Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

The Role of Neutral Rh(PONOP)H, free NMe_2H, Boronium and Ammonium Salts in the Dehydrocoupling of Dimethylamineborane using the Cationic Pincer $[Rh(PONOP)(\eta^2–H^2)]^+$ Catalyst.

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Reaction of 2 with D_2

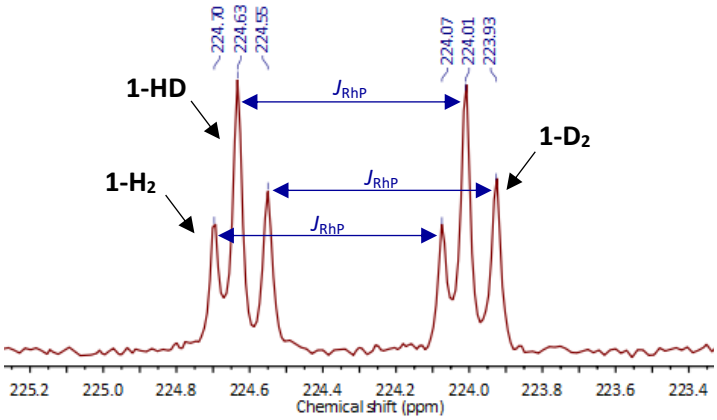


Figure S1. Partial $^{31}P\{^{1}H\}$ NMR spectrum (1,2–$F_2C_6H_4$ solvent, 298 K, 500 MHz) of the reaction mixture 30 minutes after time of mixing. **1-H_2** δ 224.4, J_{RhP} 126 Hz; **1-HD** δ 224.3, J_{RhP} 126 Hz; **1-D_2** δ 224.2, J_{RhP} 126 Hz.

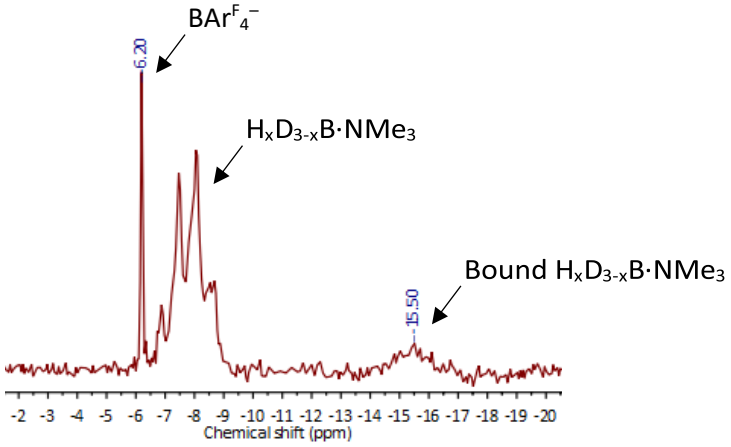


Figure S2. ^{11}B NMR spectrum (1,2–$F_2C_6H_4$ solvent, 298 K, 500 MHz) of the reaction mixture 30 minutes after time of mixing.

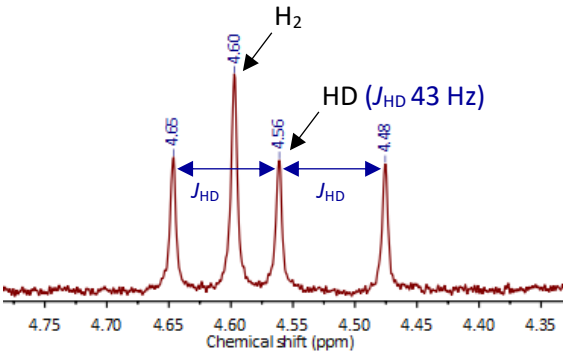


Figure S3. Partial ^{1}H NMR spectrum (1,2–$F_2C_6H_4$ solvent, 298 K, 500 MHz) of the reaction mixture 30 minutes after time of mixing.

Catalyst speciation under hydrogen evolution conditions

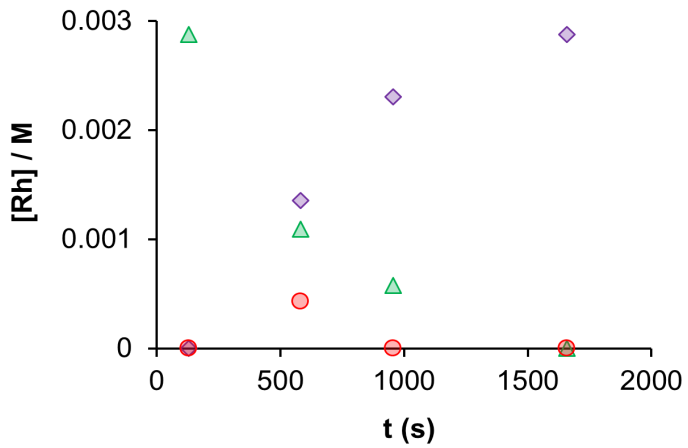


Figure S4. Time course plot for dehydrogenation of $H_3B{\cdot}NMe_2H$ [0.072 M, 298 K, 1,2–$F_2C_6H_4$ solvent] using complex **1** (4 mol%) under hydrogen evolution conditions as measured by $^{31}P\{^1H\}$ NMR spectroscopy of aliquots of the reaction mixture taken at four different times after time of mixing. ○ = complex **4,** △ = complex **3** and ◇ = complex **1**.

Application of simple kinetic models to reaction profile of catalysis, 2 mol%

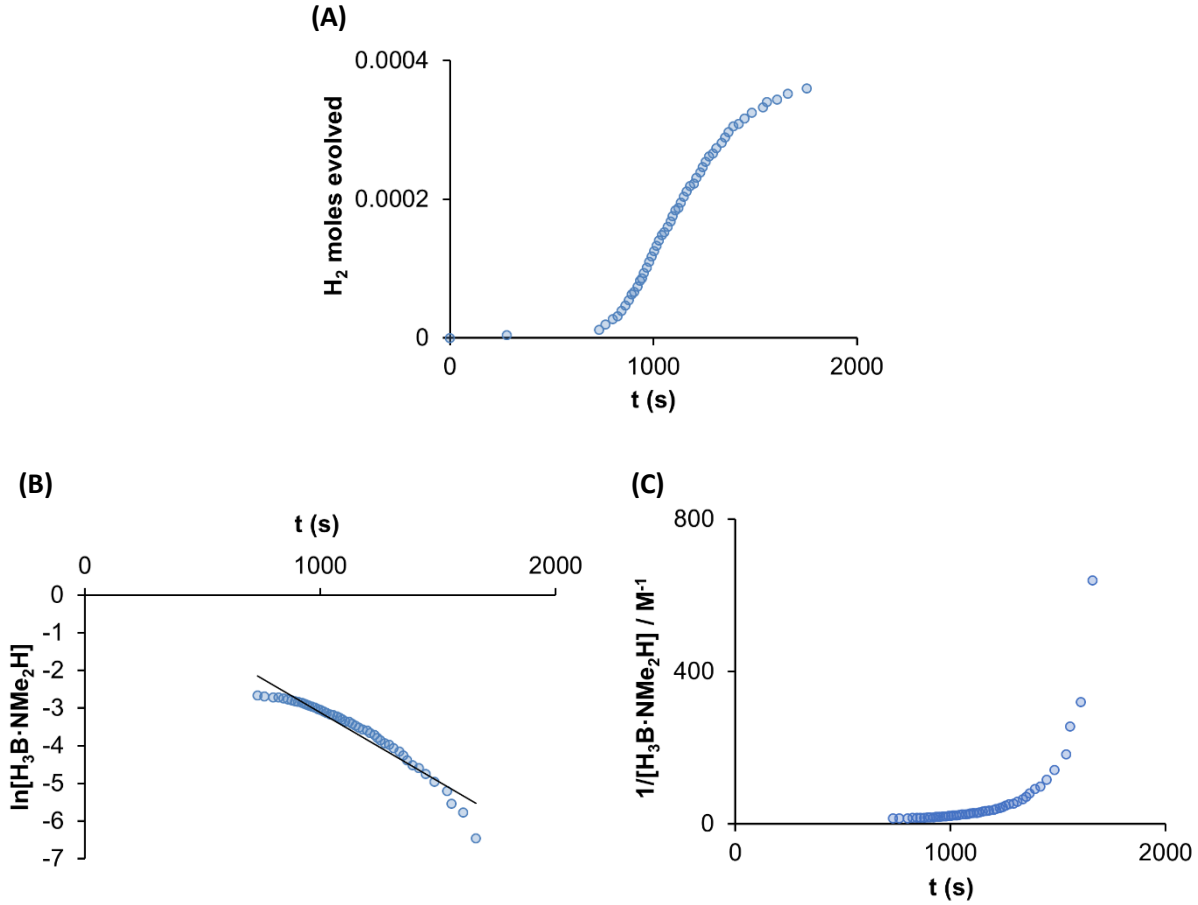


Figure S5. (A) Time course plot for the dehydrogenation of $H_3B{\cdot}NMe_2H$ [0.072 M, 298 K, 1,2–$F_2C_6H_4$ solvent] using complex **1** (2 mol%) under hydrogen evolution conditions. **(B)** Plot of the natural logarithm of [$H_3B{\cdot}NMe_2H$] vs. time (post induction period) showing poor agreement with first order rate kinetics. **(C)** Plot of 1/[$H_3B{\cdot}NMe_2H$] vs. time (post induction period) showing poor agreement with second order rate kinetics.

Tests for homogeneity

Mercury poisoning

Dehydrogenation was conducted as per standard hydrogen evolution measurement conditions at a catalyst loading of 2 mol%. After 0.25 equivalents of expected hydrogen had evolved, an excess of elemental mercury (2000 eq relative to catalyst) was added. Catalysis continued, consistent with a homogeneous system, although only 0.9 equivalents of hydrogen were evolved and a small decrease in rate of catalysis was observed.

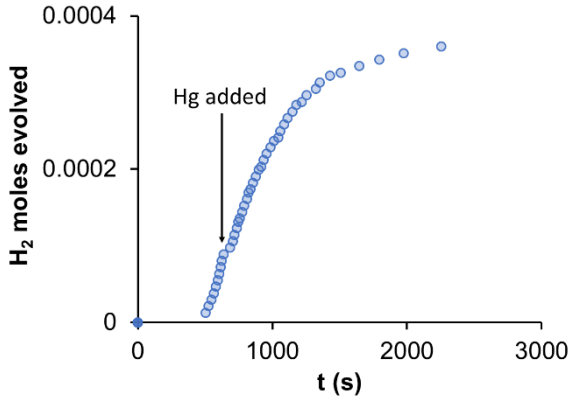


Figure S6. Time course plot for dehydrogenation of H3B·NMe2H [0.072 M, 298 K, 1,2–F2C6H4 solvent] using complex **1** (2 mol%) as measured by H2 evolution with the addition of 2000 eq. elemental mercury at 624 s.

PPh_3 fractional poisoning

Dehydrogenation was conducted as per standard hydrogen evolution measurement conditions at a catalyst loading of 2 mol%. After 0.25 equivalents of expected hydrogen had evolved, 0.2 equivalents (relative to catalyst) of PPh_3 in 0.2 mL 1,2– $F_2C_6H_4$ was added. A minor decrease in the rate of hydrogen evolution was observed, consistent with homogeneous catalysis.

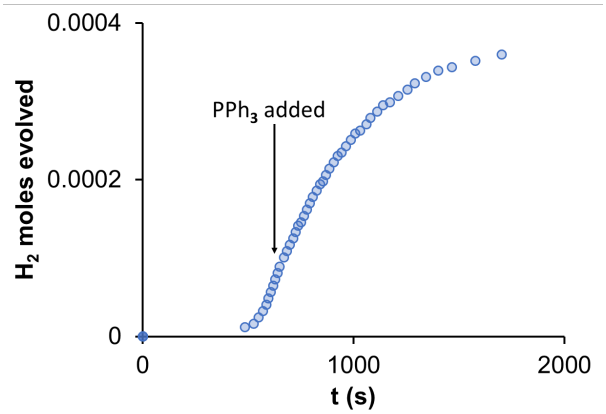


Figure S7. Time course plot for dehydrogenation of $H_3B{\cdot}NMe_2H$ [0.072 M, 298 K, 1,2–$F_2C_6H_4$ solvent] using complex **1** (2 mol%) as measured by H2 evolution with the addition of 0.2 eq. PPh_3 at 640 s.

Application of simple kinetic models to catalysis doped with 1 equivalent of NMe_2H

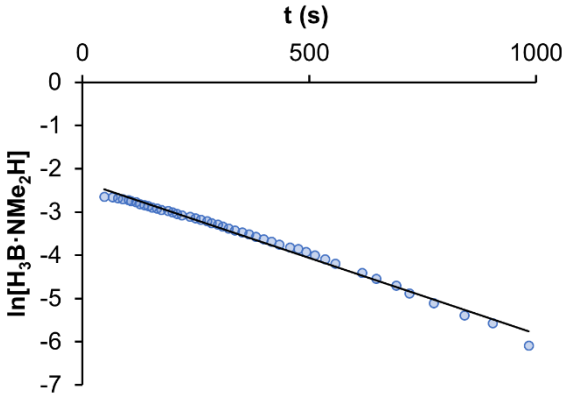


Figure S8. Plot of the natural logarithm of [$H_3B{\cdot}NMe_2H$] vs. time (post induction period) for the dehydrogenation of $H_3B{\cdot}NMe_2H$ [0.072 M, 298 K, 1,2–$F_2C_6H_4$ solvent] using complex **1** (2 mol%) + 1 eq. NMe_2H (2 mol%) as measured under hydrogen evolution conditions.

Calculation of maximum rates of dehydrogenation

For each data set of [$H_3B{\cdot}NMe_2H$] vs. time, Python 3 was run through the anaconda software distribution to fit the kinetic data to a polynomial.[1,2] A 6th order polynomial was determined by inspection to give the best fit around the point of maximum rate and fitted to the data using the SciPy packages.[3]

Maximum rate of catalysis versus [1]

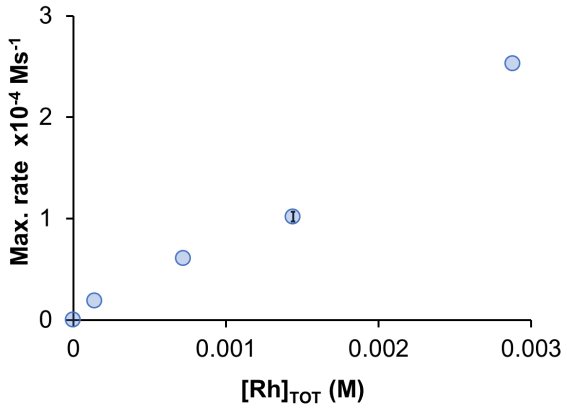


Figure S9. Maximum rate of catalysis versus [**1**] where starting [$H_3B{\cdot}NMe_2H$] = 0.072 M as measured by H_2 evolution.

Anion binding titration of $[H_2B(NMe_2H)_2][BArF_4]$ with $H_3B{\cdot}NMe_2H$

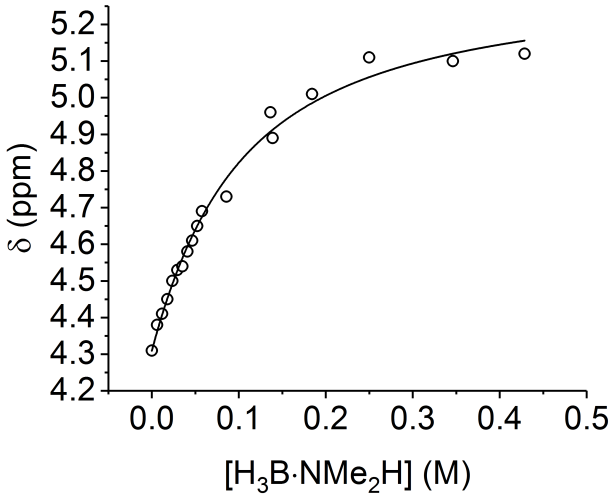


Figure S10. Anion binding titration of $[H_2B(NMe_2H)_2][BAr^F{}_4]$ (298 K, 30 mM, 1,2–$F_2C_6H_4$) with $H_3B{\cdot}NMe_2H$. Attempted 1:1 binding isotherm fit is indicated by line. Attempted calculation of corresponding association constant, using WinEQNMR2[4] monitoring the chemical shift data for the NH protons in $[H_2B(NMe_2H)_2][BAr^F{}_4]$, was unsuccessful due to large errors in fitting.

Crystallography

Crystallographic data were collected (ω-scans) on a Nonius Kappa-CCD with Mo-*Kα* radiation (*λ* = 0.71073 Å) for **2** and Oxford Diffraction/Agilent SuperNova diffractometer with Cu-*Kα* radiation (*λ* = 1.54184 Å) equipped with nitrogen gas Oxford Cryosystems Cryostream unit for **4**.[5] Raw frame data were reduced using CrysAlisPro, including unit cell determination and refinement, integration of intensities and associated correction, or the DENZO-SMN package.[6] The structures were solved using direct methods with SIR92[7] for **2** and SHELXT[8] for **4**; and then refined using full-matrix least squares refinement on all F^2 data using the CRYSTALS program suite[9,10] for **2**, and SHELXL[8] using the interface GUI OLEX2[11] for **4**. Some of the CF_3 groups in the $[BAr^F{}_4]^-$ anion refined to give highly prolate[12] displacement ellipsoids. For each structure a split site model was used and same distance restraints were applied to maintain a sensible geometry. Thermal similarity and vibrational restraints were also used to ensure the displacement ellipsoids behaved as expected. For **2**, the hydrogen atoms were located in the difference Fourier maps and refined independently using soft restraints.[10] Hydrogen atoms were refined in this way at intervals following inclusion in the refinement using a riding model. For **4**, the hydrogen atoms were set at geometric positions with exception of the hydride H atoms, which were located using the difference Fourier map, refined and the Rh–H bond lengths were restrained to refine similar lengths for the six independent molecules present in the asymmetric unit. In addition, 4 was refined as a 2-component twin, rotated by -179.9 degree around 0.00 0.45 -0.89 (reciprocal space) or -0.05 0.71 -0.71 (direct space) and BASF refined to 0.4203(7). Selected crystallographic data are summarized in the text and full details are given in the supplementary deposited CIF files (CCDC 1917326 and 1917160). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://optimized.ccdc.cam.ac.uk/data_request/cif.

Compound	2	4
Chemical formula	$C_{24}H_{51}BN_2O_2P_2Rh \cdot C_{32}H_{12}BF_{24}$	$C_{21}H_{40}NO_2P_2Rh$
Formula weight	1438.55	503.39
Temperature (K)	150	150
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
a (Å)	12.6670 (1)	9.2325(2)
b (Å)	18.7076 (2)	26.6707(4)
c (Å)	26.9666 (3)	33.1426(6)
α (deg)	90	68.569(2)
β (deg)	94.9435 (5)	89.805(2)
γ (deg)	90	88.2210(10)
V (Å^3)	6366.48 (11)	7592.7(3)
Z	4	12
ρ (calcd) (g cm^{-1})	1.501	1.321
μ (mm^{-1})	0.43	6.757
Reflections collected	22651	51748
Unique reflections	14142	51748
Restraints/parameters	924/1072	36/1555
R_{int}	0.029	0.0973
R_1 [$I > 2\sigma(I)$]	0.050	0.0592
wR_2 [$I > 2\sigma(I)$]	0.135	0.1893
GooF	0.92	1.086
Residual electron density (e Å^{-3})	1.17, −1.11	1.833, -2.100
CCDC no.	1917326	1917160

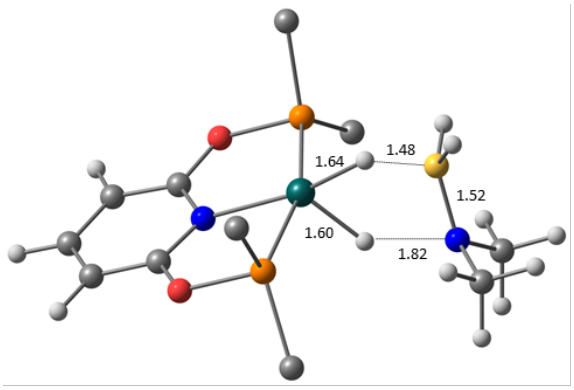
Table S1. Crystallographic data for complexes **2** and **4**.

Computational details

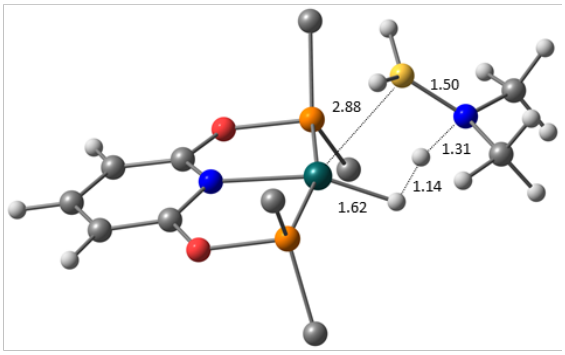
Calculations were run with Gaussian 09 Revision D.01.[13] Geometry optimisations were performed using the BP86 functional[14-15] with Rh and P centres described via Stuttgart RECPs and associated basis sets[16] (with additional d-orbital polarisation on P[17]) and 6-31G** basis sets[18-19] for all other atoms. All stationary points were fully characterized via analytical frequency calculations as either minima (no imaginary frequencies) or transition states (a single imaginary frequency). Transition states were further characterised through IRC calculations and subsequent geometry optimisations. SCF energies were re-computed at the BP86-optimised geometries with the def2-tzvp basis sets[20] on all atoms and including a correction for 2-hexanone solvent via the PCM approach[21] and dispersion using Grimme's D3 parameter set with Becke-Johnson damping.[22] 2-hexanone (ε = 14.14) was employed as solvent in the absence of parameters for 1,2-difluorobenzene (ε = 13.81).

Alternative Reaction Pathways from Cationic [Rh(PONOP)(DMAB]$^+$, 3.

Two transition states were located for concerted processes involving activation of both the B-H and the N-H bonds, **TS(3-1)$_{concerted1}$** and **TS(3-1)$_{concerted2}$**. Both were shown to lead directly to the formation of **1** and Me_2NBH_2 (Scheme S1).



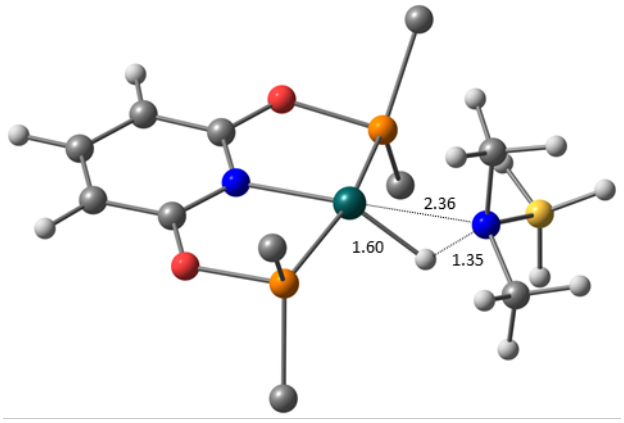
+28.5
TS(3-1)$_{concerted1}$



+32.3
TS(3-1)$_{concerted2}$

Scheme S1. Transition states for dehydrogenation from [Rh(PONOP) (DMAB)]$^+$ via concerted processes. Free energies (kcal/mol) are quoted relative to **3** set to 0.0 kcal/mol. The free energy change for **3** → **1** + free DMAB is +0.1 kcal/mol. Ball and stick representations have the ^{t}Bu Me groups removed for clarity and all distances are given in Å.

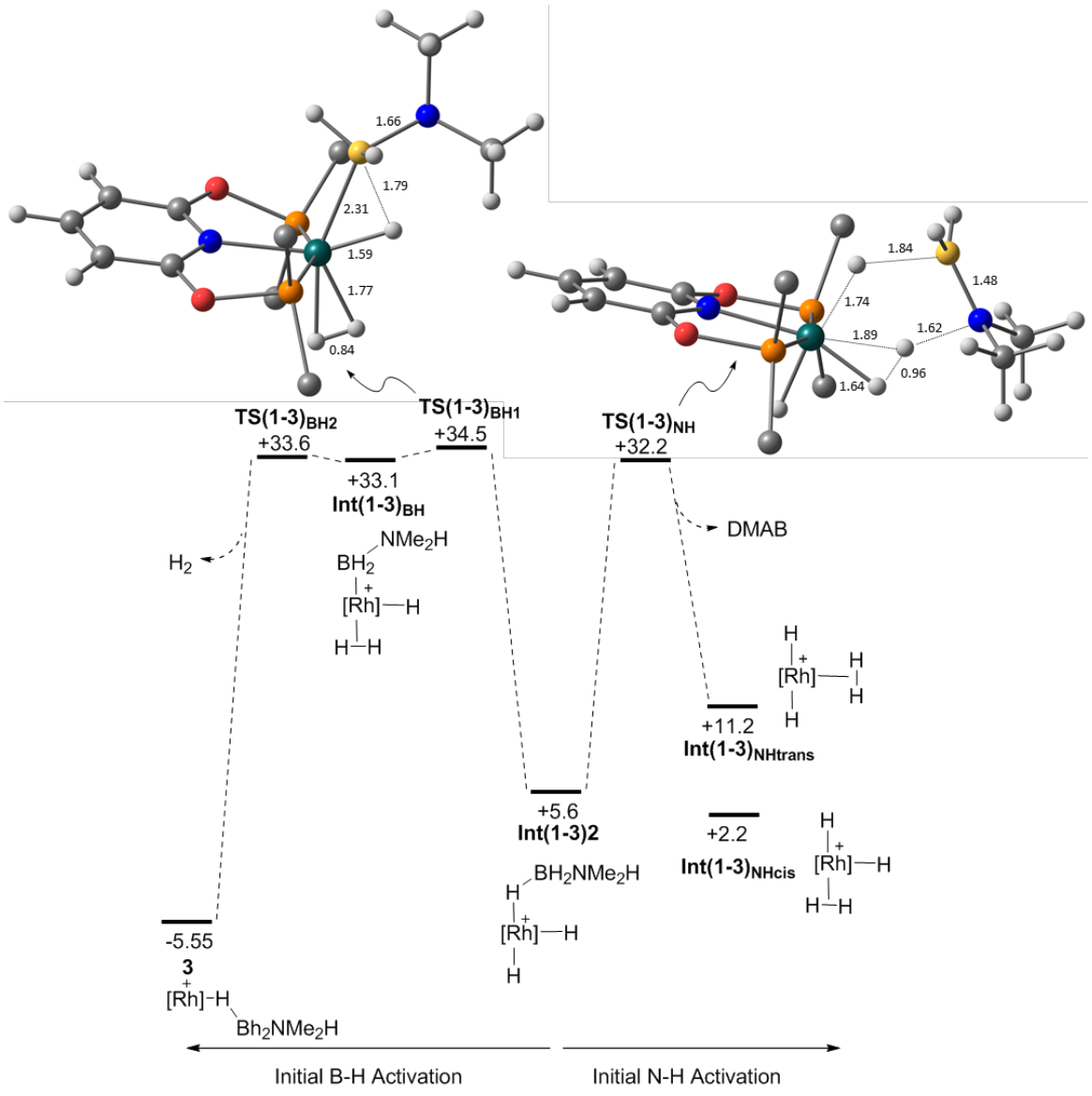
No intermediates corresponding to initial B-H activation could be located, with all attempts reverting to **3** upon optimisation. A transition for initial N-H activation, **TS(3-1)$_{NH}$** was located at +50.0 kcal/mol (Scheme S2). IRCs showed this links to **Int(3-1)$_{NH1}$** at 26.0 kcal/mol, a C-H σ-complex bound through a Me C-H bond, and [Rh(PONOP)(H)(NMe_2BH_3)]$^+$ at +23.5 kcal/mol, **Int(3-1)$_{NH2}$** (Scheme S2).



+50.0
TS(3-1)$_{NH}$

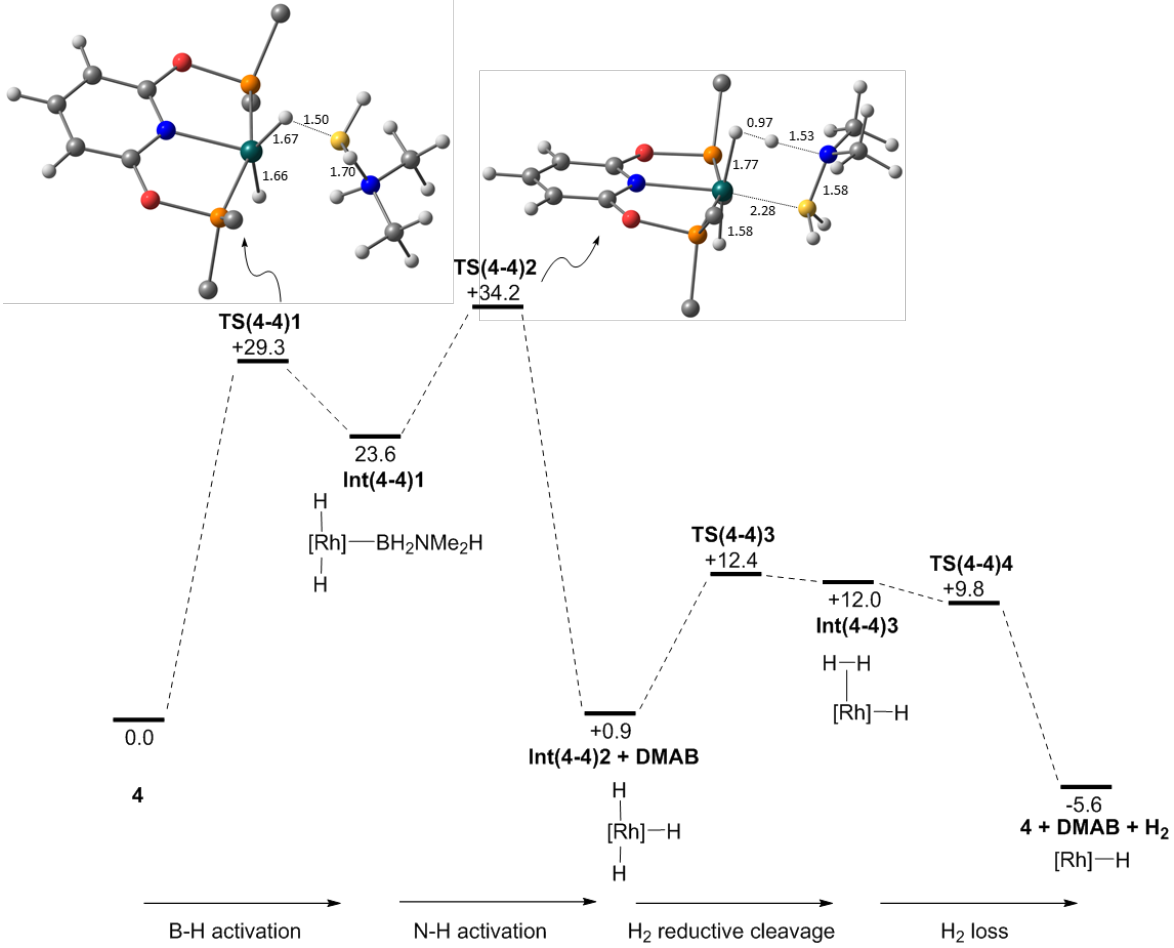
Scheme S2. Transition state for initial N-H activation from [Rh(PONOP)(DMAB)]+. Free energy (kcal/mol) is quoted relative to 3 set to 0.0 kcal/mol. Ball and stick representations have the ^{t}Bu Me groups removed for clarity and all distances are given in Å.

Dehydrogenation was also assessed from **Int(1-3)2**, $[Rh(PONOP)(H)_2(H_3BNMe_2H)]^+$ (Scheme S3, centre). B-H activation (left) led to $[Rh(PONOP)(\eta^2\text{-}H_2)(H)(H_2BNMe_2H)]^+$, **Int(1-3)$_{BH1}$**, but upon H_2 loss B-H reductive coupling occurred to return **3**. N-H activation (right) resulted in a concerted process with expulsion of H_2BNMe_2 and formation of trans-$[Rh(PONOP)(\eta^2\text{-}H_2)(H)_2]^+$, **Int(1-3)$_{NHtrans}$**.



Scheme S3. Dehydrogenation profiles from $[Rh(PONOP)(H)_2(H_3BNMe_2H)]^+$, **Int(1-3)2** (left: B-H activation; right: N-H activation). Free energies (kcal/mol) are quoted relative to **3** set to 0.0 kcal/mol. Ball and stick representations have the ^{t}Bu Me groups removed for clarity and all distances are given in Å. [Rh] = (PONOP)Rh.

Alternative Reaction Pathways from Neutral [Rh(PONOP)(H)], 4.



Scheme S4. Dehydrogenation from [Rh(PONOP) (H)], **4**, via initial B-H activation. [Rh] = (PONOP)Rh. Energies are quoted relative to **4** + free $H_3B{\cdot}NMe_2H$ set to 0.0 kcal/mol. Ball and stick representations have the ^{t}Bu Me groups removed for clarity and all distances are given in Å. Alternative pathways via formation of a cis isomer of **Int(4-4)1** were also assessed and proved higher in energy.

Computed Cartesian Cooordinates (Å) and Energies (Hartrees) for all stationary points.

In the following SCF(Corr) refers to the SCF energy recomputed with the def2-tzvp basis sets including corrections for dispersion (BJD3) and solvation (2-hexanone). The two lowest frequencies are reported for each structure to signal a minimum (no negative modes) or a TS (one negative modes)

Dihydrogen

SCF = -1.17646504316
H(0 K)= -1.166553
H(298 K)= -1.164193
G(298 K)= -1.178061
SCF (Corr) = -1.17782936552
Low Freq. = 4350.8276cm-1, cm-1

2
H 0.00000 0.00000 0.37545
H 0.00000 0.00000 -0.37545

$H_3B.NMe_2H$

SCF = -161.823572613
H(0 K)= -161.699830
H(298 K)= -161.693820
G(298 K)= -161.727716
SCF (Corr) = -161.905007688
Low Freq. = 185.5743cm^{-1}, 243.0585cm^{-1}

14
N -0.00295 -0.00000 -0.34561
B -1.58655 -0.00033 0.11879
H -2.06051 1.02018 -0.35783
H -1.55880 -0.00033 1.34154
H -2.06009 -1.02105 -0.35766
C 0.70551 1.23194 0.10243
H -0.01312 0.00000 -1.37448
C 0.70605 -1.23164 0.10242
H 1.75832 -1.23646 -0.23192
H 0.65956 -1.26474 1.20103
H 0.17142 -2.10456 -0.29681
H 1.75779 1.23719 -0.23186
H 0.17054 2.10462 -0.29683
H 0.65896 1.26503 1.20104

H_2BNMe_2

SCF = -160.644812913
H(0 K)= -160.542658
H(298 K)= -160.537208
G(298 K)= -160.569957
SCF (Corr) = -160.713428510
Low Freq. = 210.4409cm-1, 216.7701cm-1

12
C 1.22143 -0.65525 0.00000
N 0.00000 0.15126 -0.00003
C -1.22143 -0.65525 0.00000
B -0.00000 1.55271 0.00009
H 1.05686 2.13381 -0.00014
H -1.05687 2.13381 -0.00015
H -1.26482 -1.30875 -0.89312
H -1.26447 -1.30919 0.89282
H -2.10056 0.00443 0.00033
H 1.26482 -1.30874 -0.89312
H 2.10056 0.00444 0.00033
H 1.26447 -1.30918 0.89281

$[Me_2HNBH_2NHMe_2]^+$

SCF = -296.227493166
H(0 K)= -296.015344
H(298 K)= -296.005335
G(298 K)= -296.049496
SCF (Corr) = -296.424224963
Low Freq. = 70.0970cm-1, 93.6370cm-1

23
0.0000000000
N -1.32023 0.10634 -0.22792
B 0.00004 -0.79905 -0.00003
N 1.32027 0.10636 0.22795
H 0.18322 -1.44059 -1.00916
H -0.18312 -1.44084 1.00895
H -1.21350 0.66402 -1.08931
C -1.64339 1.05226 0.89333
C -2.47982 -0.82770 -0.47947
C 1.64325 1.05231 -0.89333
H 1.21355 0.66402 1.08935
C 2.47993 -0.82765 0.47948
H -3.38910 -0.24357 -0.68589
H -2.23641 -1.47229 -1.33468
H -2.62411 -1.44842 0.41569
H -2.59457 1.56953 0.69566
H -1.72324 0.47082 1.82322
H -0.84733 1.80594 0.99349
H 3.38932 -0.24344 0.68514
H 2.23683 -1.47173 1.33516
H 2.62374 -1.44888 -0.41540
H 2.59472 1.56921 -0.69607
H 1.72242 0.47096 -1.82333
H 0.84741 1.80631 -0.99298

H_3BNMe_3

SCF = -201.129588460
H(0 K)= -200.978712
H(298 K)= -200.971659
G(298 K)= -201.007875
SCF (Corr) = -201.226873730
Low Freq. = 191.0001cm-1, 278.4538cm-1

17
C -0.49327 1.21981 -0.70289
N 0.00467 0.00000 0.00046
C -0.49329 -1.21812 -0.70580
B 1.66367 -0.00001 0.00187
H 1.98509 1.02069 0.59262
H 1.98582 0.00140 -1.17721
H 1.98507 -1.02215 0.59015
C -0.49560 -0.00168 1.40675
H -1.59824 -1.23998 -0.71952
H -0.10064 -1.20902 -1.73239
H -0.10236 -2.10436 -0.18630
H -1.59822 1.24172 -0.71657

```
H  -0.10234  2.10480 -0.18128
H  -0.10061  1.21315 -1.72950
H  -1.60086 -0.00170  1.43020
H  -0.10539 -0.89582  1.91335
H  -0.10539  0.89125  1.91548
```

$NHMe_2$

```
SCF  =          -135.162935951
H(0 K)=         -135.072932
H(298 K)=       -135.068506
G(298 K)=       -135.098406
SCF (Corr) =    -135.223085470
Low Freq. = 244.6655cm-1, 265.6521cm-1

10
C  -1.21504 -0.22381  0.02066
N   0.00000  0.57276 -0.15198
C   1.21513 -0.22394  0.02059
H  -0.00001  1.32901  0.54062
H  -1.27371 -0.78672  0.98349
H  -1.28237 -0.96724 -0.79457
H   1.27396 -0.78553  0.98412
H   1.28177 -0.96796 -0.79409
H   2.10211  0.42784 -0.05201
H  -2.10224  0.42775 -0.05122
```

$[NH_2Me_2]^+$

```
SCF  =          -135.534960093
H(0 K)=         -135.429636
H(298 K)=       -135.425081
G(298 K)=       -135.455417
SCF (Corr) =    -135.675594180
Low Freq. = 196.2712cm-1, 261.0534cm-1

11
C   1.27255 -0.27757 -0.00000
N   0.00008  0.54388 -0.00000
C  -1.27266 -0.27757  0.00001
H  -0.00003  1.16824 -0.82438
H   1.28122 -0.90362 -0.90245
H   1.27923 -0.90665  0.90035
H  -1.27949 -0.90609 -0.90073
H  -1.28093 -0.90406  0.90214
H  -2.13453  0.40384 -0.00140
H   2.13459  0.40365  0.00215
H   0.00007  1.16834  0.82429
```

$[Rh(PONOP)(H_2)]^+$, 1

```
SCF  =          -1153.88317208
H(0 K)=         -1153.312833
H(298 K)=       -1153.276863
G(298 K)=       -1153.377241
SCF (Corr) =    -1824.15172136
Low Freq. = 23.7718cm-1, 31.9989cm-1

68
C  -0.00006  4.22566 -0.22320
C   1.21797  3.53617 -0.18141
C   1.18276  2.13725 -0.09564
N  -0.00001  1.44128 -0.05219
C  -1.18281  2.13722 -0.09546
C  -1.21806  3.53613 -0.18127
O   2.34607  1.45595 -0.05151
P   2.28446 -0.31333  0.02537
C   3.21262 -0.74757 -1.59385
C   4.68946 -0.30797 -1.60753
Rh  0.00001 -0.62092  0.06101
P  -2.28447 -0.31339  0.02544
C  -3.21220 -0.74749 -1.59410
C  -3.09239 -2.27721 -1.79381
O  -2.34611  1.45589 -0.05125
H  -0.00007  5.31753 -0.29063
C  -3.28860 -0.56732  1.63897
C  -3.66021 -2.06342  1.74170
C  -2.31200 -0.19035  2.77935
C  -4.54454  0.32458  1.72623
C   3.28820 -0.56717  1.63920
C   4.54398  0.32491  1.72681
C   2.31127 -0.19040  2.77936
C   3.66003 -2.06322  1.74197
C   3.09268 -2.27728 -1.79356
C   2.43469 -0.02455 -2.71910
C  -4.68899 -0.30772 -1.60823
C  -2.43386 -0.02452 -2.71910
H   2.84431 -0.34557 -3.69338
H   1.36072 -0.28133 -2.70122
H   2.53828  1.07036 -2.65452
H   3.55561 -2.54127 -2.76111
H   3.61399 -2.85446 -1.01342
H   2.03989 -2.60479 -1.82866
H   5.09578 -0.47286 -2.62174
H   4.80900  0.76178 -1.37237
H   5.30737 -0.89776 -0.91204
H   2.81077 -0.36923  3.74853
H   2.02929  0.87527  2.74302
H   1.38883 -0.79515  2.74866
H   4.98049  0.20902  2.73516
H   5.31908  0.04431  0.99973
H   4.30112  1.38980  1.58781
H   4.08811 -2.25313  2.74231
H   2.78310 -2.72507  1.63163
H  -1.38947 -0.79498  2.74890
H  -2.81168 -0.36923  3.74841
H   4.42075 -2.35757  1.00087
H  -2.03017  0.87535  2.74304
H  -4.08846 -2.25337  2.74196
H  -4.42075 -2.35792  1.00046
H  -2.78317 -2.72513  1.63154
H  -4.98124  0.20870  2.73450
H  -4.30180  1.38949  1.58720
H  -5.31944  0.04380  0.99900
H  -5.09502 -0.47256 -2.62256
H  -5.30719 -0.89742 -0.91294
H  -4.80849  0.76205 -1.37313
H  -2.84324 -0.34547 -3.69349
H  -2.53735  1.07041 -2.65452
H  -1.35992 -0.28142 -2.70089
H  -3.55510 -2.54112 -2.76149
H  -2.03964 -2.60486 -1.82861
H  -3.61401 -2.85433 -1.01382
H   0.00027 -2.15763  0.61014
H  -2.18209  4.04553 -0.21314
H   2.18198  4.04560 -0.21336
H  -0.00009 -2.19107 -0.36997
```

$[Rh(PONOP)(H_3BNMe_3)]^+$, 2

```
SCF  =          -1353.83878916
H(0 K)=         -1353.130289
H(298 K)=       -1353.086988
G(298 K)=       -1353.203033
SCF (Corr) =    -2024.20916293
Low Freq. = 13.4127cm-1, 25.1685cm-1
```

```
83
C   1.17583 -2.68798 -0.29139
C   1.21629 -4.08384 -0.41779
C   0.00613 -4.78179 -0.48386
C  -1.20613 -4.08750 -0.41655
C  -1.16972 -2.69159 -0.29007
N   0.00204 -1.97640 -0.23419
O  -2.33931 -2.02668 -0.22492
P  -2.28236 -0.28010  0.01411
C  -3.45455  0.17088 -1.45041
C  -3.95830  1.61824 -1.26700
Rh -0.00129  0.07818 -0.05221
B   0.01452  2.51095 -0.77660
N  -0.01074  4.00000 -0.06356
C  -1.26871  4.23239  0.71803
O   2.34345 -2.01969 -0.22790
P   2.28331 -0.27351  0.01390
C   3.46071  0.18243 -1.44594
C   4.64251 -0.79739 -1.61370
C  -3.14245 -0.21023  1.73895
C  -2.30049 -1.12648  2.65770
C  -3.04022  1.24216  2.25346
C  -4.60858 -0.68324  1.73989
C   3.14143 -0.20530  1.73952
C   2.29348 -1.11568  2.65862
C   4.60474 -0.68706  1.74247
C   3.04637  1.24831  2.25168
C  -2.56092  0.07207 -2.71107
C  -4.64771 -0.79627 -1.60912
C   2.56794  0.10713 -2.70876
C   3.98431  1.62106 -1.24741
C   0.05304  5.00852 -1.17898
H   0.00772 -5.87089 -0.58385
H  -3.15705  0.36734 -3.59387
H  -1.67913  0.72945 -2.65054
H  -2.21154 -0.96071 -2.87763
H  -4.52292  1.91687 -2.16875
H  -4.64125  1.71778 -0.40694
H  -3.12573  2.33168 -1.14982
H  -5.16418 -0.54953 -2.55469
H  -4.32130 -1.84540 -1.67016
H  -5.38565 -0.70519 -0.79985
H  -2.65916 -1.01559  3.69705
H  -2.39782 -2.18796  2.37966
H  -1.23130 -0.85183  2.63061
H  -4.96131 -0.73870  2.78608
H  -5.27665  0.01444  1.20987
H  -4.72023 -1.68657  1.29919
H  -3.48494  1.29847  3.26348
H  -1.98523  1.55537  2.33266
H   1.22611 -0.83408  2.63111
H   2.65283 -1.00686  3.69796
H  -3.58060  1.96079  1.61503
H   2.38387 -2.17796  2.38110
H   3.48754  1.30287  3.26335
H   3.59332  1.96306  1.61467
H   1.99357  1.56887  2.32587
H   4.95656 -0.74184  2.78902
H   4.71043 -1.69226  1.30454
H   5.27743  0.00504  1.21100
H   5.16859 -0.54026 -2.55117
H   5.37584 -0.73062 -0.79789
H   4.30318 -1.84091 -1.69560
H   3.17067  0.39812 -3.58851
H   2.20159 -0.91854 -2.88293
H   1.69738  0.77883 -2.64575
H   4.54925  1.92209 -2.14820
H   3.16336  2.34586 -1.11799
H   4.67257  1.70072 -0.38960
H  -0.01235  1.76078  0.32460
H   2.18625 -4.58129 -0.46035
H  -2.17460 -4.58791 -0.45814
H   1.05385  2.47580 -1.38940
H  -0.98564  2.46485 -1.45200
C   1.16625  4.21170  0.84048
H   0.02788  6.02813 -0.76010
H   0.98243  4.85467 -1.74415
H  -0.80523  4.85273 -1.84698
H  -1.27208  5.25264  1.13645
H  -2.13099  4.10178  0.04967
H  -1.32487  3.49694  1.53184
H   1.15895  5.24008  1.23841
H   1.11353  3.49290  1.66946
H   2.08847  4.03967  0.26842
```

[Rh(PONOP)(H_3BNMe_2H)]$^+$, 3

```
SCF  =          -1314.54155344
H(0 K)=         -1313.860279
H(298 K)=       -1313.818258
G(298 K)=       -1313.931750
SCF (Corr) =    -1984.89437408
Low Freq. = 22.8036cm-1, 25.7374cm-1

80
C   0.74220 -4.08359 -0.12195
C  -0.53507 -4.65430 -0.16194
C  -1.66852 -3.83465 -0.15473
C  -1.48720 -2.44492 -0.11370
N  -0.24694 -1.85539 -0.08960
C   0.84519 -2.68692 -0.08166
O  -2.58141 -1.65672 -0.09532
P  -2.34643  0.08650  0.00812
C  -3.24937  0.41833  1.67187
C  -3.04511  1.90809  2.03019
Rh -0.04191  0.19796 -0.00139
P   2.18454 -0.37873  0.02748
C   3.18821 -0.21540  1.66208
C   4.58274 -0.86902  1.63232
O   2.07769 -2.13510 -0.02823
C  -3.38316  0.56685 -1.54656
C  -2.43065  0.35025 -2.74659
C  -4.63347 -0.32074 -1.73013
C  -3.78613  2.05506 -1.45962
C   3.24388 -0.17085 -1.57348
C   2.25030 -0.42628 -2.73322
C   3.76613  1.27823 -1.65210
C   4.41327 -1.17207 -1.68333
C   3.30298  1.28921  1.99243
C   2.31069 -0.89941  2.73752
C  -4.74881  0.06323  1.65046
C  -2.51901 -0.45990  2.71523
H  -0.64700 -5.74174 -0.19284
H  -2.96651  0.61194 -3.67720
H  -1.52946  0.97997 -2.67598
H  -2.11186 -0.70250 -2.83171
H  -4.25036  2.35009 -2.41808
H  -4.53094  2.24011 -0.66824
H  -2.91932  2.71549 -1.29368
H  -5.10823 -0.04778 -2.69016
H  -4.37742 -1.39005 -1.77361
H  -5.38332 -0.17363 -0.93992
H  -2.90845 -0.21580  3.72011
H  -2.69035 -1.53414  2.53953
H  -1.43079 -0.27281  2.70946
```

```
H  -5.14897  0.15733  2.67646
H  -5.33254  0.74496  1.01149
H  -4.92447 -0.97298  1.31967
H  -3.48489  2.09434  3.02665
H  -1.97539  2.17015  2.07826
H   1.28065 -0.50118  2.73275
H   2.75250 -0.71161  3.73282
H  -3.53731  2.58989  1.31869
H   2.26348 -1.98985  2.58937
H   3.80440  1.40923  2.96962
H   3.90728  1.84327  1.25262
H   2.30517  1.75388  2.07714
H   4.99514 -0.87340  2.65774
H   4.54234 -1.91387  1.28644
H   5.29317 -0.31308  0.99995
H   4.83181 -1.10741 -2.70418
H   5.23043 -0.95560 -0.98063
H   4.07911 -2.20881 -1.52479
H   2.77076 -0.25666 -3.69349
H   1.88596 -1.46685 -2.73264
H   1.37569  0.24374 -2.68535
H   4.28162  1.42563 -2.61823
H   2.93945  2.01052 -1.62031
H   4.49446  1.51201 -0.85752
H   0.00314  1.78867  0.62080
H   1.65427 -4.68215 -0.11674
H  -2.68352 -4.23407 -0.17471
B  -0.01025  2.58142 -0.44002
N   1.18444  3.61797 -0.05074
H   0.21815  2.13472 -1.54778
H  -1.03282  3.22684 -0.35614
C   1.38757  4.62035 -1.14814
C   0.94461  4.31171  1.25620
H   2.05769  3.07617  0.04264
H   2.17919  5.33613 -0.87484
H   1.65359  4.09033 -2.07274
H   0.43829  5.15332 -1.30303
H   1.78587  4.97943  1.50096
H   0.01682  4.89477  1.16750
H   0.81861  3.55824  2.04637
```

[Rh(PONOP)(H)], 4

```
SCF  =          -1153.46555258
H(0 K)=         -1152.904562
H(298 K)=       -1152.869076
G(298 K)=       -1152.968545
SCF (Corr) =    -1823.69571182
Low Freq. = 26.2152cm-1, 29.1469cm-1

67
C  -1.17777  2.14531 -0.06928
N  -0.00006  1.45151 -0.02993
C   1.17759  2.14543 -0.06913
C   1.21707  3.54744 -0.14494
C  -0.00019  4.24181 -0.18154
C  -1.21739  3.54733 -0.14503
Rh  0.00001 -0.63960  0.06868
P  -2.22529 -0.34260  0.02735
C  -3.29275 -0.59340  1.61315
C  -2.32993 -0.25168  2.77539
O   2.34031  1.45242 -0.03150
P   2.22526 -0.34241  0.02733
C   3.29260 -0.59364  1.61315
C   2.32966 -0.25254  2.77547
O  -2.34044  1.45219 -0.03200
C   3.19500 -0.73413 -1.59196
C   4.66587 -0.28080 -1.61294
C   3.08544 -2.25982 -1.82022
C   2.40879 -0.00710 -2.70787
C  -3.19475 -0.73461 -1.59206
C  -3.08482 -2.26025 -1.82049
C  -4.66570 -0.28152 -1.61322
C  -2.40858 -0.00734 -2.70783
C  -4.53826  0.30992  1.70867
C  -3.68015 -2.08576  1.69557
C   3.68027 -2.08596  1.69495
C   4.53796  0.30986  1.70911
H  -0.00024  5.33462 -0.24097
H  -2.83132 -0.46736  3.73804
H  -1.40011 -0.84314  2.71293
H  -2.05278  0.81603  2.76930
H  -4.11566 -2.29399  2.69067
H  -4.43714 -2.36173  0.94217
H  -2.80217 -2.74278  1.56895
H  -4.98266  0.20086  2.71601
H  -4.27759  1.37065  1.56700
H  -5.31521  0.04332  0.97691
H  -2.80677 -0.31746 -3.69200
H  -2.50563  1.08765 -2.62785
H  -1.33533 -0.26607 -2.66524
H  -5.07606 -0.42881 -2.63027
H  -5.29284 -0.87037 -0.92368
H  -4.77157  0.78661 -1.36198
H  -3.49713 -2.50616 -2.81715
H  -2.03351 -2.59191 -1.78538
H   1.33563 -0.26622 -2.66554
H   2.80728 -0.31701 -3.69198
H  -3.65296 -2.84090 -1.07521
H   2.50543  1.08792 -2.62781
H   3.49808 -2.50579 -2.81673
H   3.65349 -2.84022 -1.07466
H   2.03418 -2.59167 -1.78536
H   5.07623 -0.42762 -2.63005
H   4.77156  0.78724 -1.36126
H   5.29312 -0.86982 -0.92365
H   4.98236  0.20037  2.71640
H   5.31496  0.04373  0.97723
H   4.27713  1.37062  1.56796
H   2.83107 -0.46838  3.73807
H   2.05223  0.81510  2.76969
H   1.39999 -0.84422  2.71278
H   4.11639 -2.29443  2.68973
H   2.80232 -2.74309  1.56865
H   4.43686 -2.36162  0.94103
H   0.00040 -2.24721  0.13359
H   2.18241  4.05580 -0.17371
H  -2.18278  4.05559 -0.17381
```

[Rh(PONOP)]$^{+}$

```
SCF  =          -1152.65482672
H(0 K)=         -1152.100117
H(298 K)=       -1152.064887
G(298 K)=       -1152.164525
SCF (Corr) =    -1822.92872472
Low Freq. = 20.3394cm-1, 31.2002cm-1

66
C  -1.21179  3.49607 -0.41308
C   0.00002  4.18894 -0.50320
C   1.21182  3.49606 -0.41308
C   1.18251  2.10794 -0.23155
N   0.00000  1.40158 -0.13859
C  -1.18249  2.10795 -0.23155
O   2.35555  1.44576 -0.14135
```

```
P    2.28202 -0.30042  0.05136
C    3.30010 -0.47236  1.66517
C    3.62693 -1.96922  1.86659
Rh  -0.00001 -0.57518  0.10612
P   -2.28202 -0.30039  0.05136
C   -3.30010 -0.47234  1.66517
C   -4.58253  0.38547  1.67292
O   -2.35555  1.44579 -0.14135
C    3.17752 -0.89788 -1.53349
C    2.48301 -0.16756 -2.70686
C    4.69272 -0.62552 -1.56700
C    2.88578 -2.41569 -1.63167
C   -3.17753 -0.89787 -1.53348
C   -2.48281 -0.16782 -2.70690
C   -2.88605 -2.41574 -1.63147
C   -4.69268 -0.62526 -1.56715
C   -3.62702 -1.96919  1.86651
C   -2.35296  0.01157  2.78994
C    4.58259  0.38537  1.67285
C    2.35301  0.01167  2.78993
H    0.00003  5.27305 -0.64562
H    2.85611 -0.59001 -3.65686
H    1.38739 -0.30427 -2.68034
H    2.70334  0.91178 -2.70677
H    3.30033 -2.79841 -2.58148
H    3.34661 -2.99535 -0.81548
H    1.79986 -2.62166 -1.64020
H    5.08251 -0.91876 -2.55864
H    4.92638  0.44160 -1.42275
H    5.24282 -1.21483 -0.81617
H    2.86142 -0.11439  3.76276
H    2.09958  1.07947  2.68194
H    1.41156 -0.56407  2.81424
H    5.03144  0.33015  2.68111
H    5.33824  0.03147  0.95732
H    4.36724  1.44451  1.46145
H    4.07713 -2.10385  2.86618
H    2.72520 -2.60658  1.82892
H   -1.41155 -0.56424  2.81421
H   -2.86136 -0.11451  3.76278
H    4.35408 -2.34456  1.12828
H   -2.09946  1.07936  2.68200
H   -4.07727 -2.10384  2.86608
H   -4.35416 -2.34445  1.12815
H   -2.72532 -2.60660  1.82884
H   -5.03135  0.33026  2.68120
H   -4.36713  1.44460  1.46153
H   -5.33823  0.03164  0.95741
H   -5.08246 -0.91859 -2.55876
H   -5.24293 -1.21436 -0.81626
H   -4.92617  0.44192 -1.42308
H   -2.85591 -0.59033 -3.65688
H   -2.70296  0.91156 -2.70697
H   -1.38721 -0.30469 -2.68028
H   -3.30063 -2.79852 -2.58124
H   -1.80017 -2.62190 -1.63992
H   -3.34701 -2.99521 -0.81521
H   -2.18069  3.99352 -0.47880
H    2.18072  3.99350 -0.47880
```

H_2/DMAB Exchange in 1

TS(1-3)1

```
SCF  =          -1153.88178801
H(0 K)=         -1153.312249
H(298 K)=       -1153.276644
G(298 K)=       -1153.376107
SCF (Corr) =    -1824.14866160
Low Freq. = -155.4258cm-1, 25.2898cm-1

68
C  -0.00000  4.23576 -0.23625
C   1.22173  3.54991 -0.19536
C   1.18488  2.15078 -0.10778
N  -0.00000  1.46571 -0.05869
C  -1.18488  2.15078 -0.10779
C  -1.22173  3.54991 -0.19537
O   2.34270  1.45646 -0.07313
P   2.28402 -0.32125  0.01312
C   3.22799 -0.75908 -1.59299
C   4.69902 -0.29846 -1.58720
Rh  0.00000 -0.63399  0.08117
P  -2.28402 -0.32125  0.01312
C  -3.22799 -0.75909 -1.59298
C  -3.13268 -2.29197 -1.77980
O  -2.34270  1.45646 -0.07314
H  -0.00000  5.32768 -0.30528
C  -3.26427 -0.56066  1.64294
C  -3.64772 -2.05326  1.75320
C  -2.25695 -0.19577  2.76103
C  -4.50727  0.34527  1.75616
C   3.26427 -0.56066  1.64293
C   4.50727  0.34528  1.75616
C   2.25695 -0.19579  2.76104
C   3.64774 -2.05326  1.75318
C   3.13267 -2.29196 -1.77981
C   2.45801 -0.05279 -2.73413
C  -4.69902 -0.29846 -1.58720
C  -2.45801 -0.05281 -2.73413
H   2.89027 -0.37223 -3.69901
H   1.38808 -0.32391 -2.73625
H   2.54495  1.04369 -2.67274
H   3.59869 -2.55465 -2.74615
H   3.66568 -2.85250 -0.99576
H   2.08697 -2.64097 -1.80757
H   5.12354 -0.46802 -2.59299
H   4.79939  0.77519 -1.36118
H   5.31338 -0.87272 -0.87584
H   2.73612 -0.36343  3.74239
H   1.95879  0.86550  2.71698
H   1.34850 -0.82227  2.71504
H   4.93004  0.22726  2.77016
H   5.29627  0.07803  1.03888
H   4.25465  1.40816  1.61959
H   4.05186 -2.23984  2.76412
H   2.78022 -2.72215  1.61723
H  -1.34850 -0.82224  2.71504
H  -2.73612 -0.36340  3.74239
H   4.43111 -2.33722  1.03192
H  -1.95880  0.86552  2.71696
H  -4.05184 -2.23984  2.76414
H  -4.43109 -2.33723  1.03194
H  -2.78019 -2.72214  1.61725
H  -4.93004  0.22726  2.77016
H  -4.25466  1.40815  1.61958
H  -5.29628  0.07801  1.03889
H  -5.12354 -0.46802 -2.59300
H  -5.31339 -0.87271 -0.87584
H  -4.79938  0.77520 -1.36119
H  -2.89027 -0.37225 -3.69901
H  -2.54493  1.04368 -2.67275
H  -1.38807 -0.32393 -2.73624
H  -3.59870 -2.55466 -2.74614
H  -2.08698 -2.64099 -1.80755
H  -3.66570 -2.85250 -0.99575
```

H 0.00000 -2.12185 0.57898
H -2.18305 4.06413 -0.23226
H 2.18304 4.06413 -0.23226
H -0.00000 -1.80836 -0.90724

Int(1-3)1

SCF =   -1153.88275501
H(0 K)=   -1153.312161
H(298 K)=   -1153.276203
G(298 K)=   -1153.376347
SCF (Corr) =   -1824.15168194
Low Freq. = 23.5197cm-1, 35.9190cm-1

68
C -0.00000 4.25089 -0.14769
C -1.22170 3.56314 -0.12744
C -1.18146 2.16167 -0.09096
N 0.00000 1.47808 -0.08379
C 1.18146 2.16167 -0.09096
C 1.22169 3.56315 -0.12744
O -2.34024 1.45937 -0.06380
P -2.28076 -0.31396 0.03908
C -3.28404 -0.59072 1.64244
C -4.76344 -0.17660 1.50723
Rh 0.00000 -0.64066 -0.00213
P 2.28076 -0.31395 0.03908
C 3.28404 -0.59072 1.64244
C 3.15898 -2.09023 2.00234
O 2.34024 1.45937 -0.06380
H -0.00000 5.34457 -0.17460
C 3.19137 -0.74087 -1.59142
C 3.59752 -2.23047 -1.54214
C 2.11416 -0.53272 -2.68502
C 4.40526 0.16335 -1.88434
C -3.19137 -0.74088 -1.59141
C -4.40532 0.16329 -1.88429
C -2.11419 -0.53264 -2.68502
C -3.59744 -2.23050 -1.54218
C -3.15894 -2.09022 2.00237
C -2.60001 0.26376 2.73506
C 4.76343 -0.17655 1.50726
C 2.59997 0.26371 2.73508
H -3.09346 0.05497 3.70072
H -1.53068 0.01566 2.84751
H -2.69285 1.34276 2.53425
H -3.65170 -2.25783 2.97656
H -3.65186 -2.74658 1.26798
H -2.10664 -2.40542 2.09705
H -5.24350 -0.26065 2.49855
H -4.87463 0.86694 1.17155
H -5.32041 -0.83425 0.82119
H -2.53667 -0.80610 -3.66872
H -1.78448 0.51831 -2.74931
H -1.23272 -1.18017 -2.51544
H -4.78116 -0.07573 -2.89558
H -5.23418 0.00255 -1.17993
H -4.13552 1.23062 -1.86877
H -3.95592 -2.53236 -2.54252
H -2.75008 -2.88830 -1.28204
H 1.23273 -1.18030 -2.51540
H 2.53664 -0.80619 -3.66871
H -4.41979 -2.41501 -0.83238
H 1.78439 0.51820 -2.74932
H 3.95600 -2.53234 -2.54248
H 4.41989 -2.41492 -0.83235
H 2.75020 -2.88830 -1.28197
H 4.78109 -0.07566 -2.89565
H 4.13541 1.23067 -1.86883
H 5.23416 0.00267 -1.18001
H 5.24347 -0.26060 2.49859
H 5.32043 -0.83418 0.82123
H 4.87459 0.86700 1.17160
H 3.09342 0.05491 3.70074
H 2.69278 1.34271 2.53430
H 1.53065 0.01558 2.84750
H 3.65174 -2.25785 2.97652
H 2.10670 -2.40546 2.09700
H 3.65193 -2.74656 1.26792
H 0.00000 -2.21706 0.03489
H 2.18328 4.07833 -0.13477
H -2.18328 4.07832 -0.13477
H 0.00000 -0.98046 1.47553

TS(1-3)2

SCF =   -1315.70998851
H(0 K)=   -1315.013927
H(298 K)=   -1314.971150
G(298 K)=   -1315.087681
SCF (Corr) =   -1986.06165227
Low Freq. = -34.5373cm-1, 17.5425cm-1

82
C -0.45137 -2.79662 2.94585
C 0.81771 -2.82844 3.54128
C 1.89420 -2.12319 2.98677
C 1.65490 -1.36978 1.82673
N 0.41487 -1.28891 1.26510
C -0.60967 -2.01896 1.78918
O 2.68055 -0.71368 1.23672
P 2.40217 0.16884 -0.28307
C 3.61593 -0.81280 -1.41105
C 3.85199 0.01109 -2.69665
Rh 0.11375 -0.12880 -0.50172
P -2.00832 -1.03475 -0.31722
C -2.58470 -2.43162 -1.51058
C -3.55338 -3.42916 -0.83669
O -1.81129 -1.99902 1.16098
C 3.04841 1.89570 0.24333
C 2.21523 2.27670 1.49010
C 4.54759 1.93347 0.59666
C 2.73204 2.86681 -0.91789
C -3.44638 0.10270 0.26963
C -2.94760 0.75640 1.58034
C -3.63365 1.18908 -0.81572
C -4.77360 -0.63038 0.54288
C -3.23322 -1.76585 -2.74499
C -1.31850 -3.20294 -1.95009
C 4.95041 -1.13397 -0.70125
C 2.92361 -2.14684 -1.77399
H 0.97372 -3.42645 4.44403
H 2.48122 3.30831 1.78180
H 1.13238 2.27334 1.28058
H 2.43087 1.61630 2.34539
H 2.98002 3.89221 -0.59069
H 3.33071 2.65507 -1.81800
H 1.66438 2.85866 -1.18877
H 4.77721 2.92995 1.01580
H 4.82065 1.18333 1.35614
H 5.19076 1.80140 -0.28764
H 3.63019 -2.75831 -2.36341
H 2.64354 -2.73118 -0.88146
H 2.02380 -1.99204 -2.39158
H 5.55349 -1.76851 -1.37505
H 5.54432 -0.23805 -0.47633

```
H    4.79200 -1.69216  0.23434
H    4.40344 -0.61491 -3.42086
H    2.90712  0.31811 -3.17758
H   -0.63677 -2.57377 -2.54522
H   -1.62954 -4.05105 -2.58605
H    4.46184  0.90970 -2.51160
H   -0.76158 -3.61753 -1.09317
H   -3.41301 -2.54082 -3.51134
H   -4.20778 -1.30781 -2.51111
H   -2.58018 -0.99991 -3.19831
H   -3.75783 -4.24561 -1.55213
H   -3.11399 -3.87701  0.06792
H   -4.51903 -2.97954 -0.56949
H   -5.48470  0.08928  0.98862
H   -5.23997 -1.01462 -0.37785
H   -4.65253 -1.46020  1.25725
H   -3.70605  1.48783  1.91573
H   -2.82179  0.01724  2.38697
H   -1.99779  1.29961  1.43510
H   -4.38858  1.91343 -0.45345
H   -2.69204  1.72465 -1.02679
H   -4.01792  0.78012 -1.76355
H    0.41328 -1.18936 -1.53419
H   -1.29834 -3.35874  3.34185
H    2.89706 -2.15335  3.41516
H   -0.09048  0.68639 -1.83165
H   -0.80759  2.65325  0.24608
B   -0.81190  3.73043 -0.36697
H    0.14586  4.42231 -0.06699
H   -0.94149  3.56069 -1.56738
N   -2.12755  4.56141  0.13196
C   -2.29919  5.82095 -0.65811
H   -2.94831  3.96781 -0.05582
C   -2.10198  4.84696  1.59842
H   -3.00746  5.39255  1.91173
H   -2.02422  3.89619  2.14379
H   -1.20873  5.45221  1.81031
H   -3.19469  6.37284 -0.32801
H   -1.40163  6.43886 -0.51052
H   -2.37899  5.56032 -1.72207

Int(1-3)2

SCF  =          -1315.71949660
H(0 K)=         -1315.021663
H(298 K)=       -1314.979244
G(298 K)=       -1315.092656
SCF (Corr) =    -1986.07313188
Low Freq. = 18.8863cm-1, 23.0869cm-1

82
C    1.38608 -1.62013  1.72678
C    1.52242 -2.54473  2.77479
C    0.35497 -3.10168  3.31131
C   -0.90277 -2.76808  2.79017
C   -0.94899 -1.83410  1.74510
N    0.16823 -1.22072  1.26711
O   -2.14650 -1.53587  1.17975
P   -2.18732 -0.52076 -0.26430
C   -2.67313 -1.80725 -1.62870
C   -2.41533 -1.12163 -2.99134
Rh   0.03536  0.18981 -0.35529
P    2.35921 -0.03128 -0.24482
C    3.26383 -1.10566 -1.57758
C    4.50127 -1.83635 -1.00595
O    2.49991 -1.12407  1.14028
C   -3.68280  0.55554  0.31325
C   -3.18939  1.29882  1.57541
C   -4.00041  1.54196 -0.83178
C   -4.94760 -0.23580  0.71703
C    3.48452  1.38878  0.41993
C    2.97709  1.69703  1.84891
C    4.98598  1.04771  0.50580
C    3.27315  2.59761 -0.52059
C   -1.73730 -3.02571 -1.45639
C   -4.13089 -2.30619 -1.56702
C    2.27987 -2.17971 -2.09159
C    3.65067 -0.17452 -2.74902
B   -0.14908  3.05611  1.05314
N   -1.21875  3.93472  0.21534
C   -0.79557  4.18104 -1.19972
C   -1.49405  5.22481  0.92938
H    0.42712 -3.82630  4.12765
H   -1.91008 -3.71892 -2.29885
H   -0.67131 -2.74701 -1.46917
H   -1.94717 -3.57128 -0.52238
H   -2.61743 -1.84926 -3.79777
H   -3.08133 -0.25760 -3.15745
H   -1.37434 -0.77573 -3.09218
H   -4.24682 -3.11876 -2.30659
H   -4.39670 -2.71764 -0.58100
H   -4.85518 -1.52273 -1.83800
H   -3.91845  2.08899  1.83382
H   -3.12922  0.61406  2.43649
H   -2.19304  1.75241  1.46223
H   -5.61897  0.45250  1.26215
H   -5.51031 -0.62675 -0.14000
H   -4.70884 -1.06754  1.39838
H   -4.73952  2.28649 -0.48398
H   -3.10282  2.08082 -1.18719
H    1.88887  1.84774  1.89759
H    3.45272  2.63299  2.19221
H   -4.44073  1.03467 -1.70653
H    3.25751  0.89576  2.55027
H    3.80469  3.46968 -0.09888
H    3.68270  2.41809 -1.52795
H    2.21009  2.86409 -0.61208
H    5.49620  1.89534  0.99872
H    5.17844  0.15074  1.11530
H    5.45506  0.92255 -0.48272
H    4.90124 -2.49988 -1.79333
H    5.31006 -1.15647 -0.71098
H    4.23924 -2.46398 -0.14002
H    2.81984 -2.83542 -2.79818
H    1.89474 -2.81783 -1.27815
H    1.42768 -1.73837 -2.63241
H    4.03335 -0.79134 -3.58184
H    2.78432  0.39314 -3.13153
H    4.44676  0.53719 -2.47854
H   -0.03766  1.06850 -1.66305
H    2.51824 -2.81695  3.12751
H   -1.82713 -3.21895  3.15412
H   -0.07520  1.90740  0.48885
H    0.91000  3.63182  0.95632
H   -0.55555  2.91899  2.18688
H   -2.10571  3.40935  0.18417
H   -2.21591  5.83255  0.36072
H   -1.88654  5.00035  1.93038
H   -0.54425  5.76948  1.03088
H   -1.57069  4.74590 -1.74253
H    0.13990  4.75860 -1.18048
H   -0.61186  3.21036 -1.68358
H    0.14649 -0.94248 -1.38460

TS(1-3)3
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```
SCF  =          -1315.69458675
H(0 K)=         -1315.001666
H(298 K)=       -1314.958168
G(298 K)=       -1315.074348
SCF (Corr) =    -1986.05099643
Low Freq. = -307.5623cm-1, 17.0405cm-1

82
C  -1.37778 -2.53853 -0.18823
C  -1.51309 -3.91843 -0.39385
C  -0.35747 -4.68021 -0.59646
C   0.89549 -4.05616 -0.59799
C   0.95155 -2.67325 -0.38463
N  -0.16189 -1.90061 -0.16670
O   2.16149 -2.06791 -0.40704
P   2.22776 -0.36837  0.01917
C   3.33015 -0.51916  1.59857
C   3.39960  0.86713  2.27755
Rh -0.01145  0.12564  0.23023
P  -2.32674 -0.05413  0.08446
C  -3.42320  0.23075  1.64295
C  -4.90719 -0.12758  1.42055
O  -2.49453 -1.80247 -0.01159
C   3.21262  0.25499 -1.52046
C   2.16047  0.43119 -2.64095
C   3.85659  1.61736 -1.18759
C   4.28618 -0.74568 -2.00181
C  -3.22918  0.40366 -1.56635
C  -2.15444  0.26136 -2.67019
C  -4.39904 -0.55252 -1.88752
C  -3.72632  1.86439 -1.50341
C   2.59669 -1.51030  2.53354
C   4.75008 -1.04997  1.31653
C  -2.85318 -0.67520  2.75964
C  -3.28139  1.71413  2.05396
B  -0.29916  2.98571 -0.55263
N   0.82590  4.10656 -0.21716
C   1.15399  4.20342  1.23967
C   0.40061  5.43954 -0.76139
H  -0.43295 -5.75889 -0.75875
H   3.12656 -1.54047  3.50249
H   1.55451 -1.20763  2.72936
H   2.59152 -2.53172  2.12156
H   3.97753  0.77717  3.21490
H   3.90681  1.62174  1.65403
H   2.39678  1.24009  2.54565
H   5.25537 -1.23464  2.28203
H   4.73385 -2.00292  0.76414
H   5.36950 -0.32690  0.76212
H   2.67029  0.79312 -3.55275
H   1.67008 -0.52425 -2.89014
H   1.37310  1.15169 -2.36760
H   4.71013 -0.36882 -2.95029
H   5.11711 -0.86181 -1.29240
H   3.85460 -1.73860 -2.19901
H   4.24616  2.07325 -2.11539
H   3.12573  2.32393 -0.75206
H  -1.29146  0.92231 -2.49462
H  -2.60954  0.53056 -3.64099
H   4.70038  1.52719 -0.48450
H  -1.78591 -0.77510 -2.75264
H  -4.11485  2.14451 -2.49951
H  -4.55275  1.99432 -0.78567
H  -2.92052  2.57121 -1.25120
H  -4.77901 -0.29667 -2.89339
H  -4.07934 -1.60537 -1.90758
H  -5.23942 -0.45751 -1.18589
H  -5.43714 -0.03456  2.38597
H  -5.40443  0.55280  0.71170
H  -5.03596 -1.16446  1.07117
H  -3.41070 -0.47294  3.69184
H  -2.97208 -1.74335  2.51950
H  -1.78797 -0.47747  2.95960
H  -3.84376  1.87700  2.99102
H  -2.23044  1.98999  2.24014
H  -3.68929  2.40396  1.29812
H   0.03801  1.17221  2.09514
H  -2.51326 -4.35440 -0.39586
H   1.82540 -4.60335 -0.75987
H   0.26024  1.86174 -0.25023
H  -1.26037  3.24258  0.13595
H  -0.48022  3.00433 -1.75114
H   1.68939  3.83981 -0.71340
H   1.16489  6.20337 -0.54631
H   0.24556  5.34708 -1.84471
H  -0.55032  5.71589 -0.28352
H   1.93795  4.95806  1.41251
H   0.23767  4.48628  1.77752
H   1.48907  3.21876  1.59420
H   0.03499  0.36773  2.09022
```

Dehydrogenation via Amine Nu Attack

3.NMe2H

```
SCF  =          -1449.71290122
H(0 K)=         -1448.940583
H(298 K)=       -1448.892073
G(298 K)=       -1449.024914
SCF (Corr) =    -2120.12257011
Low Freq. = 10.1720cm-1, 13.0852cm-1

90
C   2.39041  2.28752 -0.48043
C   3.62505  2.89578 -0.74744
C   4.75241  2.07999 -0.89038
C   4.63262  0.69192 -0.75870
C   3.36573  0.15610 -0.49166
N   2.23779  0.92758 -0.36462
O   3.25223 -1.18242 -0.34885
P   1.65658 -1.83647  0.00800
C   1.56497 -3.02495 -1.51331
C   0.42149 -4.03940 -1.30754
Rh  0.39669  0.08955  0.05817
B  -1.89225 -0.71332  0.01362
N  -2.38712 -2.16812  0.53525
C  -3.38924 -2.77572 -0.40704
O   1.30730  3.07711 -0.32837
P  -0.22816  2.30808  0.06403
C  -1.25636  3.07451 -1.37756
C  -0.85809  4.53340 -1.69026
C   2.08374 -2.72736  1.66064
C   2.61728 -1.61275  2.59159
C   0.76543 -3.27960  2.24671
C   3.13132 -3.84970  1.53594
C  -0.55627  3.13404  1.76860
C   0.66476  2.76172  2.64251
C  -0.70157  4.66676  1.70455
C  -1.82583  2.48854  2.36898
C   1.23171 -2.10240 -2.71089
C   2.88882 -3.76473 -1.80221
C  -0.94184  2.19198 -2.60915
C  -2.76040  2.98549 -1.03998
C  -2.94628 -2.12256  1.92453
H   5.72851  2.52736 -1.09794
H   1.10556 -2.72327 -3.61673
```

H	0.30454	-1.52868	-2.54687
H	2.04660	-1.38679	-2.91025
H	0.30925	-4.64689	-2.22369
H	0.61665	-4.73851	-0.47727
H	-0.54968	-3.53971	-1.14244
H	2.79590	-4.27252	-2.77951
H	3.73969	-3.06975	-1.86584
H	3.12161	-4.53537	-1.05376
H	2.74483	-2.02602	3.60850
H	3.59607	-1.23590	2.25499
H	1.91511	-0.76225	2.64708
H	3.41943	-4.18151	2.55015
H	2.73968	-4.73254	1.00561
H	4.04580	-3.50664	1.02681
H	0.96747	-3.72634	3.23689
H	0.02871	-2.47134	2.39529
H	0.83511	1.67084	2.65286
H	0.47506	3.09466	3.67895
H	0.32023	-4.07369	1.62199
H	1.58539	3.25620	2.29289
H	-1.97436	2.88536	3.38957
H	-2.73468	2.71639	1.78973
H	-1.72738	1.39309	2.44216
H	-0.75004	5.06072	2.73614
H	0.15820	5.14385	1.20737
H	-1.62666	4.97980	1.19470
H	-1.41736	4.85583	-2.58744
H	-1.11019	5.23050	-0.87847
H	0.21569	4.62892	-1.91112
H	-1.50186	2.58291	-3.47832
H	0.13051	2.21654	-2.86716
H	-1.23518	1.14211	-2.45039
H	-3.33987	3.28402	-1.93253
H	-3.06681	1.96183	-0.76907
H	-3.04553	3.66994	-0.22408
H	-0.98300	-0.41976	0.93339
H	3.67103	3.98266	-0.82959
H	5.48427	0.01635	-0.85083
H	-2.81255	0.04824	0.21540
H	-1.56026	-0.80891	-1.15341
H	-1.56111	-2.78579	0.55792
H	-3.22219	-3.13432	2.26205
H	-2.19811	-1.68940	2.60370
H	-3.83752	-1.48007	1.90860
H	-3.65440	-3.78921	-0.06330
H	-4.29789	-2.13904	-0.42797
H	-2.94325	-2.82278	-1.41045
N	-6.33668	-1.11551	-0.60408
C	-7.21629	-2.01592	-1.36665
C	-7.00063	-0.59673	0.60146
H	-6.09750	-0.31864	-1.20517
H	-8.20059	-1.56983	-1.62992
H	-6.71603	-2.32527	-2.29910
H	-7.41384	-2.92402	-0.77059
H	-7.97958	-0.10620	0.40445
H	-7.18616	-1.42891	1.30325
H	-6.34480	0.13339	1.10458

TS(3-4)B

SCF = -1449.67867447
H(0 K)= -1448.907794
H(298 K)= -1448.860366
G(298 K)= -1448.987063
SCF (Corr) = -2120.09513563
Low Freq. = -390.6967cm-1, 17.4106cm-1

90

C	3.03492	1.32063	-0.18007
C	4.43101	1.44354	-0.23362
C	5.20068	0.27648	-0.15169
C	4.57944	-0.97204	-0.02560
C	3.17818	-1.01356	0.02121
N	2.40361	0.11408	-0.04014
O	2.56496	-2.21354	0.13227
P	0.79569	-2.24093	0.01280
C	0.62873	-3.21534	-1.63929
C	-0.86986	-3.22289	-2.01771
Rh	0.31758	-0.01220	-0.00498
B	-3.03171	-0.37567	-0.30966
N	-3.25363	0.51744	1.00020
C	-3.35541	-0.28789	2.25954
O	2.27713	2.43669	-0.27514
P	0.52362	2.25435	-0.06468
C	-0.00694	3.22392	-1.64239
C	0.82144	4.49209	-1.93301
C	0.47490	-3.32159	1.57336
C	0.61662	-2.34152	2.76262
C	-0.97105	-3.85837	1.50310
C	1.47775	-4.47941	1.75822
C	0.38246	3.29797	1.55752
C	1.33664	2.61454	2.56557
C	0.76579	4.78159	1.40145
C	-1.06217	3.17318	2.08872
C	1.40323	-2.37099	-2.67936
C	1.19344	-4.64722	-1.60581
C	0.19512	2.21141	-2.79609
C	-1.50729	3.56479	-1.51746
C	-4.32626	1.55777	0.92016
H	6.29190	0.33998	-0.19230
H	1.22647	-2.79345	-3.68522
H	1.06230	-1.32033	-2.68047
H	2.48927	-2.38677	-2.49367
H	-0.98170	-3.66811	-3.02337
H	-1.47878	-3.82328	-1.32187
H	-1.27888	-2.19914	-2.04632
H	1.18030	-5.06136	-2.63083
H	2.23619	-4.67252	-1.25067
H	0.58841	-5.32086	-0.97751
H	0.34930	-2.86467	3.69936
H	1.65311	-1.97900	2.86402
H	-0.03411	-1.45705	2.64425
H	1.29831	-4.94579	2.74441
H	1.36651	-5.26576	0.99802
H	2.51853	-4.12156	1.73976
H	-1.23754	-4.31211	2.47518
H	-1.70246	-3.05823	1.29190
H	1.14332	1.52889	2.63293
H	1.18177	3.05780	3.56629
H	-1.08609	-4.64103	0.73502
H	2.39262	2.76391	2.29139
H	-1.16248	3.76170	3.01907
H	-1.81585	3.55428	1.37814
H	-1.29067	2.12225	2.34542
H	0.80960	5.24911	2.40249
H	1.75637	4.90190	0.93535
H	0.02614	5.34676	0.81132
H	0.55471	4.86308	-2.93959
H	0.62391	5.30642	-1.22114
H	1.90160	4.27960	-1.92968
H	-0.18002	2.65619	-3.73644
H	1.26213	1.97332	-2.93994
H	-0.34298	1.26596	-2.60780
H	-1.86474	3.98336	-2.47586
H	-2.11226	2.66365	-1.30919
H	-1.70371	4.32095	-0.73847

H -1.32356 -0.20943 -0.11143
H   4.87602 2.43394 -0.34071
H   5.14238 -1.90496 0.03038
H -2.96608 0.22656 -1.34416
H -2.91878 -1.55598 -0.14172
H -2.33803 1.00578 1.04416
H -4.22566 2.25610 1.76560
H -4.22922 2.10156 -0.02910
H -5.30721 1.06777 0.96503
H -3.41507 0.38177 3.13197
H -4.25608 -0.91482 2.20978
H -2.46102 -0.92193 2.33321
N -5.15702 -0.86205 -0.88577
C -6.02563 -1.65250 0.01404
C -5.92763 0.10019 -1.70548
H -4.70970 -1.52067 -1.53421
H -6.84436 -2.16762 -0.52546
H -5.41916 -2.40920 0.53679
H -6.48804 -0.98806 0.76402
H -6.70227 -0.39573 -2.32167
H -6.43426 0.82766 -1.05071
H -5.23870 0.64502 -2.36975

[4•$HMe_2NBH_2NMe_2H$]$^+$

SCF =   -1449.71627263
H(0 K)=   -1448.943769
H(298 K)=   -1448.896100
G(298 K)=   -1449.025424
SCF (Corr) =   -2120.13353152
Low Freq. = 10.1146cm-1, 19.8362cm-1

90
C   3.46608 0.02984 -0.02948
C   4.78753 -0.43936 -0.06913
C   4.99610 -1.82300 -0.12861
C   3.90612 -2.70210 -0.14474
C   2.61421 -2.15639 -0.10464
N   2.38406 -0.80800 -0.05563
O   1.55180 -2.99259 -0.11743
P -0.06605 -2.26822 0.03009
C -0.84134 -3.14627 -1.50297
C -2.37849 -3.08398 -1.38406
Rh 0.43670 -0.05294 0.01969
B -4.40432 0.38844 0.51657
N -3.39742 1.25439 -0.36270
C -3.24125 2.69655 0.00781
O   3.24850 1.36304 0.04140
P   1.56000 1.91954 0.03218
C   1.66249 2.97139 -1.58220
C   2.67702 4.12928 -1.53784
C -0.58176 -3.07749 1.69936
C   0.49306 -2.61754 2.71292
C -1.94296 -2.46807 2.10399
C -0.65276 -4.61549 1.67909
C   1.65357 2.98117 1.63915
C   2.96132 3.78223 1.80282
C   0.42901 3.91961 1.67873
C   1.54577 1.94811 2.78675
C -0.37753 -2.29621 -2.71008
C -0.37417 -4.60289 -1.70441
C   2.06598 1.96326 -2.68465
C   0.24654 3.50358 -1.89311
C -3.46008 1.09220 -1.85122
H   6.01534 -2.21898 -0.15898
H -0.85027 -2.68366 -3.63198
H -0.64565 -1.23249 -2.58588
H   0.71554 -2.35124 -2.84529
H -2.83019 -3.40369 -2.34133
H -2.76374 -3.75570 -0.59911
H -2.73629 -2.06199 -1.16664
H -0.76093 -4.96674 -2.67433
H   0.72364 -4.67582 -1.73031
H -0.74844 -5.28267 -0.92516
H   0.18137 -2.92157 3.72898
H   1.47260 -3.07844 2.50751
H   0.61328 -1.51960 2.69927
H -0.81644 -4.98156 2.70959
H -1.48989 -4.98893 1.06677
H   0.28307 -5.06600 1.31115
H -2.20625 -2.82042 3.11843
H -1.89651 -1.36628 2.12392
H   3.84714 3.13701 1.69867
H   2.98131 4.22195 2.81703
H -2.76016 -2.76820 1.42771
H   3.04818 4.61052 1.08473
H   1.50316 2.48419 3.75312
H   0.64352 1.32020 2.68489
H   2.42293 1.28023 2.81228
H   0.37374 4.40148 2.67201
H   0.49385 4.72555 0.92839
H -0.51375 3.36518 1.52640
H   2.78101 4.55620 -2.55258
H   2.35075 4.94673 -0.87446
H   3.67423 3.78962 -1.21588
H   1.99836 2.45996 -3.67001
H   3.10164 1.61122 -2.55442
H   1.39742 1.08362 -2.68860
H   0.25710 4.01824 -2.87148
H -0.47626 2.67132 -1.95335
H -0.10773 4.23057 -1.14275
H -1.08136 0.53865 0.15463
H   5.60960 0.27775 -0.04970
H   4.02676 -3.78576 -0.18409
H -4.41314 -0.73883 0.07003
H -4.05332 0.47138 1.67366
H -2.43973 0.81872 -0.09748
H -2.51143 1.43532 -2.29315
H -3.60543 0.02986 -2.08907
H -4.28794 1.68604 -2.26659
H -2.30552 3.08472 -0.42266
H -4.08557 3.28194 -0.38772
H -3.20191 2.78284 1.10257
N -5.97892 0.84798 0.51833
C -6.32797 2.08763 1.29426
C -6.69736 0.81339 -0.80026
H -6.36030 0.06159 1.06699
H -7.41663 2.14079 1.45205
H -5.80762 2.05661 2.26105
H -6.00528 2.97276 0.72990
H -7.78616 0.86239 -0.64242
H -6.38696 1.67908 -1.40197
H -6.43518 -0.11600 -1.32418

TS(4-1)$_B$

SCF =   -1449.70311239
H(0 K)=   -1448.934991
H(298 K)=   -1448.888048
G(298 K)=   -1449.012504
SCF (Corr) =   -2120.11769815
Low Freq. = -750.3122cm-1, 17.4219cm-1

90
C -3.20085 0.74065 -0.49315
C -4.34124 1.50734 -0.77595

```
C  -4.18056  2.88359 -0.97187
C  -2.91280  3.46714 -0.87037
C  -1.82038  2.63466 -0.58376
N  -1.94325  1.27921 -0.42499
O  -0.60095  3.19260 -0.45934
P   0.74553  2.16432  0.05938
C   1.99149  2.75202 -1.29462
C   3.43742  2.60170 -0.77723
Rh -0.28738  0.10176  0.05997
B   3.82325 -1.15236 -0.03524
N   2.57178 -2.00293 -0.29699
C   2.25617 -3.05620  0.68255
O  -3.35066 -0.58105 -0.27808
P  -1.90882 -1.54133  0.09502
C  -2.17140 -2.81688 -1.33653
C  -3.65175 -3.18479 -1.57854
C   1.07809  2.97214  1.77337
C  -0.23641  2.79980  2.57016
C   2.19570  2.15886  2.46547
C   1.44259  4.46766  1.70008
C  -2.45914 -2.20805  1.81501
C  -3.73765 -3.06686  1.78698
C  -1.27759 -3.00909  2.40615
C  -2.69630 -0.94862  2.68105
C   1.75566  1.79916 -2.49009
C   1.74096  4.20697 -1.74766
C  -1.62928 -2.09783 -2.59564
C  -1.35728 -4.09537 -1.05052
C   2.32393 -2.45916 -1.67667
H  -5.05147  3.50769 -1.19226
H   2.43669  2.07888 -3.31492
H   1.95015  0.74895 -2.21800
H   0.72213  1.86828 -2.86995
H   4.13102  2.77085 -1.62140
H   3.68031  3.34775 -0.00342
H   3.64169  1.59454 -0.38159
H   2.46948  4.44670 -2.54380
H   0.73068  4.34345 -2.16037
H   1.88511  4.93718 -0.93774
H  -0.07097  3.13944  3.60872
H  -1.05727  3.40152  2.14713
H  -0.55375  1.74273  2.59754
H   1.50253  4.86970  2.72805
H   2.42159  4.64321  1.22628
H   0.67850  5.05004  1.16033
H   2.31734  2.53180  3.49878
H   1.94044  1.08715  2.51970
H  -4.57385 -2.54895  1.29095
H  -4.04615 -3.27756  2.82730
H   3.16925  2.25707  1.96043
H  -3.57930 -4.03963  1.29413
H  -2.89045 -1.26283  3.72262
H  -1.81206 -0.28732  2.67832
H  -3.56788 -0.37057  2.33427
H  -1.53851 -3.32308  3.43309
H  -1.05445 -3.92393  1.83225
H  -0.36339 -2.39507  2.46314
H  -3.70701 -3.79888 -2.49612
H  -4.08467 -3.77815 -0.76080
H  -4.27713 -2.29314 -1.73246
H  -1.65865 -2.79487 -3.45306
H  -2.24922 -1.22362 -2.85622
H  -0.59269 -1.74476 -2.46360
H  -1.39353 -4.75175 -1.93893
H  -0.29522 -3.88473 -0.84305
H  -1.76894 -4.66952 -0.20409
H   0.89941 -0.69860  0.84514
H  -5.31374  1.01558 -0.82593
H  -2.74628  4.53810 -0.99431
H   4.02206 -0.41132 -0.98092
H   3.74421 -0.58727  1.04463
H   1.39942 -1.02577  0.04793
H   1.25552 -2.69930 -1.81361
H   2.59341 -1.65923 -2.38220
H   2.90299 -3.36836 -1.93519
H   1.19088 -3.34157  0.61616
H   2.85266 -3.97637  0.52097
H   2.44606 -2.68272  1.70166
N   5.29352 -1.96059  0.08601
C   5.55051 -2.69851  1.36458
C   5.67580 -2.78530 -1.10328
H   5.92746 -1.14782  0.09304
H   6.61195 -2.98656  1.43772
H   5.27788 -2.04787  2.20684
H   4.93041 -3.60476  1.38973
H   6.73504 -3.08470 -1.04684
H   5.04949 -3.68837 -1.12641
H   5.50023 -2.19638 -2.01428
```

1•$NMe_2BH_2NMe_2H$

```
SCF  =          -1449.70997640
H(0 K)=         -1448.942977
H(298 K)=       -1448.894564
G(298 K)=       -1449.026537
SCF (Corr) =    -2120.11626883
Low Freq. = 11.7487cm-1, 15.2017cm-1

90
C  -2.87288 -1.81709 -0.35572
C  -4.20526 -2.18084 -0.60084
C  -5.15214 -1.16043 -0.74841
C  -4.77723  0.18538 -0.65320
C  -3.42877  0.47989 -0.40644
N  -2.48376 -0.50426 -0.25809
O  -3.04890  1.77161 -0.31583
P  -1.34465  2.11944  0.03265
C  -0.96317  3.21644 -1.49287
C   0.40168  3.90116 -1.25757
Rh -0.51271 -0.02067  0.11476
B   3.90186  0.86545  0.15401
N   4.45103 -0.33358 -0.52027
C   5.15600 -1.38014  0.20567
O  -1.94721 -2.78691 -0.21526
P  -0.27018 -2.30655  0.11561
C   0.57538 -3.15819 -1.37728
C   0.03632 -4.57554 -1.66179
C  -1.54309  3.06459  1.68884
C  -2.29667  2.08971  2.62490
C  -0.12108  3.30726  2.24745
C  -2.32043  4.38948  1.57298
C  -0.00994 -3.17535  1.80370
C  -0.08365 -4.71276  1.73671
C   1.36307 -2.71208  2.34566
C  -1.12949 -2.63149  2.72270
C  -0.84927  2.22171 -2.67363
C  -2.06287  4.25287 -1.80224
C   0.26621 -2.24084 -2.58524
C   2.09733 -3.17951 -1.11331
C   4.70865 -0.37704 -1.95266
H  -6.19809 -1.41754 -0.93991
H  -0.56844  2.78170 -3.58403
H  -0.08170  1.45114 -2.48848
H  -1.80797  1.71577 -2.87696
H   0.71117  4.40021 -2.19357
H   0.34926  4.67777 -0.47667
```

H	1.19366	3.17815	-0.99198
H	-1.82592	4.73264	-2.76909
H	-3.05417	3.78263	-1.89656
H	-2.12371	5.04957	-1.04714
H	-2.32204	2.52300	3.64081
H	-3.33739	1.92948	2.30065
H	-1.78944	1.11047	2.68382
H	-2.50816	4.77935	2.58987
H	-1.75123	5.16087	1.03032
H	-3.29801	4.25733	1.08221
H	-0.21016	3.76240	3.25026
H	0.44249	2.36517	2.35434
H	-1.01708	-5.06577	1.26949
H	-0.05492	-5.11251	2.76660
H	0.46803	3.99843	1.62359
H	0.77206	-5.14783	1.19648
H	-0.95381	-3.00007	3.74921
H	-1.12870	-1.52751	2.75259
H	-2.12710	-2.97633	2.40665
H	1.49657	-3.12754	3.36076
H	2.20638	-3.06397	1.73111
H	1.42528	-1.61358	2.42080
H	0.48836	-4.93407	-2.60422
H	0.29950	-5.29840	-0.87643
H	-1.05725	-4.58111	-1.79114
H	0.77183	-2.64964	-3.47879
H	-0.81423	-2.19932	-2.80432
H	0.62894	-1.21208	-2.42155
H	2.60529	-3.51236	-2.03648
H	2.50367	-2.18418	-0.85234
H	2.36886	-3.89569	-0.32026
H	0.91550	0.31985	0.85793
H	-4.46584	-3.23784	-0.66956
H	-5.49110	1.00276	-0.76339
H	3.12951	1.50725	-0.56121
H	3.47149	0.63885	1.28394
H	1.08256	0.36443	-0.06646
H	4.45001	-1.37076	-2.37695
H	4.09887	0.38336	-2.46766
H	5.77581	-0.19828	-2.22381
H	4.90956	-2.38602	-0.19770
H	6.26698	-1.29584	0.15021
H	4.86965	-1.35814	1.27005
N	5.07638	2.10839	0.52050
C	6.09116	1.68780	1.52748
C	5.71899	2.69033	-0.69084
H	4.49701	2.84314	0.95183
H	6.74413	2.52863	1.81758
H	5.56972	1.29476	2.41207
H	6.70528	0.88691	1.09108
H	6.36920	3.54385	-0.43342
H	6.32205	1.90851	-1.17463
H	4.93278	3.01398	-1.38810

TS(3-4)$_N$

SCF = -1449.67207789
H(0 K)= -1448.903009
H(298 K)= -1448.854434
G(298 K)= -1448.987815
SCF (Corr) = -2120.09886137
Low Freq. = -14.9497cm-1, 7.9027cm-1

90

C	4.68785	-1.21416	-0.75981
C	3.31322	-1.17332	-0.47971
N	2.62633	0.00087	-0.34191
C	3.31216	1.17565	-0.48001
C	4.68675	1.21766	-0.76012
C	5.36917	0.00204	-0.89984
O	2.63616	-2.33745	-0.34218
P	0.89816	-2.23583	0.05248
C	0.94966	-3.20882	1.71672
C	-0.46176	-3.12269	2.34032
Rh	0.57097	0.00000	0.09215
P	0.89629	2.23610	0.05253
C	0.94756	3.20904	1.71681
C	-0.46348	3.12143	2.34106
O	2.63405	2.33920	-0.34275
B	-4.20793	0.00207	-1.23943
N	-4.15396	-0.00035	0.17945
C	-3.83742	-1.22582	0.94591
C	-3.83772	1.22255	0.95014
C	0.27056	3.30608	-1.42649
C	-1.19066	3.71518	-1.14604
C	1.13500	4.54347	-1.74283
C	0.30931	2.34031	-2.63522
C	0.27388	-3.30628	-1.42684
C	1.13960	-4.54283	-1.74300
C	-1.18704	-3.71680	-1.14695
C	0.31213	-2.34036	-2.63546
C	1.40555	4.67469	1.60711
C	1.93352	2.41809	2.60841
C	1.93440	-2.41690	2.60880
C	1.40922	-4.67399	1.60713
H	-6.01563	-0.00069	0.15327
H	-1.01085	-0.00062	0.43746
H	-4.29739	1.06042	-1.80624
H	-4.29732	-1.05438	-1.80982
H	-4.39219	-1.24564	1.90242
H	-4.08684	-2.11537	0.34938
H	-2.75374	-1.23575	1.16533
H	-4.39253	1.23895	1.90668
H	-4.08734	2.11410	0.35668
H	-2.75406	1.23199	1.16962
H	1.54414	-5.08771	2.62392
H	0.66672	-5.30813	1.09537
H	2.37288	-4.76412	1.08064
H	1.89749	-2.82267	3.63662
H	2.97114	-2.50231	2.24605
H	1.66455	-1.34617	2.64508
H	-0.43983	-3.57334	3.34993
H	-0.78187	-2.07117	2.43790
H	-1.21763	-3.66971	1.75145
H	0.79870	-4.97983	-2.70004
H	2.20120	-4.27370	-1.85526
H	1.05966	-5.32801	-0.97701
H	-1.61555	-4.17857	-2.05584
H	-1.26410	-4.45878	-0.33415
H	-1.80909	-2.84151	-0.88961
H	-0.12743	-2.84343	-3.51727
H	-0.25146	-1.41349	-2.43034
H	1.34642	-2.05624	-2.89152
H	1.89660	2.82373	3.63629
H	1.66484	1.34707	2.64472
H	2.97001	2.50466	2.24525
H	1.54049	5.08849	2.62386
H	2.36888	4.76586	1.08019
H	0.66216	5.30809	1.09572
H	-0.44160	3.57220	3.35061
H	-1.22021	3.66756	1.75246
H	-0.78239	2.06957	2.43887
H	-0.13101	2.84307	-3.51683
H	1.34379	2.05719	-2.89163
H	-0.25335	1.41290	-2.43000
H	-1.61996	4.17660	-2.05473

H -1.81178 2.83926 -0.88853
H -1.26813 4.45703 -0.33315
H   0.79342 4.98020 -2.69975
H   1.05455 5.32853 -0.97677
H   2.19683 4.27535 -1.85541
H   5.18586 -2.17990 -0.85966
H   6.44128 0.00249 -1.11772
H   5.18389 2.18382 -0.86022
N -7.09639 -0.00123 0.17610
C -7.58377 1.25834 -0.48746
C -7.58252 -1.26334 -0.48353
H -7.38248 0.00019 1.16700
H -8.68252 1.25786 -0.50837
H -7.21408 2.12443 0.07837
H -7.18338 1.28477 -1.51058
H -8.68126 -1.26403 -0.50445
H -7.18211 -1.29252 -1.50657
H -7.21197 -2.12730 0.08499

[4•H_2BNMe_2•H_2NMe]$^+$

SCF =   -1449.67389115
H(0 K)=   -1448.904704
H(298 K)=   -1448.855216
G(298 K)=   -1448.993881
SCF (Corr) =   -2120.09948909
Low Freq. = 4.7973cm-1, 5.4032cm-1

90
C   4.78276 -0.73806 -0.95149
C   3.42871 -0.85629 -0.60205
N   2.61741 0.23137 -0.43375
C   3.15417 1.47822 -0.59857
C   4.49889 1.67799 -0.94751
C   5.30931 0.54886 -1.12492
O   2.90001 -2.09083 -0.42598
P   1.19027 -2.18655 0.08063
C   1.44633 -3.10295 1.75674
C   0.06798 -3.16519 2.45442
Rh 0.60597 -0.00554 0.11440
P   0.66636 2.25238 0.07996
C   0.69418 3.19984 1.75778
C -0.66329 2.93560 2.44903
O   2.35399 2.55586 -0.41962
B -4.90912 1.35937 0.04736
N -4.27154 0.09859 0.12132
C -3.58846 -0.52355 -1.03575
C -3.85856 -0.51598 1.40337
C -0.16732 3.26378 -1.33540
C -1.64044 3.51586 -0.94993
C   0.53982 4.58929 -1.68478
C -0.10713 2.32371 -2.56318
C   0.60884 -3.36421 -1.33334
C   1.59716 -4.49513 -1.68353
C -0.76864 -3.94208 -0.94472
C   0.45221 -2.43555 -2.56128
C   0.97220 4.71066 1.65691
C   1.81254 2.51688 2.57971
C   2.37678 -2.17696 2.57500
C   2.07069 -4.50626 1.65277
H -6.05272 -0.56894 -0.07397
H -0.93116 -0.18164 0.57700
H -5.32500 1.85305 1.06419
H -5.10591 1.83881 -1.03984
H -3.83681 -1.60003 -1.10299
H -3.88503 -0.01276 -1.96324
H -2.49182 -0.43603 -0.89735
H -4.13226 -1.58810 1.42943
H -4.33396 0.01241 2.24218
H -2.75803 -0.44692 1.49588
H   2.30595 -4.87303 2.66927
H   1.38327 -5.23762 1.19670
H   3.00997 -4.49760 1.07669
H   2.44527 -2.55785 3.61062
H   3.39500 -2.14789 2.15495
H   1.98259 -1.14549 2.60674
H   0.19923 -3.56341 3.47759
H -0.38197 -2.16055 2.52729
H -0.64012 -3.82923 1.93057
H   1.24717 -5.00359 -2.60132
H   2.60592 -4.10089 -1.88101
H   1.67124 -5.25700 -0.89393
H -1.20706 -4.45940 -1.81852
H -0.69506 -4.68078 -0.12904
H -1.46947 -3.14696 -0.63340
H   0.01588 -3.00951 -3.40058
H -0.19656 -1.57110 -2.33514
H   1.42683 -2.04170 -2.89437
H   1.78641 2.90327 3.61522
H   1.66975 1.42192 2.61128
H   2.81099 2.72621 2.16328
H   1.10748 5.12122 2.67487
H   1.89136 4.92356 1.08762
H   0.13530 5.26030 1.19561
H -0.63352 3.35286 3.47261
H -1.50578 3.41416 1.92224
H -0.86477 1.85335 2.52003
H -0.65686 2.78666 -3.40437
H   0.93226 2.15717 -2.89182
H -0.54906 1.33696 -2.33988
H -2.18277 3.91970 -1.82486
H -2.14643 2.58348 -0.64053
H -1.73798 4.25245 -0.13500
H   0.08106 5.00706 -2.60032
H   0.44216 5.34662 -0.89354
H   1.61097 4.43331 -1.88557
H   5.38541 -1.63928 -1.07502
H   6.36189 0.67300 -1.39619
H   4.87614 2.69477 -1.06782
N -7.02585 -1.01379 -0.17973
C -7.86748 -0.59783 0.99718
C -7.59340 -0.60114 -1.51168
H -6.89582 -2.03690 -0.16423
H -8.87631 -1.01986 0.88923
H -7.39633 -0.96591 1.91880
H -7.91310 0.49991 1.01581
H -8.60175 -1.02340 -1.62307
H -7.63377 0.49653 -1.54241
H -6.93419 -0.97123 -2.30874

[4•H_2NMe_2]$^+$

SCF =   -1289.05350952
H(0 K)=   -1288.388813
H(298 K)=   -1288.347180
G(298 K)=   -1288.460987
SCF (Corr) =   -1959.39382531
Low Freq. = 19.2942cm-1, 24.7875cm-1

78
C -0.01150 -4.16540 -1.85943
C -1.22564 -3.52218 -1.58673
C -1.17883 -2.24526 -1.00785
N -0.00198 -1.60772 -0.72927
C   1.16991 -2.27150 -0.96743
C   1.20649 -3.54981 -1.54508

O	-2.34113	-1.61723	-0.71392
P	-2.25504	-0.06649	0.14932
C	-3.46067	0.87087	-1.03478
C	-2.61573	1.18573	-2.29204
Rh	0.00459	0.27716	0.21443
P	2.25937	-0.08706	0.16765
C	3.44139	0.80893	-1.06369
C	2.59776	0.97924	-2.34997
O	2.33514	-1.67190	-0.63311
C	-3.09159	-0.57312	1.80766
C	-4.55414	-1.03981	1.68800
C	-2.97814	0.64081	2.75942
C	-2.22224	-1.72790	2.35826
C	3.09240	-0.54048	1.84089
C	2.19291	-1.64404	2.44573
C	3.02346	0.71563	2.74033
C	4.54000	-1.05448	1.73022
C	3.80569	2.18707	-0.47252
C	4.71947	0.01971	-1.41795
C	-4.69135	0.04883	-1.47616
C	-3.91697	2.17635	-0.34888
N	-0.28867	3.54668	-0.36130
C	0.05999	4.37248	0.83421
C	0.35097	4.00497	-1.62991
H	-1.31376	3.54378	-0.48209
H	0.04189	1.56411	1.17172
H	-4.87966	-1.44173	2.66482
H	-5.23954	-0.21431	1.43655
H	-4.67440	-1.84200	0.94244
H	-2.56616	-1.97910	3.37789
H	-2.30557	-2.63625	1.73993
H	-1.15878	-1.43714	2.41578
H	-3.34080	0.34483	3.76041
H	-1.93166	0.97494	2.85899
H	-3.59209	1.49622	2.43120
H	-5.22456	0.60899	-2.26616
H	-4.39677	-0.92512	-1.89501
H	-5.40471	-0.12432	-0.65865
H	-4.42125	2.82795	-1.08522
H	-4.63296	1.98838	0.46760
H	-3.07568	2.74760	0.08907
H	-3.20055	1.82260	-2.98083
H	-1.66965	1.69722	-2.04248
H	-2.34600	0.26386	-2.83288
H	2.53686	-1.86226	3.47293
H	1.13931	-1.31755	2.49699
H	2.24369	-2.57975	1.86578
H	4.85464	-1.44305	2.71594
H	4.63565	-1.87639	1.00290
H	5.24796	-0.25524	1.45890
H	3.38529	0.45038	3.75018
H	3.66072	1.53642	2.37124
H	1.98921	1.08713	2.83399
H	3.14633	1.61829	-3.06615
H	2.41507	0.00839	-2.83913
H	1.61406	1.43342	-2.13964
H	4.31654	2.79451	-1.24182
H	2.91288	2.74482	-0.13623
H	4.49257	2.10251	0.38539
H	5.22185	0.52612	-2.26251
H	5.43896	-0.02334	-0.58827
H	4.48701	-1.00853	-1.73492
H	-2.19269	-3.98141	-1.79696
H	-0.01508	-5.16303	-2.30820
H	2.16956	-4.03063	-1.72277
H	-0.06241	2.45387	-0.10518
H	1.44194	3.95280	-1.51259
H	0.03946	3.33921	-2.44691
H	0.04899	5.04008	-1.85030
H	1.15216	4.36148	0.95844
H	-0.29192	5.40569	0.69857
H	-0.40671	3.91724	1.71946

TS(4-1)$_N$

SCF = -1289.05170281
H(0 K)= -1288.391089
H(298 K)= -1288.349911
G(298 K)= -1288.461734
SCF (Corr) = -1959.38765333
Low Freq. = -337.9922cm-1, 20.5483cm-1

78

C	-0.04674	-4.02755	-2.07926
C	-1.25805	-3.38863	-1.78335
C	-1.20270	-2.14618	-1.13399
N	-0.01908	-1.54098	-0.81817
C	1.14924	-2.20327	-1.07212
C	1.17668	-3.44860	-1.71914
O	-2.35845	-1.52385	-0.80849
P	-2.27836	-0.03806	0.16567
C	-3.47347	0.98314	-0.94872
C	-2.64474	1.33108	-2.20883
Rh	-0.00038	0.28975	0.26366
P	2.26685	-0.09050	0.18955
C	3.44959	0.84323	-1.00742
C	2.61911	1.02888	-2.30034
O	2.31472	-1.64017	-0.68495
C	-3.09611	-0.66234	1.79106
C	-4.55965	-1.12111	1.65103
C	-2.97750	0.48420	2.82266
C	-2.22239	-1.85289	2.25186
C	3.08162	-0.63966	1.84049
C	2.12393	-1.70869	2.41804
C	3.09165	0.59026	2.77771
C	4.49576	-1.23388	1.69855
C	3.79179	2.21245	-0.38347
C	4.73931	0.07169	-1.35740
C	-4.73229	0.21096	-1.40090
C	-3.87966	2.26408	-0.18767
N	-0.19129	3.41599	-0.38537
C	0.20055	4.15616	0.83435
C	0.38822	3.97033	-1.63017
H	-1.21665	3.42643	-0.46353
H	0.02305	1.39120	1.39515
H	-4.87223	-1.59651	2.59851
H	-5.24730	-0.27912	1.47244
H	-4.68925	-1.86437	0.84825
H	-2.56084	-2.17600	3.25273
H	-2.30934	-2.71576	1.57190
H	-1.15841	-1.56867	2.32889
H	-3.33878	0.11956	3.80110
H	-1.93147	0.81147	2.94475
H	-3.59093	1.36048	2.55521
H	-5.25804	0.81717	-2.16102
H	-4.47324	-0.75390	-1.86256
H	-5.44019	0.02895	-0.58078
H	-4.38575	2.95935	-0.88123
H	-4.58386	2.05106	0.63298
H	-3.01687	2.79653	0.25331
H	-3.22795	2.01616	-2.85052
H	-1.68122	1.80727	-1.96413
H	-2.42068	0.42791	-2.79973
H	2.47280	-1.99138	3.42761
H	1.09503	-1.31819	2.50925
H	2.10362	-2.62150	1.80065

```
H    4.78933 -1.68014  2.66598
H    4.53975 -2.02954  0.93793
H    5.24848 -0.46784  1.45591
H    3.43374  0.27021  3.77835
H    3.78129  1.37872  2.43457
H    2.08419  1.02587  2.88678
H    3.17478  1.68326 -2.99635
H    2.45112  0.06601 -2.80994
H    1.63396  1.48077 -2.09900
H    4.31076  2.83549 -1.13428
H    2.89012  2.75842 -0.05645
H    4.46648  2.11718  0.48278
H    5.24398  0.59738 -2.18845
H    5.45022  0.02743 -0.52030
H    4.52469 -0.95460 -1.69295
H   -2.22680 -3.82736 -2.02661
H   -0.05729 -4.99890 -2.58253
H    2.13429 -3.93417 -1.91232
H    0.00688  2.00775 -0.10951
H    1.48517  3.91374 -1.57274
H    0.04711  3.37535 -2.49078
H    0.09524  5.02524 -1.77994
H    1.29808  4.14813  0.92049
H   -0.14841  5.20318  0.80767
H   -0.22129  3.64516  1.71374
```

1•NMe_2H

```
SCF  =          -1289.05442023
H(0 K)=         -1288.392567
H(298 K)=       -1288.350285
G(298 K)=       -1288.467848
SCF (Corr) =    -1959.38626695
Low Freq. = 14.4738cm-1, 23.1170cm-1

78
C   -0.21308 -4.40174 -1.43597
C   -1.40057 -3.69656 -1.20607
C   -1.30611 -2.37604 -0.74398
N   -0.09866 -1.76495 -0.52004
C    1.05154 -2.47849 -0.74328
C    1.03094 -3.80239 -1.20531
O   -2.44153 -1.68332 -0.51564
P   -2.30405 -0.03663  0.12347
C   -3.31627  0.86252 -1.23728
C   -2.34775  0.97394 -2.43960
Rh  -0.01450  0.18055  0.18794
P    2.24799 -0.23245  0.11969
C    3.32715  0.57378 -1.24637
C    2.37153  0.74317 -2.45238
O    2.24238 -1.88725 -0.51394
C   -3.22649 -0.25768  1.79078
C   -4.71710 -0.61929  1.64588
C   -3.05406  1.05859  2.58545
C   -2.47675 -1.39448  2.52517
C    3.14869 -0.52886  1.78703
C    2.30501 -1.59678  2.52291
C    3.09047  0.79836  2.57949
C    4.60265 -1.01658  1.64068
C    3.78166  1.96057 -0.74154
C    4.53640 -0.28547 -1.67025
C   -4.58473  0.09960 -1.67256
C   -3.67128  2.27341 -0.72006
N    0.03069  4.03065 -0.16496
C    0.75672  4.68449  0.93622
C    0.46230  4.51920 -1.48513
H   -0.96789  4.24283 -0.05717
H    0.05273  1.50381  1.13921
H   -5.12187 -0.85643  2.64642
H   -5.31381  0.21593  1.24567
H   -4.87042 -1.50441  1.00787
H   -2.87920 -1.47934  3.55046
H   -2.61474 -2.36771  2.02745
H   -1.39510 -1.18446  2.59931
H   -3.49898  0.92592  3.58787
H   -1.98970  1.31415  2.72270
H   -3.56320  1.91355  2.11226
H   -5.02667  0.62573 -2.53803
H   -4.35429 -0.92958 -1.98808
H   -5.35119  0.06039 -0.88549
H   -4.09237  2.86459 -1.55287
H   -4.42888  2.24899  0.07997
H   -2.78253  2.81226 -0.34758
H   -2.84622  1.53726 -3.24934
H   -1.41543  1.49810 -2.16821
H   -2.07988 -0.01764 -2.84138
H    2.69721 -1.71230  3.54917
H    1.24459 -1.29666  2.59445
H    2.36170 -2.57939  2.02776
H    4.98632 -1.28874  2.64061
H    4.67932 -1.91048  1.00116
H    5.26765 -0.23449  1.24100
H    3.52393  0.62969  3.58155
H    3.66971  1.60598  2.10385
H    2.05225  1.14456  2.71718
H    2.91207  1.26035 -3.26586
H    2.03294 -0.23017 -2.84546
H    1.48083  1.33871 -2.18927
H    4.25248  2.50758 -1.57809
H    2.93351  2.56990 -0.38300
H    4.53134  1.88905  0.06338
H    5.01199  0.19330 -2.54531
H    5.30093 -0.36564 -0.88443
H    4.23235 -1.30077 -1.96832
H   -2.38542 -4.13586 -1.37044
H   -0.25788 -5.43379 -1.79592
H    1.97402 -4.32559 -1.36902
H    0.05262  1.86679  0.24840
H    1.51156  4.22515 -1.65774
H   -0.15347  4.05589 -2.27275
H    0.40055  5.62326 -1.59297
H    1.82493  4.41158  0.88175
H    0.69356  5.79338  0.91648
H    0.36524  4.33136  1.90468
```

[Rh(PONOP)(H_3BNMe_2)], I

```
SCF  =          -1314.09985104
H(0 K)=         -1313.435066
H(298 K)=       -1313.393344
G(298 K)=       -1313.505389
SCF (Corr) =    -1984.41564781
Low Freq. = 23.8370cm-1, 28.3151cm-1

79
N    0.33036 -1.78820 -0.38820
C    1.58563 -2.34020 -0.44444
C    1.80673 -3.70718 -0.66863
C    0.69596 -4.54561 -0.82477
C   -0.59702 -4.01488 -0.73834
C   -0.74089 -2.63785 -0.51128
O    2.65621 -1.53325 -0.27108
P    2.34142  0.18379  0.05568
Rh   0.05872  0.23020 -0.02477
P   -2.12691 -0.41136  0.05345
O   -1.98524 -2.12594 -0.40348
```

```
C   3.19162  0.33714  1.77869
C   2.48159 -0.70425  2.67414
C   2.88246  1.75505  2.31123
C   4.70843  0.07115  1.78376
C   3.43661  0.88210 -1.37413
C   2.57679  0.71322 -2.64980
C   3.68876  2.38301 -1.11418
C   4.76684  0.12452 -1.57119
C  -2.94075 -0.62862  1.78937
C  -4.34636 -1.25782  1.77039
C  -2.97180  0.76645  2.45266
C  -1.98016 -1.54211  2.58497
C  -3.41362  0.07590 -1.29723
C  -2.57043  0.32950 -2.56946
C  -4.44951 -1.02763 -1.59899
C  -4.10047  1.38762 -0.85991
B  -0.13227  2.62695 -0.26250
N  -1.45116  3.38093 -0.16666
C  -1.58390  4.16866  1.05728
C  -1.69798  4.23012 -1.33322
H  -0.13245  1.71831  0.77182
H   0.86171  3.28211  0.06529
H   0.02032  2.08320 -1.36660
H  -0.96510  5.06826 -1.43539
H  -1.64254  3.62945 -2.25718
H  -2.70740  4.68709 -1.27948
H  -2.59024  4.62925  1.12618
H  -0.83345  4.99403  1.13376
H  -1.44735  3.52095  1.94103
H  -4.66944 -1.44297  2.81222
H  -5.09640 -0.59429  1.31071
H  -4.35721 -2.22521  1.24184
H  -2.31154 -1.58006  3.63932
H  -1.97533 -2.57233  2.19262
H  -0.94814 -1.15165  2.55530
H  -3.34010  0.66211  3.49044
H  -1.96325  1.21064  2.48820
H  -3.63581  1.47121  1.92813
H  -5.06445 -0.69798 -2.45730
H  -3.96763 -1.97905 -1.87352
H  -5.13392 -1.21453 -0.75872
H  -4.67550  1.79008 -1.71489
H  -4.81639  1.22244 -0.03622
H  -3.35282  2.14704 -0.55159
H  -3.24591  0.64413 -3.38706
H  -1.81923  1.11882 -2.40990
H  -2.04544 -0.58373 -2.89935
H   2.82349 -0.57258  3.71753
H   1.38647 -0.56995  2.64302
H   2.71534 -1.73656  2.36560
H   5.06429  0.04984  2.83104
H   4.96011 -0.89977  1.32644
H   5.27239  0.86407  1.26639
H   3.23678  1.82832  3.35638
H   3.38777  2.54390  1.73157
H   1.80053  1.96528  2.29700
H   3.13960  1.11545 -3.51301
H   2.35983 -0.34884 -2.85688
H   1.62010  1.25302 -2.57188
H   4.14821  2.83031 -2.01534
H   2.75210  2.92799 -0.90458
H   4.38820  2.54553 -0.27649
H   5.24884  0.50265 -2.49220
H   5.47506  0.27877 -0.74429
H   4.60569 -0.95787 -1.69497
H  -1.49315 -4.63026 -0.83363
H   0.83818 -5.61569 -1.00234
H   2.83280 -4.07642 -0.70972
```

TS B-H activation

```
SCF  =          -1314.09912036
H(0 K)=         -1313.434862
H(298 K)=       -1313.393512
G(298 K)=       -1313.505098
SCF (Corr) =    -1984.41351229
Low Freq. = -68.4636cm-1, 24.0436cm-1

79
N   0.36750 -1.79385 -0.45655
C   1.63395 -2.31035 -0.53862
C   1.88314 -3.66323 -0.81963
C   0.78794 -4.51649 -1.00229
C  -0.51677 -4.02038 -0.88670
C  -0.68770 -2.65642 -0.60271
O   2.68541 -1.48583 -0.33958
P   2.33344  0.21371  0.07159
Rh  0.04935  0.21116  0.01476
P  -2.10562 -0.47983  0.07341
O  -1.94180 -2.17360 -0.46456
C   3.19258  0.29192  1.79484
C   2.49836 -0.80032  2.64075
C   2.86001  1.67811  2.39381
C   4.71282  0.04934  1.78687
C   3.40730  0.99260 -1.32920
C   2.54797  0.83539 -2.60725
C   3.60186  2.49148 -1.01295
C   4.76427  0.29468 -1.55653
C  -2.92149 -0.78743  1.79454
C  -4.32494 -1.41920  1.74931
C  -2.95446  0.57617  2.52237
C  -1.95461 -1.73243  2.54442
C  -3.38432  0.06418 -1.25552
C  -2.53045  0.35034 -2.51432
C  -4.44520 -1.00021 -1.60088
C  -4.03633  1.37394 -0.76203
B  -0.10966  2.87305 -0.18789
N  -1.42732  3.56955 -0.17308
C  -1.77948  4.33683  1.01426
C  -1.89963  4.20814 -1.39426
H  -0.22674  1.71503  0.66858
H   0.76412  3.36958  0.51735
H   0.26091  2.55849 -1.30803
H  -1.45441  5.21913 -1.55614
H  -1.64111  3.58942 -2.26849
H  -3.00188  4.34430 -1.38087
H  -2.87530  4.50209  1.07516
H  -1.29576  5.34227  1.04498
H  -1.46876  3.79239  1.92127
H  -4.64548 -1.65806  2.78102
H  -5.07820 -0.73519  1.32583
H  -4.33535 -2.35818  1.17177
H  -2.28458 -1.82451  3.59589
H  -1.94270 -2.74173  2.10130
H  -0.92513 -1.33395  2.53466
H  -3.30321  0.42156  3.56067
H  -1.95020  1.03062  2.55789
H  -3.63814  1.29510  2.04338
H  -5.04195 -0.63499 -2.45781
H  -3.98250 -1.95586 -1.89404
H  -5.14360 -1.19211 -0.77319
H  -4.60784  1.82645 -1.59374
H  -4.74756  1.19500  0.06246
H  -3.27235  2.10617 -0.43399
H  -3.18740  0.74631 -3.31156
H  -1.73816  1.08871 -2.30884
```

H -2.05214 -0.56788 -2.89633
H 2.84003 -0.71463 3.68908
H 1.40123 -0.67777 2.61701
H 2.74434 -1.81363 2.28268
H 5.07079 -0.02098 2.83142
H 4.97888 -0.89206 1.27880
H 5.26382 0.87669 1.31105
H 3.20951 1.70816 3.44287
H 3.35505 2.50136 1.85413
H 1.77462 1.87133 2.38306
H 3.07855 1.30970 -3.45427
H 2.39141 -0.22685 -2.86171
H 1.56256 1.31537 -2.49690
H 4.04021 2.99097 -1.89711
H 2.64681 2.99272 -0.78077
H 4.29833 2.64747 -0.17148
H 5.22407 0.71478 -2.47085
H 5.47252 0.45588 -0.73079
H 4.64480 -0.78983 -1.70712
H -1.39860 -4.65292 -1.00133
H 0.95180 -5.57552 -1.22332
H 2.91578 -4.01051 -0.88250

[Rh(PONOP)(NMe_2BH_3)], **II**

SCF = -1314.08726071
H(0 K)= -1313.419802
H(298 K)= -1313.378992
G(298 K)= -1313.487037
SCF (Corr) = -1984.40664093
Low Freq. = 26.1688cm-1, 27.1802cm-1

79
C 1.11834 2.35665 -0.27378
N -0.06403 1.65922 -0.15176
C -1.22597 2.38592 -0.13660
C -1.26695 3.78315 -0.24626
C -0.05378 4.47146 -0.37610
C 1.14916 3.76210 -0.38952
Rh -0.07068 -0.39629 -0.06164
N 0.18341 -2.53023 -0.09816
B 1.53166 -2.89853 0.66513
O -2.39552 1.72240 -0.00830
P -2.32284 -0.05261 0.03061
C -3.46868 -0.30880 -1.51263
C -4.84152 0.38215 -1.40328
O 2.26914 1.69176 -0.28832
P 2.26059 -0.13618 0.03820
C 3.52322 -0.39738 -1.45005
C 4.01413 -1.85347 -1.58392
C -3.31784 -0.25545 1.69214
C -4.34732 0.86767 1.94026
C 3.18649 0.03419 1.77595
C 2.06700 -0.01283 2.84061
C -2.24017 -0.19158 2.80025
C -4.02549 -1.62666 1.73411
C -2.67240 0.30733 -2.68782
C -3.65528 -1.81864 -1.77390
C 3.92889 1.38400 1.91335
C 4.19210 -1.11072 2.02276
C 2.73873 0.00439 -2.72180
C 4.75555 0.52434 -1.31277
C -0.88178 -3.34641 0.53861
C 0.27152 -2.95422 -1.51999
H 4.38064 1.41508 2.92275
H 4.74237 1.50626 1.18301
H 3.25260 2.24562 1.81873
H 2.52206 0.10100 3.84352
H 1.34086 0.80556 2.70013
H 1.52080 -0.96738 2.80946
H 4.65138 -0.96436 3.01897
H 3.71069 -2.09898 2.01327
H 5.01267 -1.11044 1.28580
H 5.35042 0.45197 -2.24302
H 4.47145 1.57761 -1.17271
H 5.41379 0.21647 -0.48394
H 4.70400 -1.90849 -2.44785
H 4.56371 -2.19400 -0.69239
H 3.19735 -2.56925 -1.75656
H 3.36825 -0.18939 -3.61052
H 1.80333 -0.56945 -2.83151
H 2.47876 1.07441 -2.71400
H -2.72174 -0.34288 3.78512
H -1.45973 -0.95828 2.66550
H -1.73707 0.78975 2.81636
H -4.78123 0.72730 2.94833
H -3.88051 1.86326 1.90588
H -5.17767 0.85246 1.21891
H -4.44368 -1.78286 2.74608
H -4.86654 -1.68257 1.02300
H -3.33934 -2.46433 1.53130
H -3.19161 0.07976 -3.63764
H -2.59691 1.40298 -2.59616
H -1.64817 -0.10296 -2.73930
H -4.23548 -1.95371 -2.70599
H -2.68953 -2.33150 -1.91105
H -4.20613 -2.32805 -0.96697
H -5.35190 0.32787 -2.38368
H -5.49960 -0.11072 -0.66866
H -4.74406 1.44588 -1.13387
H 2.11962 4.25218 -0.48473
H -0.04942 5.56229 -0.46446
H -2.23439 4.28747 -0.22903
H -0.59200 -4.41765 0.53489
H -1.01161 -3.02821 1.58285
H -1.83648 -3.24146 -0.00479
H 0.47554 -4.04393 -1.57813
H -0.66397 -2.73061 -2.06192
H 1.09291 -2.42224 -2.01920
H 1.94773 -4.00253 0.31954
H 2.40591 -2.04893 0.31594
H 1.37555 -2.80172 1.86956

Alternative Dehydrogenation Pathways from 3.

TS(3-1)$_{concerted1}$

SCF = -1314.48903314
H(0 K)= -1313.816000
H(298 K)= -1313.774315
G(298 K)= -1313.886260
SCF (Corr) = -1984.84198582
Low Freq. = -295.0495cm-1, 14.8966cm-1

80
C 1.14164 -3.57741 -1.52883
C -0.08338 -4.18375 -1.83017
C -1.28771 -3.52834 -1.54918
C -1.22673 -2.24560 -0.98493
N -0.04067 -1.60499 -0.74117
C 1.12136 -2.29285 -0.96617
O -2.37970 -1.62804 -0.66405
P -2.33999 -0.05733 0.14774
C -3.13761 -0.54197 1.82645

C	-3.10951	0.70884	2.73587
Rh	-0.00340	0.25960	0.24977
P	2.31102	-0.12618	0.13803
C	3.11307	-0.59266	1.81610
C	4.49615	-1.25844	1.68329
O	2.29159	-1.71960	-0.62704
C	-3.54802	0.80179	-1.09247
C	-2.68327	1.10295	-2.33963
C	-4.71086	-0.12492	-1.51751
C	-4.12125	2.09504	-0.47475
C	3.56016	0.66272	-1.11834
C	2.69119	1.21290	-2.27304
C	4.37281	1.79364	-0.45259
C	4.53865	-0.39129	-1.68819
C	3.19055	0.70011	2.66215
C	2.12315	-1.57749	2.48149
C	-4.56923	-1.09848	1.70754
C	-2.20508	-1.62568	2.41688
H	-0.09996	-5.18574	-2.26864
H	-3.29495	1.65963	-3.07201
H	-1.79331	1.70648	-2.10505
H	-2.34646	0.17344	-2.82861
H	-4.70219	2.62600	-1.25017
H	-4.81285	1.87955	0.35632
H	-3.34320	2.78002	-0.10543
H	-5.27003	0.39253	-2.31804
H	-4.35627	-1.08390	-1.92215
H	-5.41960	-0.32538	-0.70210
H	-2.54733	-1.87205	3.43789
H	-2.21765	-2.55513	1.82481
H	-1.16230	-1.26773	2.49644
H	-4.88106	-1.47640	2.69811
H	-5.29463	-0.32278	1.41591
H	-4.63504	-1.93654	0.99558
H	-3.48703	0.42202	3.73387
H	-2.09021	1.10830	2.86099
H	1.11944	-1.12915	2.59460
H	2.49147	-1.82496	3.49324
H	-3.75278	1.52061	2.36124
H	2.03106	-2.52043	1.91819
H	3.52435	0.43435	3.68116
H	3.91319	1.42755	2.26102
H	2.20796	1.19403	2.75219
H	4.82873	-1.58521	2.68514
H	4.46405	-2.14958	1.03612
H	5.26199	-0.56693	1.29832
H	5.20670	0.12708	-2.39958
H	5.17291	-0.85166	-0.91670
H	4.01902	-1.19103	-2.23448
H	3.35332	1.66442	-3.03361
H	2.11838	0.41034	-2.76826
H	1.97906	1.98133	-1.93443
H	4.95458	2.31085	-1.23647
H	3.74576	2.55228	0.03737
H	5.09492	1.40689	0.28407
H	0.09611	1.47865	1.33916
H	2.09983	-4.07000	-1.69978
H	-2.26185	-3.98231	-1.73628
B	-0.45162	2.80807	0.96639
N	0.12735	3.35475	-0.32354
H	-1.65311	2.76902	1.01550
H	0.09033	3.15160	2.00396
C	-0.75054	4.13619	-1.20549
C	1.43233	4.00916	-0.18260
H	0.12466	1.56384	-0.66182
H	-0.29964	4.24396	-2.20838
H	-1.72814	3.64759	-1.31003
H	-0.92200	5.15576	-0.80120
H	1.93841	4.12642	-1.15782
H	1.32045	5.01827	0.26654
H	2.07124	3.42058	0.49177

TS(3-1)$_{concerted2}$

SCF = -1314.48200677
H(0 K)= -1313.810038
H(298 K)= -1313.767307
G(298 K)= -1313.882581
SCF (Corr) = -1984.83260740
Low Freq. = -1180.4201cm-1, 20.6198cm-1

80

C	-0.00008	-4.56891	-0.61626
C	1.21352	-3.87965	-0.51484
C	1.17155	-2.48781	-0.34441
N	-0.00003	-1.77759	-0.33346
C	-1.17164	-2.48774	-0.34463
C	-1.21366	-3.87958	-0.51507
O	2.33253	-1.82906	-0.16548
P	2.30428	-0.07558	0.07779
C	3.16830	0.00210	1.79563
Rh	-0.00000	0.29077	0.10798
P	-2.30431	-0.07550	0.07774
C	-3.48407	0.27384	-1.42529
O	-2.33261	-1.82893	-0.16593
C	3.48391	0.27343	-1.42545
B	0.00004	2.61626	-1.59198
N	0.00019	3.52034	-0.39166
C	-3.16820	0.00186	1.79566
H	-2.18048	-4.38424	-0.53924
H	-0.00010	-5.65507	-0.74569
H	2.18032	-4.38436	-0.53883
C	-4.57793	-0.61789	1.84804
C	-2.22887	-0.77312	2.75009
C	-3.21451	1.48751	2.21986
C	-4.73216	-0.63793	-1.43398
C	-3.92688	1.75021	-1.43701
C	-2.63473	-0.05114	-2.67880
C	4.57792	-0.61791	1.84806
C	3.21488	1.48783	2.21947
C	2.22890	-0.77249	2.75032
C	4.73193	-0.63842	-1.43413
C	2.63438	-0.05169	-2.67880
C	3.92681	1.74977	-1.43751
H	-1.05107	2.40506	-2.11705
H	1.05105	2.40492	-2.11722
H	-0.00001	1.58771	1.07414
C	-1.23188	4.26584	-0.04272
H	0.00015	2.37648	0.24890
C	1.23238	4.26575	-0.04293
H	3.21335	0.22397	-3.57866
H	2.41394	-1.12954	-2.74499
H	1.68239	0.50014	-2.70284
H	5.21550	-0.53544	-2.42265
H	5.47588	-0.35171	-0.67773
H	4.47626	-1.69969	-1.29804
H	4.56851	1.91921	-2.32099
H	3.07558	2.44225	-1.52120
H	4.52367	2.01697	-0.54952
H	4.89265	-0.68466	2.90526
H	4.60176	-1.63612	1.42912
H	5.32614	-0.00090	1.32712
H	3.61419	1.55164	3.24765
H	3.87672	2.09137	1.57596
H	2.21046	1.94378	2.22279

```
H   2.60474 -0.66556  3.78396
H   1.19882 -0.37580  2.71723
H   2.19904 -1.84815  2.51226
H  -3.61368  1.55113  3.24811
H  -2.21003  1.94331  2.22315
H  -3.87636  2.09129  1.57658
H  -4.89257 -0.68491  2.90526
H  -5.32609 -0.00056  1.32738
H  -4.60203 -1.63596  1.42878
H  -2.60462 -0.66640  3.78379
H  -2.19920 -1.84872  2.51176
H  -1.19873 -0.37659  2.71704
H  -4.56874  1.91985 -2.32035
H  -4.52355  2.01729 -0.54886
H  -3.07562  2.44264 -1.52075
H  -5.21569 -0.53495 -2.42253
H  -4.47657 -1.69922 -1.29788
H  -5.47612 -0.35116 -0.67762
H  -3.21372  0.22488 -3.57854
H  -1.68262  0.50050 -2.70279
H  -2.41452 -1.12902 -2.74527
H  -1.16902  4.63084  0.99556
H  -1.36586  5.12970 -0.71566
H  -2.10260  3.60266 -0.13650
H   1.16982  4.63056  0.99543
H   2.10306  3.60257 -0.13708
H   1.36618  5.12972 -0.71576
```

TS(3-1)$_{NH}$

```
SCF  =          -1314.45230236
H(0 K)=         -1313.777272
H(298 K)=       -1313.736008
G(298 K)=       -1313.845277
SCF (Corr) =    -1984.81195635
Low Freq. = -801.8131cm-1, 24.9289cm-1

80
C  -1.12536  2.38298 -0.20594
N   0.06299  1.68780 -0.12266
C   1.23298  2.40863 -0.07726
C   1.26336  3.80678 -0.12438
C   0.04582  4.49322 -0.21532
C  -1.15882  3.78865 -0.25355
Rh  0.06643 -0.34775 -0.13587
N  -0.17658 -2.69629 -0.02598
B  -1.60306 -3.11897  0.62929
H  -1.46682 -3.13320  1.83795
O   2.40079  1.74498  0.02291
P   2.37677 -0.01326  0.02022
C   3.30516 -0.27942  1.69856
C   2.21111 -0.23456  2.79089
O  -2.27294  1.71394 -0.24993
P  -2.30037 -0.07870  0.01872
C  -3.18677 -0.01542  1.77692
C  -2.07071 -0.19737  2.82914
C  -3.53612 -0.33017 -1.47898
C  -4.01976 -1.78677 -1.63099
C  -4.76600  0.59341 -1.31369
C  -2.74784  0.09634 -2.74066
C  -3.85761  1.36190  1.99395
C  -4.24915 -1.12445  1.93423
C   3.49463 -0.26213 -1.52914
C   4.86440  0.43499 -1.40415
C   3.68743 -1.77231 -1.78912
C   2.69426  0.36128 -2.69866
C   4.00747 -1.65431  1.71142
C   4.33507  0.83864  1.97586
H  -1.94392 -4.17959  0.14073
H   2.22705  4.31646 -0.08791
H   0.03952  5.58639 -0.25264
H  -2.12858  4.28405 -0.31814
H  -0.01644 -1.64566  0.80457
C  -0.22909 -2.84242 -1.51896
C   0.89695 -3.59589  0.49810
H  -2.36703 -2.19287  0.29531
H  -3.39131 -0.05339 -3.62608
H  -2.46350  1.15981 -2.71033
H  -1.83360 -0.50266 -2.89258
H  -5.36949  0.52239 -2.23673
H  -5.41475  0.28158 -0.48026
H  -4.48624  1.64810 -1.17720
H  -4.71840 -1.82316 -2.48665
H  -3.20469 -2.49613 -1.83603
H  -4.55923 -2.14906 -0.74323
H  -4.34234  1.33574  2.98636
H  -3.13342  2.18973  1.99899
H  -4.63630  1.58696  1.25093
H  -2.51956 -0.10804  3.83538
H  -1.59800 -1.18868  2.75620
H  -1.28980  0.57665  2.74014
H  -4.67787 -1.04089  2.94938
H  -5.08324 -1.01187  1.22337
H  -3.82702 -2.13392  1.83252
H   3.23553  0.17036 -3.64258
H   1.68576 -0.07959 -2.79314
H   2.58884  1.45264 -2.59006
H   5.37605  0.38253 -2.38231
H   4.76675  1.49861 -1.13592
H   5.51957 -0.06010 -0.66986
H   4.26019 -1.89853 -2.72528
H   4.25216 -2.27759 -0.99048
H   2.72874 -2.29915 -1.92748
H   2.69026 -0.35724  3.77899
H   1.67489  0.72907  2.79736
H   1.46345 -1.03572  2.67123
H   4.77611  0.65273  2.97176
H   5.15937  0.85346  1.24864
H   3.86965  1.83497  1.99437
H   4.39864 -1.83778  2.72809
H   3.32714 -2.48795  1.47359
H   4.86664 -1.69191  1.02268
H   0.58593 -4.63556  0.30012
H   1.85827 -3.39894 -0.00073
H   0.99101 -3.46056  1.58492
H  -0.43056 -3.90957 -1.72969
H  -1.05481 -2.24639 -1.92613
H   0.71926 -2.54485 -1.99171
```

Int(3-1)$_{NH1}$

```
SCF  =          -1314.49023712
H(0 K)=         -1313.813031
H(298 K)=       -1313.771952
G(298 K)=       -1313.881338
SCF (Corr) =    -1984.85207847
Low Freq. = 13.9563cm-1, 24.3693cm-1

80
C  -1.09845  2.36338 -0.21702
N   0.09026  1.66751 -0.14286
C   1.26331  2.37358 -0.14512
C   1.31454  3.76693 -0.24267
C   0.09893  4.46176 -0.33371
C  -1.11255  3.77167 -0.32130
Rh  0.05706 -0.40695 -0.00851
```

```
N  -0.23015 -2.51471  0.01143
B  -1.64954 -2.83732  0.65951
H  -1.58875 -2.73785  1.86474
O   2.43022  1.69247 -0.05273
P   2.40858 -0.05717  0.05712
C   3.44985 -0.18850  1.67579
C   2.58299  0.46773  2.77658
O  -2.24401  1.70561 -0.19801
P  -2.31534 -0.15145  0.06557
C  -3.34276  0.00970  1.74134
C  -2.32236 -0.03051  2.90101
C  -3.39499 -0.34656 -1.56615
C  -3.87304 -1.79522 -1.78586
C  -4.62946  0.58188 -1.51147
C  -2.48184  0.09405 -2.73450
C  -4.10489  1.35399  1.81308
C  -4.35458 -1.14896  1.87498
C   3.37834 -0.40867 -1.57572
C   4.58195  0.53079 -1.79839
C   3.83775 -1.88166 -1.60355
C   2.33358 -0.15027 -2.69102
C   3.70604 -1.66701  2.03594
C   4.79113  0.56732  1.55828
H  -2.10933 -3.88825  0.24916
H   2.28308  4.26853 -0.24325
H   0.10338  5.55304 -0.41104
H  -2.07687  4.27805 -0.38408
H   0.00543 -0.39143  1.50220
C  -0.18006 -2.95018 -1.41092
C   0.75511 -3.33648  0.76931
H  -2.46837 -1.93104  0.24978
H  -3.03404 -0.02863 -3.68354
H  -2.18891  1.15220 -2.65339
H  -1.56719 -0.52007 -2.81339
H  -5.13174  0.53631 -2.49493
H  -5.36418  0.25165 -0.76001
H  -4.35983  1.62997 -1.31858
H  -4.47736 -1.81960 -2.71088
H  -3.04860 -2.51323 -1.90812
H  -4.50901 -2.15695 -0.96314
H  -4.65890  1.36100  2.76887
H  -3.43131  2.22187  1.80685
H  -4.83984  1.47952  1.00588
H  -2.87243  0.07315  3.85407
H  -1.77017 -0.98206  2.93457
H  -1.60668  0.80781  2.84375
H  -4.90038 -1.01801  2.82669
H  -5.10710 -1.14021  1.06943
H  -3.87354 -2.13723  1.90119
H   2.79111 -0.37071 -3.67231
H   1.44335 -0.79792 -2.59580
H   2.00394  0.90190 -2.71097
H   4.94942  0.38072 -2.82981
H   4.30628  1.59073 -1.69084
H   5.41957  0.31443 -1.12013
H   4.24110 -2.11105 -2.60613
H   4.64188 -2.07914 -0.87675
H   3.01575 -2.59271 -1.41410
H   3.12417  0.39605  3.73678
H   2.39559  1.53512  2.57782
H   1.61377 -0.04402  2.90459
H   5.24075  0.63026  2.56549
H   5.51081  0.03657  0.91633
H   4.66542  1.59467  1.18363
H   4.29230 -1.69845  2.97159
H   2.77297 -2.22060  2.21658
H   4.29104 -2.20034  1.26978
H   0.45105 -4.39998  0.73582
H   1.76340 -3.24382  0.33418
H   0.76788 -3.01491  1.81936
H  -0.46764 -4.01614 -1.48645
H  -0.89542 -2.37014 -2.01444
H   0.83346 -2.82694 -1.82968
```

Int(3-1)$_{NH2}$

```
SCF  =          -1314.49347724
H(0 K)=         -1313.814193
H(298 K)=       -1313.772093
G(298 K)=       -1313.885592
BP86 (D3) =     -1.17646507316
SCF (Corr) =    -1984.85507582
Low Freq. = 23.0470cm-1, 28.8021cm-1

80
C  -1.46826 -2.43922 -0.11709
N  -0.23370 -1.83487 -0.04515
C   0.87173 -2.65348 -0.05101
C   0.78142 -4.05079 -0.10312
C  -0.48745 -4.63584 -0.16155
C  -1.63038 -3.82942 -0.17181
Rh -0.05308  0.19124  0.05642
N   1.12068  3.51961  0.03137
B   1.00502  4.01714 -1.53907
H   1.98187  4.71277 -1.74261
O   2.09682 -2.09337 -0.01230
P   2.20888 -0.33944  0.01401
C   3.24308 -0.10620 -1.59427
C   2.21742 -0.23731 -2.74620
O  -2.57309 -1.66557 -0.14439
P  -2.36310  0.07022  0.00117
C  -3.27390  0.61069 -1.60330
C  -2.27477  0.31995 -2.74957
C  -3.34890  0.35016  1.62863
C  -3.18557  1.82810  2.05008
C  -4.84153 -0.01604  1.51208
C  -2.66526 -0.55619  2.68019
C  -4.57576 -0.18145 -1.85070
C  -3.55826  2.12717 -1.53162
C   3.21462 -0.15926  1.64493
C   4.61301 -0.80468  1.58398
C   3.33305  1.34419  1.98213
C   2.36122 -0.85445  2.73259
C   3.86146  1.30858 -1.60896
C   4.33927 -1.18088 -1.75972
H  -0.05749  4.61591 -1.59876
H   1.70110 -4.63758 -0.10209
H  -0.58609 -5.72410 -0.20391
H  -2.63997 -4.23943 -0.22436
H   2.00483  2.99832  0.12254
C   0.00816  2.58804  0.36028
C   1.16659  4.67154  0.98397
H   0.99919  2.97764 -2.19039
H  -3.10715 -0.34479  3.67035
H  -2.82004 -1.62543  2.46511
H  -1.57950 -0.36378  2.74301
H  -5.29057  0.01541  2.52135
H  -5.39945  0.69885  0.88694
H  -4.99148 -1.03190  1.11348
H  -3.72242  1.98370  3.00290
H  -2.12921  2.09024  2.22687
H  -3.60940  2.53490  1.31866
H  -4.95223  0.08460 -2.85475
H  -4.40541 -1.26903 -1.83538
H  -5.36892  0.06020 -1.12909
H  -2.73659  0.62833 -3.70478
```

```
H  -1.33042  0.87702 -2.63163
H  -2.03763 -0.75442 -2.82591
H  -3.96436  2.45424 -2.50531
H  -4.30968  2.37924 -0.76559
H  -2.64683  2.72402 -1.35424
H   2.82216 -0.66970  3.71948
H   1.32926 -0.46091  2.75687
H   2.31519 -1.94441  2.58161
H   5.05234 -0.79156  2.59794
H   4.57044 -1.85463  1.25415
H   5.30077 -0.25192  0.92462
H   3.87751  1.45391  2.93708
H   3.89919  1.91150  1.22430
H   2.34220  1.80995  2.12614
H   2.74658 -0.09435 -3.70556
H   1.75038 -1.23636 -2.77038
H   1.42271  0.52397 -2.67995
H   4.77890 -1.06456 -2.76660
H   5.15646 -1.07604 -1.03195
H   3.93333 -2.20142 -1.68784
H   4.38824  1.44760 -2.57006
H   3.09903  2.10625 -1.56523
H   4.60871  1.45396 -0.81115
H   0.24660  5.25906  0.85026
H   1.25303  4.32830  2.02882
H   2.02491  5.30145  0.71367
H  -0.93122  3.15289  0.29610
H  -0.02535  1.88160 -0.57429
H   0.10854  2.13639  1.36867
```

TS(1-3)$_{BH1}$

```
SCF  =          -1315.66799222
H(0 K)=         -1314.972668
H(298 K)=       -1314.930668
G(298 K)=       -1315.042876
SCF (Corr) =    -1986.02532325
Low Freq. = -450.7307cm-1, 10.1419cm-1

82
C   1.05570 -1.69969 -1.67733
C   1.03057 -2.66478 -2.69362
C  -0.20086 -3.26171 -2.99672
C  -1.35812 -2.89899 -2.29619
C  -1.24585 -1.91080 -1.30493
N  -0.06366 -1.30597 -1.00865
O  -2.34446 -1.55341 -0.60403
P  -2.35750 -0.02719  0.29519
C  -3.53601  0.91892 -0.93774
C  -3.80887  2.35627 -0.43538
Rh  0.01305  0.26916  0.47110
B  -0.01994  2.25770 -0.70875
N   0.89475  3.58318 -0.32493
C   3.38494  1.57605 -1.51842
C   3.71624  0.94009 -0.14572
C   5.14598  0.36745 -0.23892
O   2.24142 -1.13851 -1.32207
P   2.27435 -0.29869  0.22183
C   2.89203 -1.77821  1.34435
C   1.79487 -2.87003  1.39053
C  -3.39151 -0.64472  1.83936
C  -2.44452 -1.14864  2.94847
C  -4.19502  0.54861  2.40649
C  -4.33192 -1.81397  1.46317
C   4.16080 -2.46145  0.77929
C   3.14867 -1.22378  2.76210
C  -2.78460  0.94498 -2.29241
C  -4.88069  0.19281 -1.16056
C   3.67471  1.97782  1.00409
H   0.36587  1.91600 -1.80972
H  -1.12625  2.73844 -0.72662
H  -0.25693 -4.02192 -3.78118
H  -3.36513  1.57135 -2.99393
H  -1.77428  1.37068 -2.21824
H  -2.71816 -0.06241 -2.73441
H  -4.31946  2.91214 -1.24284
H  -4.47177  2.37494  0.44182
H  -2.88588  2.90144 -0.19125
H  -5.40456  0.70203 -1.99024
H  -4.74310 -0.85975 -1.45350
H  -5.54652  0.24106 -0.28515
H  -3.06658 -1.53679  3.77481
H  -1.79898 -1.97573  2.60919
H  -1.81136 -0.34677  3.35872
H  -4.88508 -2.10837  2.37340
H  -5.07289 -1.55286  0.69721
H  -3.76810 -2.69140  1.11213
H  -4.63213  0.24646  3.37494
H  -3.56112  1.43194  2.59808
H   0.82672 -2.51068  1.76837
H   2.14012 -3.66599  2.07435
H  -5.02920  0.84771  1.75454
H   1.63513 -3.33439  0.40398
H   3.42437 -2.05864  3.43112
H   3.98301 -0.50291  2.78499
H   2.25605 -0.73868  3.19260
H   4.29345 -3.42262  1.30725
H   4.06468 -2.68730 -0.29473
H   5.07620 -1.87959  0.93949
H   5.81046  1.17731 -0.59256
H   5.53661  0.03592  0.73474
H   5.22359 -0.45892 -0.96146
H   4.01110  2.47704 -1.65572
H   3.62179  0.87713 -2.33569
H   2.32364  1.84427 -1.63631
H   4.26965  2.86635  0.72396
H   2.65014  2.29541  1.26469
H   4.11663  1.57537  1.93047
H   1.95650 -2.93745 -3.20219
H  -2.33141 -3.34825 -2.49904
H   0.06795  1.76580  1.00507
H   0.07459 -0.10166  2.20506
H  -0.04203 -0.88837  1.92021
C   0.88983  4.52960 -1.48914
C   0.46631  4.29948  0.91731
H   1.87214  3.28823 -0.18510
H  -0.58040  4.61102  0.78852
H   0.52987  3.61300  1.77387
H   1.09957  5.18374  1.09367
H  -0.15344  4.80479 -1.70102
H   1.47708  5.43252 -1.25467
H   1.30810  4.01987 -2.36715
```

Int(1-3)$_{BH1}$

```
SCF  =          -1315.67192357
H(0 K)=         -1314.974939
H(298 K)=       -1314.932716
G(298 K)=       -1315.043961
SCF (Corr) =    -1986.03033427
Low Freq. = 23.0413cm-1, 30.7524cm-1

82
C  -1.09677 -1.50470  1.75509
C  -1.08491 -2.40640  2.82917
C   0.12673 -3.04340  3.13151
```

```
C   1.27993 -2.78438  2.37892
C   1.18725 -1.84879  1.33585
N   0.02456 -1.20674  1.04365
O   2.27724 -1.58574  0.57757
P   2.35485 -0.05436 -0.32408
C   3.57220  0.84153  0.91951
C   3.80082  2.30473  0.47364
Rh -0.02351  0.26668 -0.52527
B   0.01341  2.02333  0.83451
N  -0.73321  3.42203  0.37272
C  -3.49963  1.74104  1.34219
C  -3.72664  1.06572 -0.03283
C  -5.18546  0.56427 -0.05962
O  -2.26842 -0.92506  1.38001
P  -2.30270 -0.23476 -0.24151
C  -2.94808 -1.81179 -1.20542
C  -1.89705 -2.94588 -1.11295
C   3.37742 -0.68289 -1.87029
C   2.42267 -1.15811 -2.98600
C   4.18464  0.51350 -2.42844
C   4.30356 -1.86937 -1.51581
C  -4.24819 -2.38939 -0.59261
C  -3.16568 -1.40016 -2.67762
C   2.90069  0.78798  2.31608
C   4.93569  0.12700  1.04836
C  -3.53841  2.05247 -1.21425
H  -0.50675  1.69145  1.88595
H   1.14447  2.41759  0.97912
H   0.16973 -3.75864  3.95814
H   3.49575  1.41785  3.00217
H   1.87093  1.16967  2.32250
H   2.90945 -0.23523  2.72395
H   4.40761  2.81048  1.24679
H   4.35567  2.37547 -0.47370
H   2.85806  2.86147  0.37317
H   5.48721  0.60836  1.87675
H   4.82377 -0.93822  1.30420
H   5.56477  0.21996  0.15017
H   3.04020 -1.48468 -3.84173
H   1.81169 -2.02217 -2.67838
H   1.75827 -0.35547 -3.34320
H   4.80876 -2.19441 -2.44333
H   5.08427 -1.61575 -0.78829
H   3.73265 -2.72592 -1.12585
H   4.63632  0.21096 -3.38997
H   3.54580  1.39069 -2.63263
H  -0.90107 -2.67183 -1.48819
H  -2.25616 -3.78713 -1.73234
H   5.00747  0.82281 -1.76765
H  -1.79156 -3.32258 -0.08289
H  -3.48887 -2.28415 -3.25616
H  -3.95445 -0.63679 -2.78600
H  -2.24530 -1.01648 -3.14946
H  -4.39196 -3.40711 -0.99721
H  -4.18291 -2.47955  0.50369
H  -5.14465 -1.81381 -0.85024
H  -5.83851  1.43205  0.14805
H  -5.48444  0.16796 -1.04187
H  -5.38894 -0.18966  0.71510
H  -4.08080  2.68075  1.38046
H  -3.85840  1.09103  2.15542
H  -2.44220  1.95053  1.56071
H  -4.13675  2.96353 -1.03249
H  -2.48553  2.33541 -1.38407
H  -3.89355  1.61735 -2.16369
H  -2.00620 -2.60695  3.37810
H   2.23379 -3.27374  2.58136
H  -0.07337  1.48659 -1.52674
H  -0.08865 -0.47039 -2.19646
H   0.03526 -1.17485 -1.81104
C  -0.80428  4.34728  1.55250
C  -0.08800  4.12615 -0.77881
H  -1.70311  3.21416  0.09492
H   0.94444  4.37474 -0.49348
H  -0.06561  3.45057 -1.64485
H  -0.63766  5.04929 -1.02400
H   0.22114  4.52284  1.90872
H  -1.27132  5.30373  1.26556
H  -1.38099  3.86853  2.35480
```

TS(1-3)$_{BH2}$

```
SCF  =          -1315.67017251
H(0 K)=         -1314.974899
H(298 K)=       -1314.932646
G(298 K)=       -1315.044137
SCF (Corr) =    -1986.02766937
Low Freq. = -273.8401cm-1, 17.5143cm-1

82
C   1.08725 -1.58217 -1.69746
C   1.07397 -2.52693 -2.73338
C  -0.13759 -3.17602 -3.00880
C  -1.28972 -2.88220 -2.26820
C  -1.19496 -1.90485 -1.26421
N  -0.03063 -1.25585 -0.98970
O  -2.28925 -1.60183 -0.53015
P  -2.35741 -0.03919  0.31422
C  -3.55555  0.82511 -0.96976
C  -3.82319  2.29034 -0.55250
Rh  0.01661  0.30683  0.48845
B  -0.02656  2.06796 -0.82803
N   0.75559  3.44271 -0.36490
C   3.49601  1.69228 -1.41228
C   3.74815  1.02680 -0.03706
C   5.18729  0.47140 -0.05456
O   2.25778 -0.98105 -1.35843
P   2.29805 -0.22836  0.23591
C   2.92291 -1.78253  1.25033
C   1.81239 -2.86416  1.25418
C  -3.40083 -0.62609  1.86090
C  -2.44446 -1.07399  2.98413
C  -4.21549  0.57828  2.38770
C  -4.32319 -1.82169  1.52819
C   4.16456 -2.44886  0.60768
C   3.23708 -1.32141  2.69022
C  -2.84751  0.76436 -2.34714
C  -4.90368  0.08597 -1.11840
C   3.63289  2.03754  1.13283
H   0.48137  1.71737 -1.87785
H  -1.15841  2.46871 -0.93422
H  -0.18182 -3.92459 -3.80529
H  -3.44355  1.36020 -3.06217
H  -1.82997  1.17765 -2.33509
H  -2.81270 -0.26670 -2.73390
H  -4.41196  2.77433 -1.35306
H  -4.41178  2.36339  0.37392
H  -2.89619  2.86804 -0.42694
H  -5.44302  0.54116 -1.96927
H  -4.76918 -0.98262 -1.34768
H  -5.55427  0.18853 -0.23664
H  -3.05688 -1.42639  3.83344
H  -1.79974 -1.91358  2.67637
H  -1.81121 -0.25093  3.34732
H  -4.84615 -2.11196  2.45749
H  -5.08964 -1.59244  0.77774
```

H -3.74788 -2.69289 1.17996
H -4.65950 0.29955 3.36009
H -3.58487 1.46753 2.56309
H 0.83598 -2.50838 1.61065
H 2.13524 -3.67630 1.93009
H -5.04477 0.85920 1.72175
H 1.67595 -3.30857 0.25519
H 3.53818 -2.19943 3.28956
H 4.07565 -0.60593 2.72392
H 2.36829 -0.86440 3.19131
H 4.27997 -3.45135 1.05752
H 4.04378 -2.58847 -0.47840
H 5.09775 -1.90478 0.79505
H 5.86585 1.30722 -0.30666
H 5.50821 0.08313 0.92393
H 5.32953 -0.30704 -0.81890
H 4.11404 2.60571 -1.48788
H 3.79248 1.01641 -2.22943
H 2.44108 1.94680 -1.59173
H 4.25881 2.92259 0.91897
H 2.59714 2.36619 1.32724
H 3.99682 1.60461 2.07962
H 1.99438 -2.74709 -3.27624
H -2.24599 -3.37420 -2.45193
H 0.05194 1.53351 1.48396
H 0.20849 -0.22842 2.37188
H 0.16250 -1.00235 2.46124
C 0.83608 4.36769 -1.54509
C 0.13901 4.15936 0.79539
H 1.72264 3.20710 -0.09807
H -0.89166 4.42896 0.52304
H 0.11467 3.48367 1.66121
H 0.71128 5.07048 1.03303
H -0.18840 4.56893 -1.89039
H 1.32779 5.31201 -1.26033
H 1.39404 3.87778 -2.35392

TS(1-3)$_{NH}$

SCF = -1315.66529167
H(0 K)= -1314.977092
H(298 K)= -1314.934586
G(298 K)= -1315.047162
SCF (Corr) = -1986.02205294
Low Freq. = -878.0562cm-1, 22.9812cm-1

82
C -1.17118 -2.53168 -0.26543
C -1.21281 -3.92211 -0.44420
C 0.00026 -4.61156 -0.54563
C 1.21327 -3.92193 -0.44463
C 1.17150 -2.53151 -0.26584
N 0.00012 -1.82899 -0.23661
O 2.33364 -1.86860 -0.10059
P 2.32719 -0.12213 0.09052
C 3.29948 0.05663 1.75014
C 3.08978 1.51358 2.22423
Rh 0.00005 0.23934 0.17938
P -2.32709 -0.12238 0.09056
C -3.29953 0.05698 1.75002
C -4.80715 -0.24938 1.63920
O -2.33336 -1.86895 -0.09975
C 3.40275 0.23176 -1.48591
C 2.48570 -0.04482 -2.69943
C 3.85629 1.70498 -1.47999
C 4.62836 -0.70798 -1.58345
C -3.40263 0.23081 -1.48603
C -2.48535 -0.04551 -2.69943
C -4.62783 -0.70945 -1.58361
C -3.85677 1.70385 -1.48026
C 2.66532 -0.92097 2.76513
C 4.80715 -0.24946 1.63935
C -2.66537 -0.92010 2.76552
C -3.09007 1.51416 2.22349
B -0.00046 2.88069 -1.72144
N -0.00049 3.59975 -0.43081
C -1.21711 4.27628 0.05176
C 1.21618 4.27611 0.05188
H 0.00031 -5.69634 -0.68497
H 3.14160 -0.75583 3.74805
H 1.58191 -0.75584 2.88219
H 2.83306 -1.97178 2.48037
H 3.60516 1.64795 3.19189
H 3.51288 2.25305 1.52344
H 2.02329 1.74439 2.37943
H 5.24349 -0.19319 2.65280
H 5.00136 -1.26204 1.25305
H 5.34406 0.48258 1.01618
H 3.04759 0.19928 -3.61863
H 2.20341 -1.10933 -2.76012
H 1.56942 0.56298 -2.68438
H 5.05490 -0.59015 -2.59572
H 5.42192 -0.46097 -0.86647
H 4.35385 -1.76656 -1.46136
H 4.45059 1.89515 -2.39169
H 3.00022 2.39651 -1.50426
H -1.56913 0.56239 -2.68418
H -3.04712 0.19858 -3.61870
H 4.49873 1.94962 -0.61753
H -2.20290 -1.10999 -2.76016
H -4.45043 1.89394 -2.39239
H -4.49994 1.94809 -0.61823
H -3.00095 2.39573 -1.50374
H -5.05450 -0.59165 -2.59583
H -4.35280 -1.76792 -1.46172
H -5.42143 -0.46295 -0.86653
H -5.24366 -0.19246 2.65255
H -5.34407 0.48215 1.01544
H -5.00115 -1.26226 1.25358
H -3.14207 -0.75485 3.74822
H -2.83260 -1.97105 2.48101
H -1.58206 -0.75452 2.88293
H -3.60543 1.64884 3.19112
H -2.02360 1.74520 2.37857
H -3.51330 2.25326 1.52240
H -0.00002 1.62087 1.06336
H -2.18072 -4.42389 -0.48072
H 2.18124 -4.42358 -0.48149
H 0.00042 1.08269 -1.34283
H -1.04535 2.78334 -2.30708
H 1.04433 2.78370 -2.30736
H -0.00040 2.13080 0.24609
H 1.21371 4.33950 1.15555
H 2.11026 3.72493 -0.26962
H 1.28211 5.30572 -0.34710
H -1.21569 4.33802 1.15553
H -1.28181 5.30656 -0.34571
H -2.11131 3.72637 -0.27154
H -0.00006 -0.31805 1.67857

Alternative Dehydrogenation Pathways from 4.

TS(4-4)1

SCF = -1315.25522724

```
H(0 K)=          -1314.571897
H(298 K)=        -1314.530288
G(298 K)=        -1314.640564
SCF (Corr) =     -1985.57584587
Low Freq. = -332.8164cm-1, 28.3797cm-1

81
N    0.00000  1.86064 -0.17606
C    1.16784  2.55479 -0.17038
C    1.21588  3.95879 -0.18729
C    0.00001  4.65704 -0.20135
C   -1.21586  3.95880 -0.18728
C   -1.16783  2.55479 -0.17037
O    2.32426  1.85304 -0.15031
H    2.18297  4.46500 -0.18683
H    0.00001  5.75136 -0.21457
H   -2.18295  4.46502 -0.18681
O   -2.32425  1.85305 -0.15029
Rh   0.00000 -0.32357 -0.12102
P   -2.24755  0.07036 -0.00165
C   -3.48408 -0.25895 -1.47295
C   -3.16264 -0.04750  1.71955
P    2.24755  0.07035 -0.00166
H    0.00000 -0.95869 -1.66521
C   -4.67239  0.72739 -1.53692
C   -2.65437 -0.08364 -2.76602
C   -3.99664 -1.71180 -1.38373
C   -4.62936  0.42266  1.71368
C   -3.07816 -1.51101  2.19926
C    3.48408 -0.25898 -1.47295
C    3.16264 -0.04749  1.71955
C    3.99663 -1.71183 -1.38372
C    2.65438 -0.08367 -2.76602
C    4.67240  0.72736 -1.53692
C    3.07816 -1.51100  2.19928
C    4.62936  0.42267  1.71367
C    2.35607  0.84380  2.69012
H    0.00000 -0.76798  1.48217
B   -0.00001 -2.40789 -1.27655
N   -0.00002 -3.39909  0.10564
H   -1.00359 -2.74364 -1.88591
H    1.00355 -2.74366 -1.88592
H   -0.00004 -2.65168  0.83461
C   -1.22460 -4.23046  0.23167
C    1.22458 -4.23042  0.23171
C   -2.35607  0.84378  2.69013
H   -3.31520 -0.26625 -3.63467
H   -2.25647  0.94125 -2.85373
H   -1.80836 -0.78384 -2.81281
H   -5.19390  0.57566 -2.50081
H   -5.41125  0.56904 -0.73933
H   -4.33397  1.77409 -1.49817
H   -4.62814 -1.92832 -2.26611
H   -3.16275 -2.43274 -1.39086
H   -4.61824 -1.88524 -0.48832
H   -5.00110  0.44072  2.75585
H   -4.73460  1.44058  1.30577
H   -5.28763 -0.25737  1.14868
H   -2.73522  0.68863  3.71770
H   -1.28470  0.58127  2.66861
H   -2.46549  1.91230  2.44412
H   -3.50245 -1.58688  3.21818
H   -3.64877 -2.20051  1.55310
H   -2.02799 -1.84597  2.23940
H    3.31520 -0.26629 -3.63467
H    1.80836 -0.78387 -2.81281
H    2.25648  0.94122 -2.85374
H    5.19390  0.57562 -2.50082
H    4.33398  1.77406 -1.49819
H    5.41125  0.56902 -0.73933
H    4.62815 -1.92835 -2.26609
H    4.61823 -1.88527 -0.48830
H    3.16274 -2.43276 -1.39085
H    2.73521  0.68866  3.71769
H    2.46549  1.91231  2.44410
H    1.28470  0.58128  2.66860
H    5.00110  0.44073  2.75584
H    5.28763 -0.25737  1.14868
H    4.73460  1.44058  1.30576
H    3.50245 -1.58686  3.21820
H    2.02799 -1.84596  2.23942
H    3.64877 -2.20050  1.55313
H   -1.20990 -4.82157  1.16434
H   -2.09993 -3.56689  0.22812
H   -1.28634 -4.90626 -0.63525
H    1.20988 -4.82153  1.16438
H    1.28639 -4.90621 -0.63520
H    2.09990 -3.56681  0.22820
```

Int(4-4)1

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SCF  =           -1315.26431493
H(0 K)=          -1314.578894
H(298 K)=        -1314.537201
G(298 K)=        -1314.648163
SCF (Corr) =     -1985.58633570
Low Freq. = 25.1338cm-1, 27.8278cm-1

81
N   -0.15979  1.88173 -0.17021
C   -1.36608  2.49622 -0.10971
C   -1.49809  3.89604 -0.15040
C   -0.32491  4.65960 -0.22311
C    0.93194  4.03887 -0.23633
C    0.96637  2.63346 -0.19242
O   -2.47623  1.73087  0.00822
H   -2.49098  4.34774 -0.11351
H   -0.39030  5.75184 -0.25518
H    1.86518  4.60410 -0.26626
O    2.16117  1.99899 -0.16607
Rh  -0.03780 -0.29892  0.08017
P    2.19291  0.21665  0.04372
C    3.21831  0.15410  1.69910
C    3.36052 -0.05938 -1.50139
P   -2.29576 -0.04820  0.05328
H   -0.01402 -0.05965  1.69770
C    4.70135  0.55912  1.61018
C    2.50684  1.09878  2.69273
C    3.09633 -1.30123  2.20526
C    4.54631  0.92806 -1.59734
C    3.88245 -1.51094 -1.47997
C   -3.43867 -0.37330  1.59489
C   -3.27141 -0.39707 -1.59313
C   -3.99024 -1.81530  1.51334
C   -2.54368 -0.25748  2.84819
C   -4.59189  0.64634  1.72690
C   -3.12084 -1.89810 -1.91964
C   -4.75842  0.00704 -1.55873
C   -2.56381  0.42681 -2.69338
H   -0.06241 -0.78711 -1.51452
B   -0.18640 -2.40764  0.70331
N    0.87009 -3.41204 -0.10494
H    0.13156 -2.55997  1.87713
H   -1.27102 -2.93723  0.47080
H    1.75330 -2.88259 -0.12930
C    1.09963 -4.68226  0.64158
```

C	0.47448	-3.68866	-1.51378
C	2.47361	0.14930	-2.74845
H	2.94916	0.95748	3.69670
H	2.63636	2.15532	2.40664
H	1.42786	0.87465	2.74919
H	5.13051	0.55248	2.63019
H	5.29816	-0.14488	1.00703
H	4.83212	1.57477	1.20376
H	3.55697	-1.37953	3.20818
H	2.03948	-1.60947	2.28201
H	3.63156	-2.01391	1.55004
H	4.98899	0.84458	-2.60793
H	4.21393	1.96874	-1.46207
H	5.34618	0.71799	-0.87431
H	3.05175	-0.12601	-3.65082
H	1.55167	-0.45320	-2.70175
H	2.17436	1.20616	-2.84863
H	4.51791	-1.68747	-2.36807
H	4.49575	-1.73175	-0.58936
H	3.05692	-2.24262	-1.53403
H	-3.16919	-0.44965	3.74086
H	-1.71336	-0.97919	2.82738
H	-2.10645	0.74985	2.94666
H	-5.12713	0.44372	2.67371
H	-4.21487	1.67987	1.76504
H	-5.32722	0.57815	0.91290
H	-4.51362	-2.04843	2.45973
H	-4.72018	-1.94451	0.69741
H	-3.18073	-2.55299	1.38475
H	-2.98411	0.14014	-3.67563
H	-2.72588	1.50858	-2.55830
H	-1.47922	0.22472	-2.70102
H	-5.18400	-0.12392	-2.57183
H	-5.35623	-0.61708	-0.87520
H	-4.88819	1.06533	-1.27945
H	-3.56549	-2.09764	-2.91305
H	-2.05672	-2.17974	-1.94971
H	-3.62972	-2.54589	-1.18784
H	1.79085	-5.34912	0.09549
H	1.50164	-4.44191	1.63515
H	0.12518	-5.17829	0.76810
H	1.25138	-4.27170	-2.03892
H	-0.46720	-4.25781	-1.49362
H	0.30306	-2.71666	-2.00314

TS(4-4)2

SCF = -1315.24311257
H(0 K)= -1314.564234
H(298 K)= -1314.522509
G(298 K)= -1314.633189
SCF (Corr) = -1985.56322065
Low Freq. = -744.9623cm-1, 17.7423cm-1

81

N	-0.04923	-1.73145	-0.64589
C	1.10237	-2.43002	-0.69704
C	1.14114	-3.77680	-1.10960
C	-0.07542	-4.38185	-1.45382
C	-1.28394	-3.67457	-1.36625
C	-1.21931	-2.33769	-0.93340
O	2.24685	-1.81120	-0.33462
H	2.09240	-4.31095	-1.14570
H	-0.08449	-5.42645	-1.78147
H	-2.24812	-4.12815	-1.60292
O	-2.36324	-1.62218	-0.78921
Rh	-0.03496	0.41467	0.07650
P	-2.29009	-0.05801	0.07731
C	-3.07999	-0.63921	1.75534
C	-3.61738	0.81621	-1.03831
P	2.24997	-0.07192	0.13036
H	-0.05717	-0.07912	1.57962
C	-4.55625	-1.07284	1.66160
C	-2.25314	-1.85248	2.23977
C	-2.92100	0.52012	2.76424
C	-4.75709	-0.11459	-1.51017
C	-4.18726	2.02464	-0.26175
C	-2.86486	1.31332	-2.29272
C	3.16650	-0.32383	1.81841
C	3.55521	0.43626	-1.25625
C	3.27233	1.07156	2.47502
C	2.27147	-1.22577	2.69659
C	4.55047	-0.99427	1.70133
C	4.45524	1.59943	-0.78513
C	4.44597	-0.74505	-1.70545
C	2.72846	0.90499	-2.47402
H	-0.00982	1.20505	-1.51178
B	-0.27233	2.50618	0.95471
N	0.10085	3.38789	-0.29727
C	-0.87820	4.40156	-0.70592
C	1.44583	3.96034	-0.24961
H	0.05300	2.04367	-1.02076
H	0.50301	2.64619	1.88910
H	-1.43863	2.68682	1.26656
H	1.75249	4.36724	-1.23356
H	1.52181	4.77597	0.50118
H	2.15357	3.17227	0.05182
H	-1.86820	3.93796	-0.83540
H	-0.98146	5.20723	0.05306
H	-0.58302	4.87160	-1.66420
H	3.65575	0.95775	3.50631
H	3.96732	1.73822	1.93873
H	2.28714	1.56628	2.52742
H	4.95202	-1.16005	2.71874
H	4.48422	-1.97618	1.20500
H	5.28485	-0.37546	1.16262
H	2.74556	-1.33038	3.69028
H	1.26942	-0.78993	2.83485
H	2.15926	-2.23388	2.26460
H	5.13697	-0.37674	-2.48744
H	5.05729	-1.15948	-0.89100
H	3.85199	-1.56449	-2.13554
H	3.41949	1.13350	-3.30724
H	2.02544	0.12860	-2.81969
H	2.14208	1.81021	-2.25532
H	5.06237	1.94473	-1.64305
H	3.87886	2.46706	-0.42849
H	5.15631	1.29976	0.00971
H	-4.78612	2.64794	-0.95188
H	-4.85412	1.71497	0.55993
H	-3.38981	2.65603	0.16505
H	-3.58952	1.80548	-2.96796
H	-2.07518	2.03673	-2.04595
H	-2.39796	0.48034	-2.84484
H	-5.39557	0.45181	-2.21410
H	-4.36623	-0.99594	-2.04089
H	-5.40097	-0.46055	-0.69035
H	-4.86822	-1.47048	2.64571
H	-5.23193	-0.23559	1.42500
H	-4.70498	-1.87330	0.91872
H	-2.58114	-2.11467	3.26267
H	-2.40778	-2.73592	1.59892
H	-1.17602	-1.62218	2.27370
H	-3.26753	0.17731	3.75744
H	-1.87011	0.83872	2.84914
H	-3.51912	1.40363	2.48810

Int(4-4)2

```
SCF  =          -1154.64704428
H(0 K)=         -1154.069755
H(298 K)=       -1154.034068
G(298 K)=       -1154.134114
SCF (Corr) =    -1824.88077472
Low Freq. = 10.2801cm-1, 22.1738cm-1

69
N  -0.00000  1.46645 -0.16825
C  -1.17520  2.14053 -0.28623
C  -1.21823  3.52549 -0.51975
C  -0.00000  4.20943 -0.63303
C   1.21823  3.52550 -0.51972
C   1.17520  2.14053 -0.28620
O  -2.33462  1.44936 -0.17003
H  -2.18314  4.02773 -0.60655
H  -0.00000  5.28863 -0.81497
H   2.18314  4.02774 -0.60650
O   2.33461  1.44937 -0.16997
Rh -0.00000 -0.63699  0.14907
P   2.24711 -0.31908  0.07524
C   3.36727 -0.38690  1.65387
C   3.20116 -0.91881 -1.50709
P  -2.24711 -0.31908  0.07523
H   0.00001 -0.58142  1.78614
C   4.68513  0.41095  1.53406
C   2.54813  0.22876  2.80989
C   3.63372 -1.87888  1.95159
C   4.72550 -0.69599 -1.50876
C   2.88525 -2.42681 -1.64196
C   2.58720 -0.15707 -2.70324
C  -3.36726 -0.38686  1.65387
C  -3.20115 -0.91886 -1.50709
C  -3.63367 -1.87882  1.95167
C  -2.54814  0.22890  2.80985
C  -4.68515  0.41095  1.53403
C  -2.88525 -2.42686 -1.64190
C  -4.72550 -0.69603 -1.50877
C  -2.58720 -0.15716 -2.70325
H  -0.00001 -1.01719 -1.46162
H  -0.00000 -2.19795  0.37852
H   2.98277 -0.59342 -3.63917
H   1.48855 -0.25287 -2.71274
H   2.85473  0.91202 -2.68393
H   3.31393 -2.79946 -2.59102
H   3.32538 -3.02179 -0.82326
H   1.79722 -2.60146 -1.65321
H   5.12112 -0.99592 -2.49735
H   4.99481  0.36102 -1.35258
H   5.24363 -1.31190 -0.75594
H   5.14422  0.47924  2.53780
H   5.42183 -0.06234  0.87156
H   4.50315  1.43902  1.18131
H   3.13223  0.13071  3.74391
H   2.35751  1.30230  2.64110
H   1.57573 -0.27220  2.93454
H   4.15599 -1.96982  2.92198
H   2.69163 -2.44972  2.02221
H   4.27430 -2.35231  1.18801
H  -3.13224  0.13087  3.74389
H  -1.57573 -0.27203  2.93453
H  -2.35756  1.30243  2.64101
H  -4.15592 -1.96974  2.92207
H  -4.27424 -2.35232  1.18813
H  -2.69156 -2.44963  2.02231
H  -5.14422  0.47930  2.53778
H  -4.50321  1.43900  1.18120
H  -5.42186 -0.06242  0.87159
H  -5.12111 -0.99601 -2.49735
H  -5.24363 -1.31191 -0.75592
H  -4.99481  0.36098 -1.35264
H  -3.31392 -2.79954 -2.59096
H  -1.79722 -2.60151 -1.65314
H  -3.32538 -3.02182 -0.82319
H  -2.98275 -0.59353 -3.63917
H  -2.85472  0.91194 -2.68398
H  -1.48855 -0.25296 -2.71275
```

TS(4-4)3

```
SCF  =          -1154.62574810
H(0 K)=         -1154.052336
H(298 K)=       -1154.016500
G(298 K)=       -1154.115506
SCF (Corr) =    -1824.85972296
Low Freq. = -663.8201cm-1, 20.9569cm-1

69
N  -0.00000  1.42519 -0.35206
C  -1.17420  2.11866 -0.41421
C  -1.21654  3.50854 -0.60023
C  -0.00001  4.19946 -0.70231
C   1.21653  3.50854 -0.60022
C   1.17419  2.11866 -0.41420
O  -2.33290  1.42881 -0.27814
H  -2.18301  4.01302 -0.65182
H  -0.00001  5.28393 -0.84713
H   2.18300  4.01303 -0.65181
O   2.33289  1.42882 -0.27812
Rh -0.00000 -0.69078 -0.16581
P   2.23179 -0.32233  0.05424
C   3.12643 -0.29912  1.77752
C   3.42050 -0.94928 -1.34665
P  -2.23179 -0.32233  0.05423
H  -0.00000 -1.55358  1.21105
C   4.38532  0.59273  1.83415
C   2.08893  0.26787  2.77152
C   3.44948 -1.75975  2.15638
C   4.90477 -0.57286 -1.17661
C   3.26662 -2.48667 -1.40419
C   2.89947 -0.33320 -2.66586
C  -3.12642 -0.29911  1.77752
C  -3.42051 -0.94929 -1.34665
C  -3.44942 -1.75975  2.15642
C  -2.08892  0.26794  2.77150
C  -4.38534  0.59270  1.83415
C  -3.26663 -2.48669 -1.40416
C  -4.90478 -0.57286 -1.17661
C  -2.89947 -0.33323 -2.66586
H   0.00000 -1.30318 -1.75017
H   0.00000 -2.10508 -1.00782
H   3.46413 -0.77270 -3.50921
H   1.82812 -0.54453 -2.81758
H   3.04610  0.75881 -2.68717
H   3.83885 -2.87421 -2.26764
H   3.65653 -2.98191 -0.49914
H   2.21222 -2.78222 -1.53028
H   5.45355 -0.87594 -2.08833
H   5.04754  0.51246 -1.04957
H   5.37657 -1.09558 -0.32895
H   4.69276  0.70245  2.89099
H   5.24011  0.16965  1.28884
H   4.18234  1.60105  1.43881
```

```
H    2.51290  0.22561  3.79233
H    1.84814  1.32152  2.54945
H    1.15178 -0.30967  2.74552
H    3.79382 -1.79880  3.20656
H    2.55637 -2.40408  2.07314
H    4.25200 -2.18698  1.53141
H   -2.51288  0.22568  3.79232
H   -1.15175 -0.30957  2.74550
H   -1.84817  1.32159  2.54941
H   -3.79374 -1.79878  3.20661
H   -4.25193 -2.18701  1.53147
H   -2.55628 -2.40404  2.07319
H   -4.69276  0.70244  2.89099
H   -4.18239  1.60102  1.43878
H   -5.24012  0.16958  1.28887
H   -5.45355 -0.87594 -2.08833
H   -5.37658 -1.09558 -0.32895
H   -5.04754  0.51246 -1.04957
H   -3.83886 -2.87423 -2.26761
H   -2.21224 -2.78224 -1.53025
H   -3.65655 -2.98191 -0.49911
H   -3.46414 -0.77274 -3.50921
H   -3.04610  0.75878 -2.68718
H   -1.82812 -0.54456 -2.81757
```

Int(4-4)3

```
SCF  =          -1154.62961213
H(0 K)=         -1154.054876
H(298 K)=       -1154.019177
G(298 K)=       -1154.116467
SCF (Corr) =    -1824.86326191
Low Freq. = -5.6204cm-1, 41.9243cm-1

69
N  -0.00000  1.41272 -0.44872
C  -1.17553  2.10897 -0.45094
C  -1.21646  3.50627 -0.58745
C   0.00000  4.19778 -0.67283
C   1.21646  3.50627 -0.58745
C   1.17553  2.10897 -0.45093
O  -2.33144  1.42516 -0.29683
H  -2.18227  4.01417 -0.60426
H   0.00000  5.28704 -0.77812
H   2.18227  4.01416 -0.60425
O   2.33144  1.42515 -0.29681
Rh -0.00001 -0.69712 -0.27898
P   2.21871 -0.33151  0.05961
C   3.06420 -0.28860  1.81076
C   3.48889 -0.94307 -1.27923
P  -2.21872 -0.33150  0.05961
H  -0.00001 -2.14316  0.41985
C   4.27137  0.66393  1.93346
C   1.95582  0.19969  2.76806
C   3.44404 -1.73815  2.18057
C   4.96263 -0.56568 -1.03668
C   3.33913 -2.48092 -1.35011
C   3.04105 -0.32360 -2.62331
C  -3.06420 -0.28858  1.81076
C  -3.48890 -0.94309 -1.27923
C  -3.44411 -1.73811  2.18055
C  -1.95578  0.19964  2.76806
C  -4.27131  0.66402  1.93351
C  -3.33921 -2.48095 -1.35000
C  -4.96263 -0.56561 -1.03676
C  -3.04097 -0.32374 -2.62334
H  -0.00001 -1.14081 -2.11367
H  -0.00001 -1.86993 -1.70830
H   3.64891 -0.76016 -3.43773
H   1.98120 -0.53259 -2.84056
H   3.18734  0.76833 -2.63296
H   3.95049 -2.86836 -2.18663
H   3.68507 -2.97848 -0.42875
H   2.29119 -2.77695 -1.52305
H   5.56126 -0.88295 -1.91182
H   5.09768  0.52188 -0.92017
H   5.38851 -1.07221 -0.15554
H   4.53782  0.76578  3.00251
H   5.16498  0.29907  1.40825
H   4.02954  1.66881  1.55149
H   2.33115  0.15909  3.80810
H   1.66367  1.24218  2.55461
H   1.05462 -0.42725  2.68318
H   3.73881 -1.78040  3.24576
H   2.59125 -2.42705  2.04416
H   4.29578 -2.11380  1.58906
H  -2.33109  0.15904  3.80811
H  -1.05461 -0.42733  2.68315
H  -1.66359  1.24213  2.55464
H  -3.73887 -1.78036  3.24575
H  -4.29587 -2.11371  1.58904
H  -2.59135 -2.42705  2.04413
H  -4.53772  0.76589  3.00256
H  -4.02944  1.66888  1.55152
H  -5.16496  0.29920  1.40833
H  -5.56123 -0.88292 -1.91190
H  -5.38856 -1.07204 -0.15560
H  -5.09763  0.52197 -0.92034
H  -3.95056 -2.86842 -2.18651
H  -2.29128 -2.77704 -1.52289
H  -3.68521 -2.97842 -0.42861
H  -3.64881 -0.76033 -3.43775
H  -3.18721  0.76821 -2.63308
H  -1.98112 -0.53279 -2.84052
```

TS(4-4)4

```
SCF  =          -1154.62842193
H(0 K)=         -1154.054941
H(298 K)=       -1154.018272
G(298 K)=       -1154.118993
SCF (Corr) =    -1824.86306319
Low Freq. = -451.6964cm-1, 15.4653cm-1

69
N   0.00358  1.42393 -0.38977
C  -1.17051  2.12351 -0.36294
C  -1.20986  3.52455 -0.45690
C   0.00659  4.21665 -0.53267
C   1.22223  3.52067 -0.48158
C   1.18026  2.11991 -0.38655
O  -2.32900  1.44004 -0.22268
H  -2.17502  4.03397 -0.45101
H   0.00758  5.30857 -0.60561
H   2.18892  4.02704 -0.49480
O   2.33885  1.43196 -0.26933
Rh  0.00084 -0.67939 -0.23624
P   2.22436 -0.33439  0.03983
C   3.06535 -0.34103  1.78851
C   3.48251 -0.90980 -1.32303
P  -2.22088 -0.33336  0.04475
H   0.00045 -2.20396  0.28763
C   4.28954  0.58623  1.93354
C   1.96366  0.14798  2.75417
C   3.41969 -1.80503  2.12660
C   4.95954 -0.54813 -1.07679
```

C	3.32378	-2.44413	-1.43938
C	3.02987	-0.24617	-2.64432
C	-3.07852	-0.38749	1.78507
C	-3.47580	-0.86547	-1.33980
C	-3.49130	-1.84976	2.05904
C	-1.97260	0.01517	2.78496
C	-4.26930	0.57832	1.95521
C	-3.33852	-2.39880	-1.48957
C	-4.94878	-0.48490	-1.09735
C	-3.00322	-0.18045	-2.64317
H	0.00407	-1.06719	-2.16159
H	-0.00168	-1.85713	-2.10551
H	3.63329	-0.65768	-3.47493
H	1.96989	-0.44686	-2.86615
H	3.17864	0.84504	-2.61940
H	3.93106	-2.80943	-2.28882
H	3.67009	-2.97019	-0.53411
H	2.27387	-2.73004	-1.61622
H	5.55163	-0.84006	-1.96509
H	5.10160	0.53416	-0.92507
H	5.38656	-1.08594	-0.21491
H	4.55205	0.66335	3.00554
H	5.17882	0.21358	1.40631
H	4.06847	1.60226	1.56890
H	2.33055	0.06386	3.79467
H	1.70453	1.20494	2.57153
H	1.04483	-0.44880	2.64203
H	3.71977	-1.87363	3.18891
H	2.55381	-2.47472	1.97976
H	4.26169	-2.18326	1.52266
H	-2.36788	-0.07080	3.81498
H	-1.08899	-0.63387	2.68052
H	-1.64620	1.05811	2.63337
H	-3.79756	-1.95087	3.11699
H	-4.34490	-2.16986	1.43844
H	-2.65133	-2.54621	1.88767
H	-4.55670	0.60396	3.02329
H	-3.99979	1.60360	1.65522
H	-5.15795	0.27311	1.38521
H	-5.53949	-0.75176	-1.99443
H	-5.39107	-1.02939	-0.24748
H	-5.07341	0.59708	-0.92854
H	-3.94035	-2.73542	-2.35460
H	-2.29081	-2.69588	-1.66129
H	-3.70328	-2.94080	-0.60135
H	-3.60591	-0.56515	-3.48705
H	-3.13681	0.91203	-2.59627
H	-1.94449	-0.39169	-2.86118

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