15 1.0

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16 17 1.0 18 1.0 19 1.0

17

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19 20 1.0 21 1.0 22 1.0

20  
21  
22

# **Ni(PH<sub>3</sub>)P(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>**

%Mem=4GB

%Nprocs=4

%chk=C6F5\_freq\_2.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-0.70136114	0.07128756	-0.00212580
P	1.49863518	0.07470181	-0.00425160
H	1.95064652	-0.52141142	1.11950761
H	1.94863929	-0.59977439	-1.08363946
H	1.94661691	1.34738641	-0.04992741
P	-2.90135746	0.06787330	0.00000000
C	-3.50802445	0.97434493	1.45693664
C	-3.73859278	0.29619968	2.65419546
C	-3.74235996	2.34700235	1.37664597
C	-4.20403461	0.99051466	3.77066864
C	-4.20700522	3.04185324	2.49364951
C	-4.43799234	2.36385233	3.69051907
C	-3.50530538	-1.64800943	0.05825273
C	-4.40713114	-2.10310538	-0.90407226
C	-3.06652681	-2.50810433	1.06486004
C	-4.87054119	-3.41781859	-0.85932784
C	-3.52922242	-3.82353511	1.10918295
C	-4.43119790	-4.27845376	0.14740009
C	-3.51073876	0.87445993	-1.51343069
C	-4.77167393	1.47140721	-1.52638735
C	-2.71716537	0.89594494	-2.66030810
C	-5.23912615	2.08908787	-2.68620664
C	-3.18420861	1.51463369	-3.82026704
C	-4.44502502	2.11104423	-3.83343716
F	-4.83230020	-1.27007367	-1.87761703
F	-5.74377039	-3.85804722	-1.79001012
F	-4.87986675	-5.55098891	0.19041803
F	-3.10394309	-4.65585631	2.08328710
F	-2.19372603	-2.06800542	1.99600544
F	-5.53983164	1.44957866	-0.41645166
F	-6.45954869	2.66606567	-2.69906856
F	-4.89772301	2.70905884	-4.95590902



F	-2.41566242	1.53567830	-4.92994892
F	-1.49692544	0.31857068	-2.64791983
F	-3.51256850	-1.03251306	2.73123755
F	-4.42790179	0.33426597	4.92899552
F	-4.88844404	3.03566112	4.77138271
F	-4.43321954	4.37048191	2.41572045
F	-3.51911173	3.00342822	0.21830003

1 2 1.0 6 1.0

2 3 1.0 4 1.0 5 1.0

3

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6 7 1.0 13 1.0 19 1.0

7 8 1.5 9 1.5

8 10 1.5 35 1.0

9 11 1.5 39 1.0

10 12 1.5 36 1.0

11 12 1.5 38 1.0

12 37 1.0

13 14 1.5 15 1.5

14 16 1.5 25 1.0

15 17 1.5 29 1.0

16 18 1.5 26 1.0

17 18 1.5 28 1.0

18 27 1.0

19 20 1.5 21 1.5

20 22 1.5 30 1.0

21 23 1.5 34 1.0

22 24 1.5 31 1.0

23 24 1.5 33 1.0

24 32 1.0

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\$END

**{HNi(PH<sub>3</sub>)(PCF<sub>5</sub>)<sub>3</sub>}<sup>+</sup>**

%mem=4GB

%Nprocs=4

%chk=C6F5\_prod\_freq\_2.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savento) geom=connectivity

Title Card Required

1 1

Ni	-0.82312700	0.29987000	2.48107200
H	0.32639700	-0.40466600	2.97710600
P	-1.36371700	0.44003500	4.60861800
H	-2.55436000	1.07911800	5.00474100
H	-1.49684000	-0.77473900	5.29999900
H	-0.44544800	1.09452900	5.44515400
P	0.02476700	0.05385700	0.49093400
C	0.01834900	-1.64093700	-0.15986200
C	-0.98705400	-2.48661100	0.31576800
C	0.90367200	-2.16944100	-1.10233500
C	-1.11137000	-3.80094400	-0.09812400
C	0.80569900	-3.48663100	-1.52931800
C	-0.20286800	-4.30268500	-1.02627000
C	1.65037500	0.77962300	0.17184500
C	1.87980800	1.99551400	-0.47416300
C	2.76282600	0.11908900	0.70011800
C	3.16009000	2.51237900	-0.61642700
C	4.04885900	0.61086100	0.57009800
C	4.24636000	1.81824400	-0.09506700
C	-1.23717900	0.89928300	-0.50908600
C	-2.33528900	1.42892400	0.15017000
C	-1.23311600	0.98078600	-1.90053400
C	-3.39081500	2.04375900	-0.49469600
C	-2.26821300	1.59059900	-2.59271300
C	-3.34734500	2.12175100	-1.88583000
F	1.87503800	-1.42299100	-1.61856900
F	1.65901900	-3.96494900	-2.41536700
F	-0.30407700	-5.54840800	-1.43450700
F	-2.07779500	-4.56967800	0.37141500
F	-1.88372600	-2.01194800	1.19612100
F	-2.39269000	1.33879000	1.52363700

F	-4.41437800	2.53740600	0.17513600
F	-4.33315100	2.69717100	-2.53542700
F	-2.24458300	1.67126600	-3.90773600
F	-0.20599500	0.47847600	-2.57556100
F	0.86898500	2.71002300	-0.97006500
F	3.34683400	3.66287200	-1.23760500
F	5.46120600	2.30486400	-0.22425000
F	5.07777700	-0.04964200	1.06848100
F	2.58145800	-1.04218100	1.33632500

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3 4 1.0 5 1.0 6 1.0

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7 8 1.0 14 1.0 20 1.0

8 9 1.5 10 1.5

9 11 2.0 30 1.0

10 12 1.5 26 1.0

11 13 1.5 29 1.0

12 13 1.5 27 1.0

13 28 1.0

14 15 1.5 16 1.5

15 17 1.5 36 1.0

16 18 2.0 40 1.0

17 19 1.5 37 1.0

18 19 1.5 39 1.0

19 38 1.0

20 21 2.0 22 1.5

21 23 2.0 31 1.0

22 24 1.5 35 1.0

23 25 1.5 32 1.0

24 25 1.5 34 1.0

25 33 1.0

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\$END

# **Ni(PH<sub>3</sub>)(PPh<sub>3</sub>)**

%Mem=4GB

%Nprocs=4

%chk=Ph\_freq\_5.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savenbos) geom=connectivity

Title Card Required

0 1

Ni	-2.30621652	0.08371873	-0.00803287
P	-0.16671151	0.01222662	-0.00196824
P	-4.41472881	0.11331538	0.00345940
H	-5.16956437	-1.00583526	-0.43349004
H	-5.13763651	0.29228748	1.21061503
H	-5.15527157	1.07018305	-0.73862938
C	0.67460464	1.34261761	-0.94875909
C	0.11783622	1.70622412	-2.17951869
C	1.83271813	1.98997373	-0.51075567
C	0.71537705	2.68388402	-2.96467455
H	-0.79443078	1.21512762	-2.51184991
C	2.42431151	2.97759725	-1.29441542
H	2.27776841	1.72662880	0.44448853
C	1.87068560	3.32273908	-2.52237823
H	0.27385333	2.95342162	-3.91887091
H	3.32097533	3.47762417	-0.94167620
H	2.33509018	4.09304902	-3.12989897
C	0.62598269	0.12726544	1.65102393
C	1.74710908	-0.62104598	2.01953355
C	0.07886126	1.02851382	2.57133141
C	2.31247152	-0.46287674	3.28092395
H	2.17958755	-1.33096342	1.32052579
C	0.65113347	1.19204075	3.82662085
H	-0.80568780	1.59706116	2.29036790
C	1.77053458	0.44411475	4.18415178
H	3.18189536	-1.05120383	3.55760436
H	0.21963184	1.89724457	4.52990436
H	2.21559327	0.56696556	5.16636397

C	0.57003542	-1.51929735	-0.69763297
C	1.69692826	-1.52871063	-1.52159208
C	-0.03850425	-2.73646914	-0.36571343
C	2.20662078	-2.73094446	-2.00274021
H	2.17495926	-0.59206319	-1.79221549
C	0.47841804	-3.93670535	-0.83940904
H	-0.92988513	-2.72974514	0.25832578
C	1.60227186	-3.93523897	-1.66135840
H	3.08034406	-2.72415477	-2.64684317
H	-0.00063188	-4.87394562	-0.57405804
H	2.00470156	-4.87102819	-2.03593666

1 2 1.0 3 1.0

2 7 1.0 18 1.0 29 1.0

3 4 1.0 5 1.0 6 1.0

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7 8 1.5 9 1.5

8 10 1.5 11 1.0

9 12 1.5 13 1.0

10 14 1.5 15 1.0

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12 14 1.5 16 1.0

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14 17 1.0

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18 19 1.5 20 1.5

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 25 1.5 26 1.0

22

23 25 1.5 27 1.0

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25 28 1.0

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29 30 1.5 31 1.5

30 32 1.5 33 1.0

31 34 1.5 35 1.0

32 36 1.5 37 1.0

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33
34 36 1.5 38 1.0
35
36 39 1.0
37
38
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$END

```

**{HNi(PH<sub>3</sub>)(PPh<sub>3</sub>)}<sup>+</sup>**

%mem=4GB

%Nprocs=4

%chk=Ph\_prod\_freq.chk

# opt freq m06l/6-311++g(d,p) pop=(nbo6,savento) geom=connectivity

Title Card Required

1 1

Ni	-0.79912534	0.17907769	-0.00001402
H	-0.66315642	-1.24273795	0.00006523
P	-3.00879522	-0.06629823	-0.00000302
H	-3.87213238	1.04566148	-0.00005994
H	-3.55717058	-0.78750739	-1.07286975
H	-3.55716876	-0.78739811	1.07293820
P	1.38402676	-0.01770582	0.00000411
C	2.04865576	-0.90161521	1.44547029
C	2.20908106	-0.23248158	2.65914048
C	2.39753525	-2.24798189	1.33998089
C	2.71891077	-0.90946277	3.76683714
H	1.93465853	0.82917088	2.74177293
C	2.90661027	-2.92557464	2.44818690
H	2.27099320	-2.77556409	0.38354315
C	3.06746907	-2.25654163	3.66147016
H	2.84597619	-0.38194555	4.72332889
H	3.18121543	-3.98723252	2.36482748
H	3.46937707	-2.79012373	4.53500118
C	2.24042420	1.58821554	-0.00013481
C	3.27740019	1.82564936	-0.90278503
C	1.86002096	2.58164021	0.90205637
C	3.93421829	3.05601992	-0.90271959
H	3.57757696	1.04197419	-1.61341076
C	2.51628154	3.81279078	0.90158911
H	1.04262424	2.39473705	1.61343449
C	3.55333319	4.05007082	-0.00049685
H	4.75200087	3.24301832	-1.61374684

H	2.21586043	4.59602052	1.61276599
H	4.07131823	5.02011608	-0.00067126
C	2.04866564	-0.90186835	-1.44530270
C	1.29075841	-0.99929049	-2.61258886
C	3.31574997	-1.48198621	-1.38606837
C	1.79962384	-1.67727665	-3.72011424
H	0.29153473	-0.54248989	-2.65870884
C	3.82531966	-2.15936658	-2.49417688
H	3.91330679	-1.40514458	-0.46620412
C	3.06745744	-2.25721344	-3.66105642
H	1.20203490	-1.75464683	-4.64000436
H	4.82455950	-2.61631136	-2.44732149
H	3.46849387	-2.79168082	-4.53444679

1 2 1.0 3 1.0 7 1.0

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3 4 1.0 5 1.0 6 1.0

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7 8 1.0 19 1.0 30 1.0

8 9 1.5 10 1.5

9 11 1.5 12 1.0

10 13 1.5 14 1.0

11 15 1.5 16 1.0

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13 15 1.5 17 1.0

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15 18 1.0

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19 20 1.5 21 1.5

20 22 1.5 23 1.0

21 24 1.5 25 1.0

22 26 1.5 27 1.0

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24 26 1.5 28 1.0

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26 29 1.0

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30 31 1.5 32 1.5

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31 33 1.5 34 1.0
32 35 1.5 36 1.0
33 37 1.5 38 1.0
34
35 37 1.5 39 1.0
36
37 40 1.0
38
39
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$END

```

## NRT Full Results

### NV(NH<sub>2</sub>)<sub>2</sub>(P(OCH<sub>2</sub>)<sub>3</sub>CH)

NATURAL RESONANCE THEORY ANALYSIS:

Parent structure threshold: 50% of leading weight

Delocalization list threshold: 1 kcal/mol

Maximum search cycles: 3

C1 symmetry, 1 symmetry operator(s), 1 unique atom permutation(s)

User-requested resonance units:

1. <V1,N2,N5,N8,P9,O10,O11,O12>

1 initial TOPO matrices: NLS = 1; NBI = 0; SYM = 0

cycle	structures	D(w)	kmax	CHOOSE	ION	E2	SYM	dbmax	dbrms
1	3/3	0.08339449	3	4	0	34	0	3.000	1.161
2	11/100	0.07615967	13	230	-25	34	0	0.605	0.128
3	18/130	0.07365067	21	278	-90	113	0	0.221	0.062

QPNRT(18/130): D(0)=0.08576650; D(w)=0.07365067; dbmax=0.221; dbrms=0.062

Timing(sec): search=20.55; Gram matrix=3.28; minimize=0.01; other=0.84

TOPO matrix for the leading resonance structure:

Atom	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1. V	0	2	0	0	1	0	0	3	0	0	0	0	0	0	0	0	0



2.N	2	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3.H	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.H	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5.N	1	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0
6.H	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
7.H	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
8.N	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
9.P	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0
10.O	0	0	0	0	0	0	0	0	1	2	0	0	1	0	0	0	0
11.O	0	0	0	0	0	0	0	0	1	0	2	0	0	1	0	0	0
12.O	0	0	0	0	0	0	0	0	1	0	0	2	0	0	1	0	0
13.C	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1
14.C	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0
15.C	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0
16.C	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0
17.H	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
18.H	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
19.H	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
20.H	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
21.H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
22.H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
23.H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0

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1.V	0	0	0	0	0	0
2.N	0	0	0	0	0	0
3.H	0	0	0	0	0	0
4.H	0	0	0	0	0	0
5.N	0	0	0	0	0	0
6.H	0	0	0	0	0	0
7.H	0	0	0	0	0	0
8.N	0	0	0	0	0	0
9.P	0	0	0	0	0	0
10.O	0	0	0	0	0	0
11.O	0	0	0	0	0	0
12.O	0	0	0	0	0	0
13.C	1	0	0	0	0	0
14.C	0	1	1	0	0	0
15.C	0	0	0	1	1	0
16.C	0	0	0	0	0	1
17.H	0	0	0	0	0	0
18.H	0	0	0	0	0	0

19. H 0 0 0 0 0 0  
 20. H 0 0 0 0 0 0  
 21. H 0 0 0 0 0 0  
 22. H 0 0 0 0 0 0  
 23. H 0 0 0 0 0 0

Resonance		
RS	Weight(%)	Added(Removed)
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1	14.55	
2	14.49	( V 1- N 2), V 1- N 5, N 2, ( N 5)
3	7.94	( V 1- N 2), V 1- P 9, ( P 9- O 10), P 9- O 11, N 2, ( P 9), O 10, ( O 11)
4	7.81	( V 1- N 2), V 1- P 9, P 9- O 10, ( P 9- O 11), N 2, ( P 9), ( O 10), O 11
5	7.36	( V 1- N 2), V 1- N 5, ( V 1- N 8), V 1- P 9, N 2, ( N 5), N 8, ( P 9)
6	7.27	( V 1- N 8), V 1- P 9, N 8, ( P 9)
7	6.21	( V 1- N 2), V 1- P 9, ( P 9- O 11), P 9- O 12, N 2, ( P 9), O 11, ( O 12)
8	6.09	( V 1- N 2), V 1- P 9, ( P 9- O 10), P 9- O 12, N 2, ( P 9), O 10, ( O 12)
9	5.84	( V 1- N 2), V 1- P 9, P 9- O 10, ( P 9- O 12), N 2, ( P 9), ( O 10), O 12
10	5.74	( V 1- N 2), V 1- P 9, P 9- O 11, ( P 9- O 12), N 2, ( P 9), ( O 11), O 12
11	4.69	( V 1- N 8), V 1- P 9, N 8, ( P 9)
12	4.67	( V 1- N 2), V 1- N 5, ( V 1- N 8), V 1- P 9, N 2, ( N 5), N 8, ( P 9)
13	2.53	( V 1- N 2), ( V 1- N 8), V 1, N 2, N 8, ( P 9)
14	2.32	( V 1- N 2), V 1- P 9, N 8- O 12, ( P 9- O 12), N 2, ( N 8)
15	0.84	( V 1- N 2), ( V 1- N 8), V 1- P 9, V 1- P 9, ( P 9- O 12), N 2, ( P 9), O 12
16	0.83	( V 1- N 2), ( V 1- N 8), V 1- P 9, V 1- P 9, ( P 9- O 12), N 2, ( P 9), O 12
17	0.58	( V 1- N 2), ( V 1- N 8), V 1- P 9, V 1- P 9, ( P 9- O 12), N 2, ( P 9), O 12
18	0.22	( V 1- N 2), ( V 1- N 8), V 1- P 9, V 1- P 9, ( P 9- O 12), N 2, ( P 9), O 12
others	0.00	
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100.00 \* Total \*

# **NV(NH<sub>2</sub>)<sub>2</sub>(P(CH<sub>2</sub>CH<sub>2</sub>)<sub>3</sub>CH)**

## NATURAL RESONANCE THEORY ANALYSIS:

Parent structure threshold: 50% of leading weight

Delocalization list threshold: 1 kcal/mol

Maximum search cycles: 3

C1 symmetry, 1 symmetry operator(s), 1 unique atom permutation(s)

User-requested resonance units:

1. <V1,N2,N5,N8,P9,C21,C24,C27>

1 initial TOPO matrices: NLS = 1; NBI = 0; SYM = 0

cycle structures	D(w)	kmax	CHOOSE	ION	E2	SYM	dbmax	dbrms
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1	3/3	0.07140929	3	4	0	24	0	3.000	1.130
2	8/64	0.06374856	8	134	-25	43	0	0.625	0.124
3	17/175	0.06226301	24	229	-51	28	0	0.356	0.070

QPNRT(17/175): D(0)=0.07392188; D(w)=0.06226301; dbmax=0.356; dbrms=0.070

Timing(sec): search=16.59; Gram matrix=4.46; minimize=0.01; other=0.68

TOPO matrix for the leading resonance structure:

Atom	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1. V	0	0	0	0	2	0	0	3	1	0	0	0	0	0	0	0	0
2. N	0	2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3. H	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4. H	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5. N	2	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0
6. H	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
7. H	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
8. N	3	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
9. P	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10. C	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0
11. C	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1
12. C	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
13. C	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0
14. H	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0

15. H	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
16. H	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
17. H	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
18. H	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
19. H	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
20. H	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
21. C	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0
22. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24. C	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0
25. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27. C	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0
28. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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1. V	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2. N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5. N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8. N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9. P	0	0	0	1	0	0	1	0	0	1	0	0	0	0	0	0	0
10. C	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
11. C	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
12. C	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
13. C	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20. H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21. C	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
22. H	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23. H	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
24. C	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
25. H	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0

26. H	0	0	0	0	0	0	1	0	0	0	0	0
27. C	0	0	0	0	0	0	0	0	0	0	1	1
28. H	0	0	0	0	0	0	0	0	0	1	0	0
29. H	0	0	0	0	0	0	0	0	0	1	0	0

Resonance		
RS	Weight(%)	Added(Removed)
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1	22.25	
2	22.23	V 1- N 2, V 1- N 2, ( V 1- N 5), ( V 1- N 5), ( N 2), ( N 2), N 5, N 5
3	16.50	V 1- N 2, V 1- N 2, ( V 1- N 8), ( V 1- P 9), ( N 2), ( N 2), N 8, P 9
4	7.36	V 1- N 2, V 1- N 2, ( V 1- N 5), ( V 1- P 9), ( N 2), ( N 2), N 5, P 9
5	7.31	V 1- N 2, ( V 1- P 9), ( N 2), P 9
6	5.47	V 1- N 2, ( V 1- N 8), ( N 2), N 8
7	5.47	V 1- N 2, V 1- N 2, ( V 1- N 5), ( V 1- N 8), ( N 2), ( N 2), N 5, N 8
8	1.97	V 1- N 2, ( V 1- N 5), ( V 1- N 8), V 1- P 9, ( P 9- C 27), ( N 2), N 5, C 27
9	1.96	V 1- N 2, ( V 1- N 5), ( V 1- N 8), V 1- P 9, ( P 9- C 27), ( N 2), N 5, C 27
10	1.42	( V 1- N 8), ( V 1- P 9), V 1, ( N 2), N 8, P 9
11	1.42	V 1- N 2, V 1- N 2, ( V 1- N 5), ( V 1- N 5), ( V 1- N 8), ( V 1- P 9), V 1, ( N 2), ( N 2), N 5, N 8, P 9
12	1.21	V 1- N 2, ( V 1- N 5), ( V 1- N 8), ( V 1- P 9), V 1, ( N 2), ( N 2), N 5, N 8, P 9
13	1.21	V 1- N 2, ( V 1- N 5), ( V 1- N 8), ( V 1- P 9), V 1, ( N 2), N 8, P 9
14	1.17	V 1- N 2, ( V 1- N 5), ( V 1- N 5), ( V 1- P 9), V 1, ( N 2), N 5, N 5
15	1.17	( V 1- N 5), ( V 1- P 9), V 1, N 5
16	0.95	V 1- N 2, ( V 1- N 5), ( V 1- N 8), V 1- P 9, ( P 9- C 27), ( N 2), N 5, C 27
17	0.92	V 1- N 2, ( V 1- N 5), ( V 1- N 8), V 1- P 9, ( P 9- C 27), ( N 2), N 5, C 27
others	0.00	
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100.00	* Total *	