--Supporting Information--

Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N_2O by Ru Pincer Complexes

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Table S1. Comparisons of the Gibbs free energies of activation computed from SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 and SMD(THF)-B3LYP-GD3BJ/BS2.

TS	SMD(THF)-B3LYP-GD3BJ/BS2	SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1
TS-1-2	23.2	24.1
TS-2-3	5.0	5.5
TS-3-4	26.9	26.6
TS-1-2b	26.3	26.4
TS-2b-3b	6.0	5.8
TS-1-2d	40.7	40.6
TS-3-4-OH_2	14.3	15.1
TS-3-4-OH_2-b	17.0	16.2
MSD = –0.1, MAD = 0.5		

MSD: mean signed deviation. MAD: mean absolute deviation.

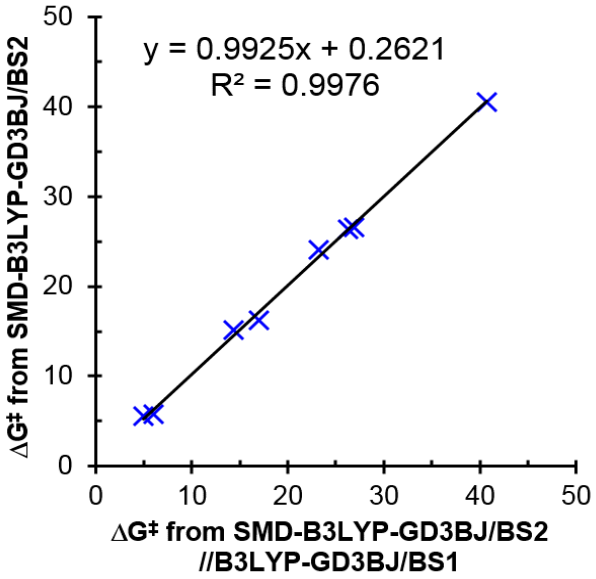
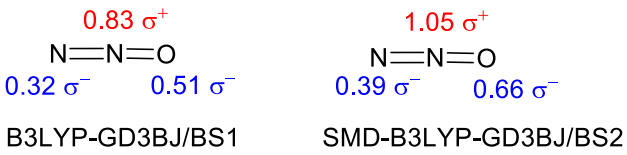


Figure S1. Linear relationship between the SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 computed Gibbs free energies of activation and SMD(THF)-B3LYP-GD3BJ/BS2 computed Gibbs free energies of activation.



Scheme S1. B3LYP-GD3BJ/BS1 and SMD(THF)-B3LYP-GD3BJ/BS2 computed APT charges of N_2O.

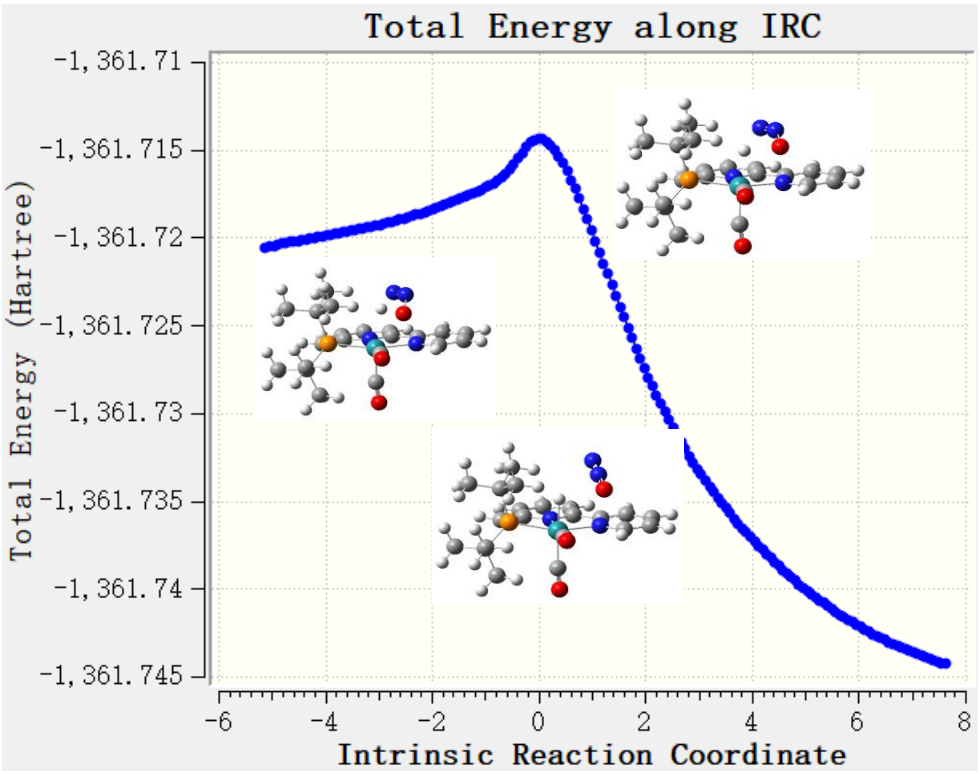


Figure S2. IRC plots for **TS-1-2.**

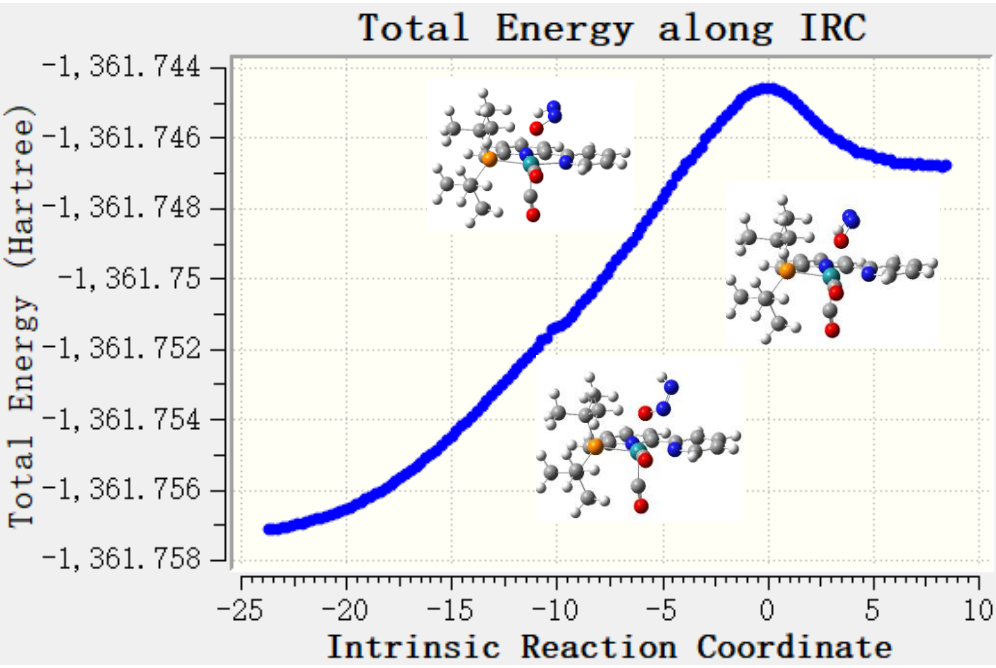


Figure S3. IRC plots for **TS-2-3.**

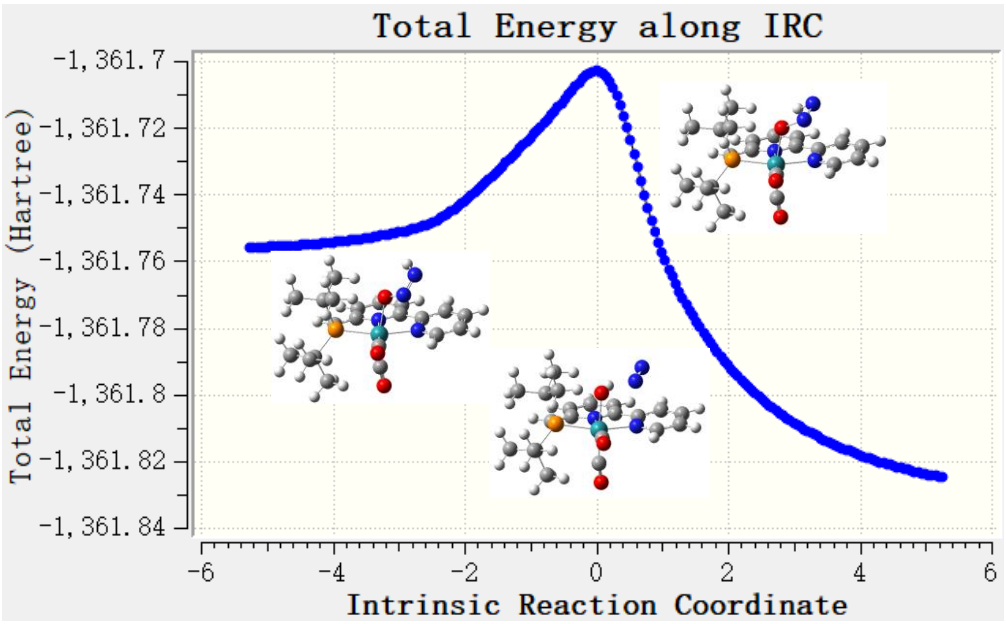


Figure S4. IRC plots for **TS-3-4.**

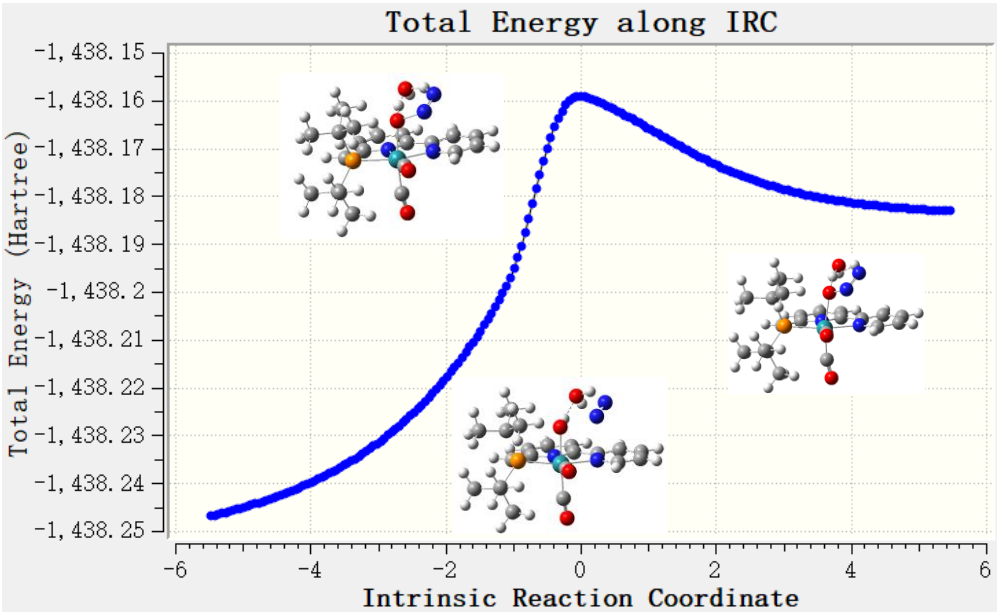


Figure S5. IRC plots for **TS-3-4-OH$_2$.**

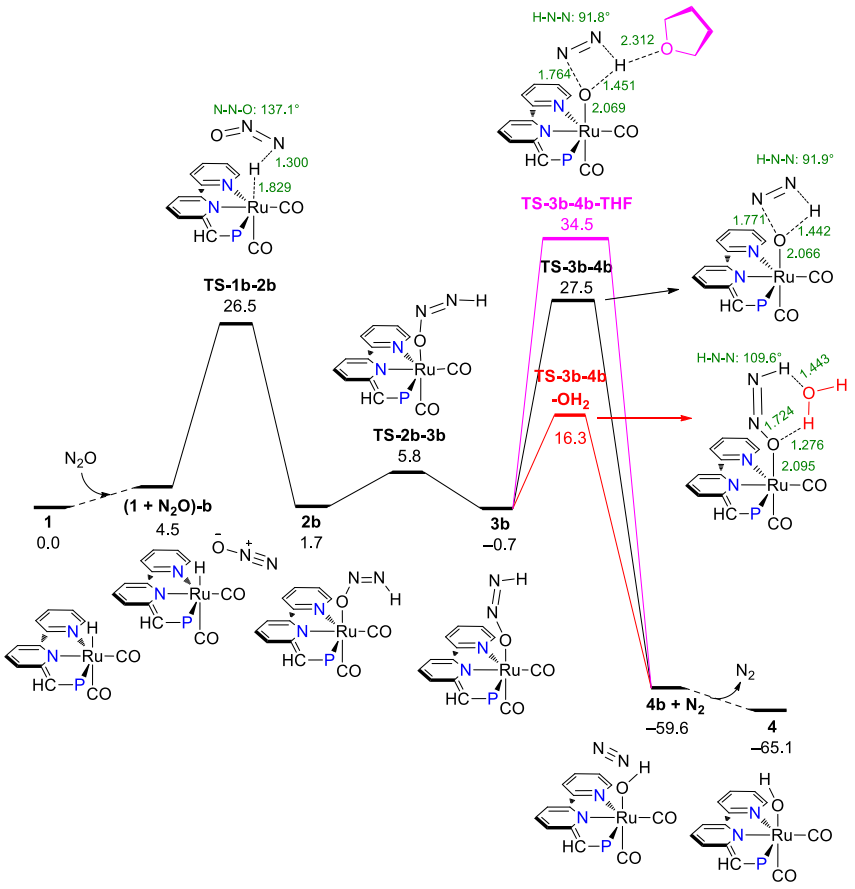
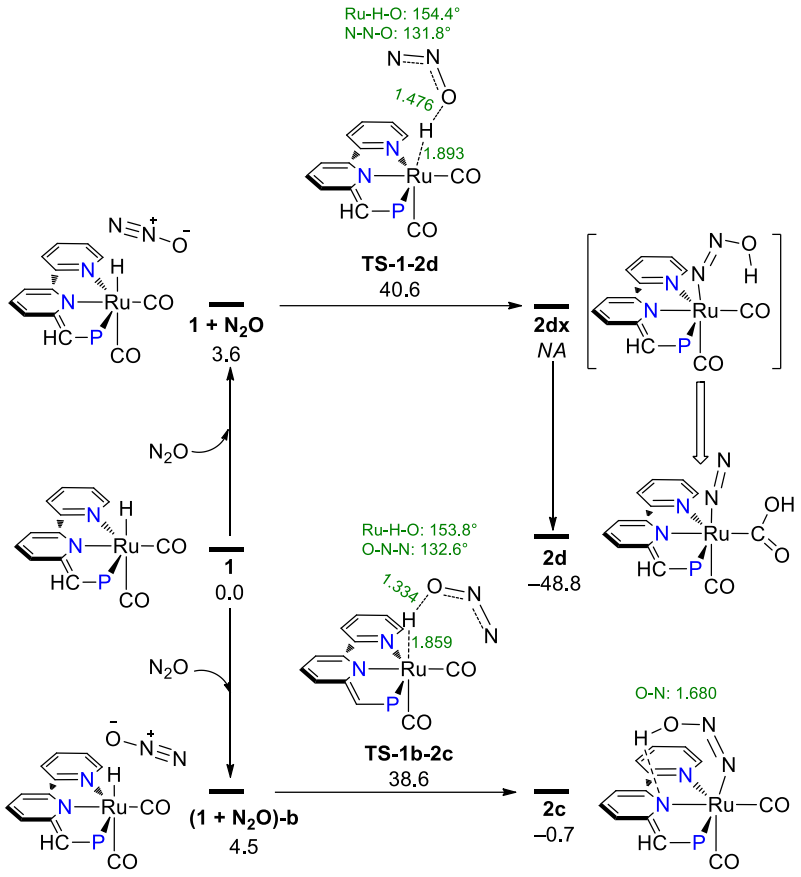


Figure S6. Free energy diagram for an alternative higher-energy pathway for proton transfer to the terminal N of endo N_2O.

Selected atom distances are given in Å and selected bond angles are given in °. $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Energy values are the results from SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 computations.



Scheme S2. Free energy diagram for proton transfer to the terminal O of endo N_2O. Selected atom distances are given in Å and selected bond angles are given in °. $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Energy values are the results from SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 computations.

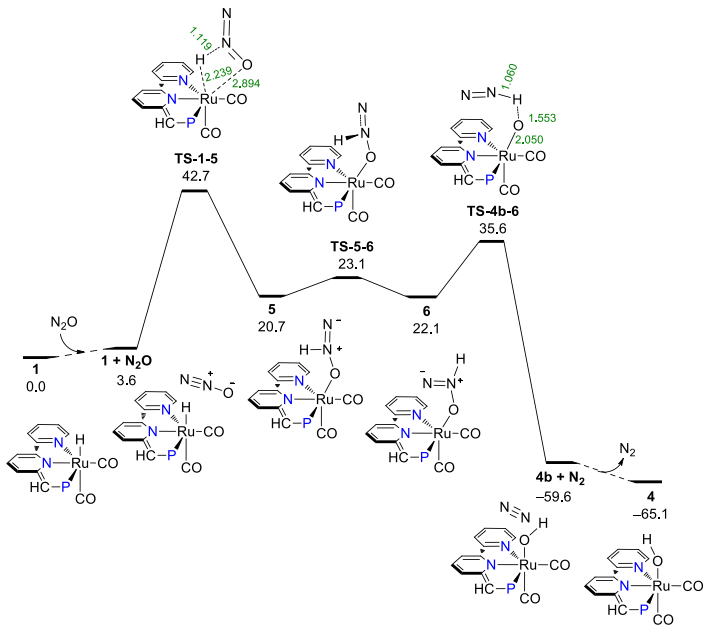


Figure S7. Free energy diagram for N_2 generation from hydride transfer to the central N of N_2O. Selected atom distances are given in Å and selected bond angles are given in °. $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Energy values are the results from SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 computations.

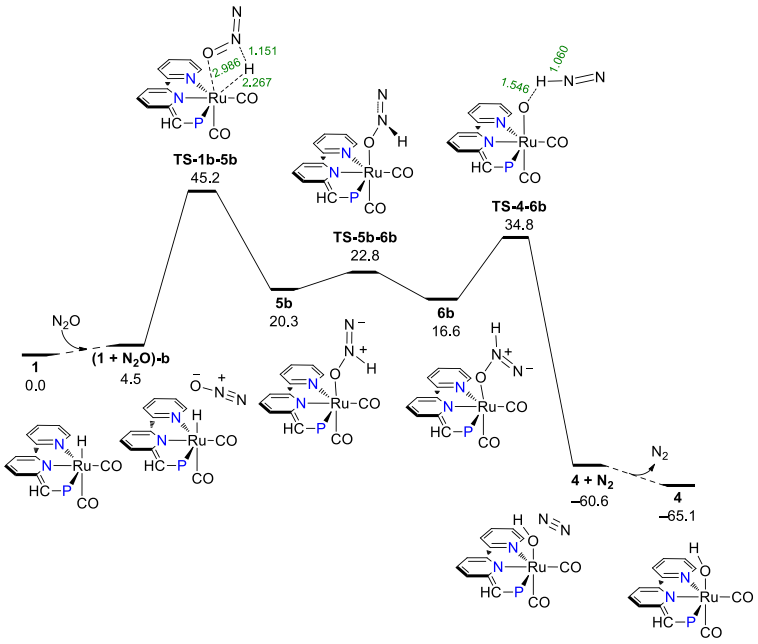


Figure S8. Free energy diagram for a higher-energy hydride transfer to the central N of N_2O. Selected atom distances are given in Å and selected bond angle are given in °. $\Delta G°/\Delta G^{‡}$ are in kcal mol^{-1}. Energy values are the results from SMD(THF)-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1 computations.

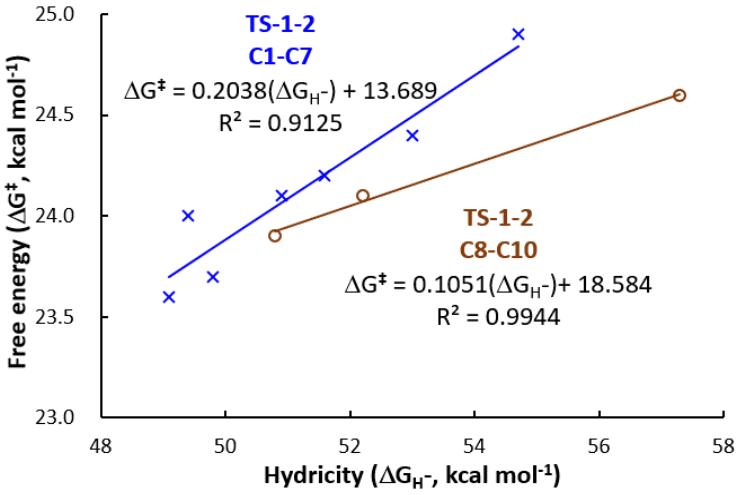


Figure S9. Linear fitting between the Gibbs free energies of activation ($\Delta G^{\ddagger}$) of TS-1-2 and the computed hydricities (ΔG_{H^-}).

Table S2. DFT computed energies (in Hartrees) of various species.

Species	$E_{(gas, B3LYP-GD3BJ/BS1)}$	$G_{(gas, B3LYP-GD3BJ/BS1)}$	$E_{(soln, SMD-B3LYP-GD3BJ/BS2//B3LYP-GD3BJ/BS1)}$
N_2O	-184.658971	-184.669064	-184.729755
N_2	-109.522714	-109.535552	-109.562406
H_2O	-76.404046	-76.400591	-76.468124
THF	-232.458409	-232.369444	-232.556171
H^-	-0.461817	-0.471816	-0.640209
PNN-Ru-H			
1	-1177.076496	-1176.694021	-1513.420072
1^+	-1176.29006	-1175.914815	-1512.681440
1 + N_2O	-1361.746471	-1361.360602	-1698.157617
TS-1-2	-1361.714377	-1361.326746	-1698.126602
2	-1361.746818	-1361.350500	-1698.167746
TS-2-3	-1361.744605	-1361.348820	-1698.164476
3	-1361.757287	-1361.362485	-1698.176070
TS-3-4	-1361.702945	-1361.315754	-1698.122212
TS-3-4-OH_2	-1438.159165	-1437.747611	-1774.629635
TS-3-4-THF	-1594.182441	-1593.684062	-1930.688574
4 + N_2	-1361.836090	-1361.448272	-1698.261804
4	-1252.305472	-1251.917193	-1588.694276
(1 + N_2O)-b	-1361.746481	-1361.359522	-1698.157177
TS-1b-2b	-1361.708821	-1361.320808	-1698.123250
2b	-1361.750857	-1361.354982	-1698.170667
TS-2b-3b	-1361.744437	-1361.349049	-1698.163557
3b	-1361.755117	-1361.359682	-1698.174062
TS-3b-4b	-1361.701942	-1361.314568	-1698.120922
TS-3-4-OH_2-b	-1438.153973	-1437.743244	-1774.626866
TS-3-4-THF-b	-1594.178357	-1593.682332	-1930.685657
4b + N_2	-1361.835250	-1361.446815	-1698.260860
TS-1b-2c	-1361.691213	-1361.303696	-1698.103418
2c	-1361.741680	-1361.346638	-1698.173557
TS-1-2d	-1361.686499	-1361.299174	-1698.100007
2d	-1361.831591	-1361.436126	-1698.250650
TS-1-5	-1361.676495	-1361.282872	-1698.103096
5	-1361.713785	-1361.320041	-1698.138157
TS-5-6	-1361.713371	-1361.318623	-1698.135348
6	-1361.716408	-1361.320888	-1698.137760
TS-4b-6	-1361.685224	-1361.296878	-1698.109106
TS-1b-5b	-1361.670462	-1361.278386	-1698.097493
5b	-1361.714536	-1361.320310	-1698.139327
TS-5b-6b	-1361.713817	-1361.318396	-1698.136456
6b	-1361.727886	-1361.331373	-1698.147478

TS-4-6b	-1361.686063	-1361.297124	-1698.110919
C1: ($P^{CF3}N^{CF3}N$)-Ru-H			
1	-1850.976846	-1850.59951	-2187.787988
1^+	-1850.173125	-1849.803300	-2187.043046
TS-1-2	-2035.598630	-2035.216043	-2372.493412
TS-3-4	-2035.588764	-2035.206933	-2372.488753
C2: (P^{CF3}NN)-Ru-H			
1	-1513.952517	-1513.573328	-1850.607073
1^+	-1513.154242	-1512.782303	-1849.865128
TS-1-2	-1698.574853	-1698.190510	-2035.313161
TS-3-4	-1698.565036	-1698.181282	-2035.308550
C3: (PN^{CF3}N)-Ru-H			
1	-1513.947804	-1513.568055	-1850.601204
1^+	-1513.151224	-1512.779332	-1849.860861
TS-1-2	-1698.570297	-1698.185900	-2035.307290
TS-3-4	-1698.560379	-1698.176589	-2035.302632
C5: (P^{CH3}NN)-Ru-H			
1	-1216.240843	-1215.834182	-1552.757351
1^+	-1215.451886	-1215.052567	-1552.021086
TS-1-2	-1400.864128	-1400.452246	-1737.463945
TS-3-4	-1400.854288	-1400.443127	-1737.45966
C6: (PN^{CH3}N)-Ru-H			
1	-1216.241681	-1215.835729	-1552.758306
1^+	-1215.452962	-1215.054682	-1552.021097
TS-1-2	-1400.864974	-1400.454456	-1737.465119
TS-3-4	-1400.855148	-1400.445154	-1737.460670
C7: ($P^{CH3}N^{CH3}$N)-Ru-H			
1	-1255.559771	-1255.128396	-1592.095785
1^+	-1254.772981	-1254.349159	-1591.359732
TS-1-2	-1440.183250	-1439.747106	-1776.802770
TS-3-4	-1440.173436	-1439.737828	-1776.798416
C8: (PNC)-Ru-H			
1	-1177.086698	-1361.333714	-1513.429164
1^+	-1176.287746	-1361.322393	-1512.687162
TS-1-2	-1361.723160	-1176.702347	-1698.135827
TS-3-4	-1361.711472	-1175.911987	-1698.128442
C9: ($P^{CH3}N^{CH3}$C)-Ru-H			
1	-1255.734791	-1255.302448	-1592.105303
1^+	-1254.940848	-1254.516589	-1591.366038
TS-1-2	-1440.371736	-1439.934039	-1776.812405
TS-3-4	-1440.360174	-1439.923261	-1776.805252
C10: ($P^{CF3}N^{CF3}$N)-Ru-H			
1	-1851.155122	-1850.774037	-2187.799190
1^+	-1850.341863	-1849.969473	-2187.048895
TS-1-2	-2035.790170	-2035.404167	-2372.504742

TS-3-4	-2035.778013	-2035.392503	-2372.496714

1^{+} stands for the cationic complex without hydride in the computation of hydricity (Scheme S3).

Table S3. SMD(THF)-B3LYP-GD3BJ/BS2 computed energies (in Hartrees) of various species.

Species	E	G
N_2O	-184.730065	-184.740340
H_2O	-76.468140	-76.464831
1	-1513.422084	-1513.041319
TS-1-2	-1698.128890	-1697.744655
TS-2-3	-1698.167004	-1697.773734
TS-3-4	-1698.124980	-1697.738864
TS-1-2b	-1698.125180	-1697.739675
TS-2b-3b	-1698.166366	-1697.772165
TS-1-2d	-1698.102479	-1697.716775
TS-3-4-OH_2	-1774.633290	-1774.223726
TS-3-4-OH_2-b	-1774.629891	-1774.219387

Table S4. Cartesian coordinates of optimized various species.

```
3
N2O     el energy= -184.658970633
N      0.000000   0.000000 -1.203650
N      0.000000   0.000000 -0.070912
O      0.000000   0.000000   1.115242

2
N2      el energy= -109.522713860
N      0.000000   0.000000   0.551536
N      0.000000   0.000000 -0.551536

3
H2O     el energy= -76.4040457810
O      0.000000   0.000000   0.117189
H      0.000000   0.767693 -0.468755
H      0.000000 -0.767693 -0.468755

13
THF     el energy= -232.458408733
O      0.000000   0.000000   1.251234
C      0.000000   1.171004   0.430813
C      0.309271   0.703178 -0.997047
C     -0.309271 -0.703178 -0.997047
C      0.000000 -1.171004   0.430813
H     -0.990120   1.653365   0.482290
H      0.742863   1.876342   0.825298
H     -0.108083   1.366691 -1.762259
H      1.394189   0.641374 -1.152855
H     -1.394189 -0.641374 -1.152855
H      0.108083 -1.366691 -1.762259
H      0.990120 -1.653365   0.482290
H     -0.742863 -1.876342   0.825298

54
Complex-1    el energy= -1177.07649613
Ru    -0.357659 -0.741267   0.023784
H     -0.354653 -0.587322 -1.612569
P      1.785199   0.282155 -0.057707
O      0.625904 -3.574869 -0.504812
O     -0.837724 -0.996328   3.105193
N     -2.509151 -0.847091 -0.224041
N     -0.973063   1.280460   0.131099
C     -3.214889 -1.968893 -0.436610
H     -2.639513 -2.888848 -0.452917
C     -4.591145 -1.966379 -0.628334
H     -5.116394 -2.901390 -0.798121
```

C	-5.260978	-0.740885	-0.598550
H	-6.336870	-0.691948	-0.746822
C	-4.532373	0.421654	-0.378950
H	-5.031207	1.383935	-0.359456
C	-3.144792	0.354798	-0.190133
C	-2.297496	1.542533	0.043432
C	-2.804989	2.827513	0.170121
H	-3.867228	3.030724	0.109982
C	-1.880986	3.875972	0.398680
H	-2.244821	4.895897	0.506064
C	-0.537210	3.617222	0.481755
H	0.176420	4.418965	0.652068
C	-0.032939	2.275658	0.339587
C	1.317446	1.942381	0.393859
H	2.053284	2.736141	0.485964
C	2.522093	0.362474	-1.839779
C	3.920776	1.001658	-1.878918
H	3.932894	1.981436	-1.386240
H	4.211707	1.159346	-2.927204
H	4.689594	0.370992	-1.422527
C	1.580856	1.262821	-2.663354
H	0.550500	0.895832	-2.644634
H	1.923897	1.273653	-3.707651
H	1.582698	2.290410	-2.285869
C	2.561558	-1.034134	-2.482060
H	3.201612	-1.734239	-1.936606
H	2.957197	-0.953185	-3.504763
H	1.557701	-1.464250	-2.542956
C	3.148023	-0.272460	1.168888
C	4.159618	0.858169	1.440387
H	4.722965	1.156443	0.554350
H	4.884145	0.515442	2.192629
H	3.655485	1.743073	1.844033
C	3.866235	-1.538959	0.675212
H	3.155100	-2.335972	0.426979
H	4.522771	-1.917445	1.471527
H	4.492491	-1.352943	-0.202296
C	2.460203	-0.598037	2.505096
H	1.820003	0.226002	2.838427
H	3.227748	-0.764765	3.273671
H	1.856467	-1.506970	2.434704
C	0.238786	-2.509230	-0.279929
C	-0.570285	-0.890476	1.994081

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Complex-1-no-hydride el energy= -1176.29006046

Ru	-0.311246	-0.674193	0.086993
P	1.838005	0.336482	-0.020898
O	0.589944	-3.591930	-0.329843
O	-0.308908	-1.014065	3.057397
N	-2.449660	-0.830726	-0.234788
N	-0.910323	1.295922	0.109298
C	-3.148407	-1.970647	-0.406501
H	-2.564574	-2.883767	-0.460823
C	-4.531398	-1.988643	-0.509570
H	-5.051907	-2.930122	-0.653352
C	-5.219662	-0.774211	-0.421096
H	-6.303547	-0.746342	-0.492612
C	-4.503273	0.402543	-0.237785
H	-5.024182	1.350247	-0.163263
C	-3.106111	0.361694	-0.147632
C	-2.259696	1.551218	0.036722
C	-2.752512	2.833228	0.119474
H	-3.815045	3.032128	0.049752
C	-1.838555	3.909791	0.300298
H	-2.218815	4.924633	0.380125
C	-0.496408	3.669900	0.368289
H	0.213877	4.480178	0.503458
C	0.019051	2.328169	0.255352
C	1.369287	2.027280	0.278335
H	2.103747	2.806719	0.449943
C	2.213399	0.176490	-1.892087
C	3.076296	1.348009	-2.388353
H	2.606049	2.311002	-2.164055
H	3.190916	1.269599	-3.477914
H	4.078972	1.342756	-1.952368
C	0.832189	0.262775	-2.581447
H	0.187156	-0.603403	-2.336704
H	0.958340	0.234071	-3.672215
H	0.302323	1.187197	-2.331259
C	2.877328	-1.164393	-2.236991
H	3.888839	-1.242450	-1.827553
H	2.962536	-1.248477	-3.328510
H	2.297633	-2.024935	-1.886654
C	3.282591	-0.132080	1.101381
C	4.601071	0.476461	0.588581
H	4.925683	0.032963	-0.357257
H	5.388900	0.284008	1.328198
H	4.531524	1.562944	0.459050

C 3.394553 -1.664583 1.193924
H 2.496386 -2.106341 1.639457
H 4.242840 -1.921366 1.840977
H 3.566249 -2.138750 0.223288
C 2.973817 0.440810 2.498833
H 2.922848 1.533664 2.492634
H 3.776860 0.140312 3.184058
H 2.034255 0.058894 2.909242
C 0.254845 -2.509220 -0.168906
C -0.271396 -0.898112 1.916521

57
Complex-1 + N2O el energy= -1361.74647122
Ru 0.169816 -0.429272 -0.567479
H 0.363645 -0.912701 0.985279
P -1.995495 0.216184 0.159810
O -0.518888 -3.346264 -1.113785
O 0.191085 0.599057 -3.523469
N 2.336601 -0.374667 -0.615718
N 0.632823 1.524572 0.094005
C 3.135020 -1.399677 -0.956346
H 2.627806 -2.305067 -1.272018
C 4.520949 -1.323894 -0.893662
H 5.123205 -2.183312 -1.172247
C 5.099889 -0.127035 -0.463800
H 6.180116 -0.026102 -0.394781
C 4.275828 0.937643 -0.121374
H 4.704193 1.871805 0.223241
C 2.883172 0.800678 -0.202371
C 1.937666 1.876637 0.157824
C 2.339721 3.151859 0.527175
H 3.385197 3.432251 0.566293
C 1.327743 4.091352 0.840817
H 1.607412 5.102413 1.129990
C 0.004385 3.736703 0.788358
H -0.775621 4.452025 1.035262
C -0.388705 2.402767 0.414096
C -1.709168 1.963624 0.368584
H -2.499626 2.636028 0.689550
C -2.448023 -0.498782 1.895774
C -3.866852 -0.112802 2.348107
H -4.027896 0.970815 2.296415
H -4.001476 -0.413490 3.396844
H -4.648950 -0.610774 1.767175
C -1.460324 0.126114 2.900609
H -0.419785 -0.056312 2.616614
H -1.630727 -0.321022 3.890272
H -1.604295 1.208450 2.978959
C -2.283920 -2.027810 1.921408
H -2.940268 -2.536999 1.209059
H -2.531748 -2.403239 2.924743
H -1.251968 -2.315226 1.700066
C -3.490446 0.023133 -1.019447
C -4.606483 1.033918 -0.691108
H -5.045285 0.887140 0.297437
H -5.413210 0.926947 -1.429997
H -4.232326 2.061651 -0.754728
C -4.034069 -1.414881 -1.003157
H -3.239361 -2.148520 -1.184224
H -4.779454 -1.530252 -1.802807
H -4.526358 -1.668885 -0.059705
C -2.995572 0.335860 -2.441522
H -2.470435 1.296427 -2.481756
H -3.858887 0.391226 -3.119137
H -2.328533 -0.446014 -2.814791
C -0.249456 -2.237286 -0.935474
C 0.097767 0.226469 -2.442020
N 2.773622 -1.001153 2.584209
N 2.471119 -1.991035 2.128054
O 2.160464 -3.028497 1.645035

57
Complex-2 el energy= -1361.74681755
Ru 0.260545 -0.649995 -0.330150
H 1.299521 0.559779 1.957289
P -1.903639 0.311064 0.059050
O -0.772388 -3.482057 -0.881671
O 0.584108 0.124626 -3.245926
N 2.434971 -0.782665 -0.317245
N 0.889296 1.346837 -0.006829
C 3.131101 -1.928210 -0.319213
H 2.544053 -2.837039 -0.396982
C 4.515929 -1.956795 -0.211220
H 5.040206 -2.907303 -0.214705
C 5.195624 -0.742987 -0.086008
H 6.278155 -0.722173 0.010463
C 4.471356 0.442866 -0.064362
H 4.975564 1.392816 0.071784
C 3.076359 0.406975 -0.178410

C 2.221505 1.610285 -0.111542
C 2.711224 2.901938 -0.110631
H 3.771230 3.106755 -0.199087
C 1.774580 3.961889 0.005523
H 2.131408 4.989232 0.027979
C 0.432100 3.703540 0.083361
H -0.288742 4.512643 0.162571
C -0.065994 2.351894 0.035988
C -1.417649 2.027029 0.027830
H -2.149421 2.820765 0.145475
C -2.637158 -0.093304 1.790469
C -4.050532 0.481272 1.988951
H -4.086301 1.560267 1.794791
H -4.340831 0.329793 3.037890
H -4.806587 -0.012117 1.371777
C -1.719804 0.578132 2.827525
H -0.699545 0.204281 2.770575
H -2.099024 0.347592 3.832647
H -1.702630 1.666317 2.706052
C -2.635389 -1.614736 2.027453
H -3.242959 -2.158082 1.297038
H -3.057834 -1.820187 3.021516
H -1.613562 -2.004295 2.008274
C -3.267192 0.086263 -1.272339
C -4.279427 1.249048 -1.224077
H -4.830825 1.306298 -0.284598
H -5.013384 1.111803 -2.030276
H -3.778988 2.209016 -1.391571
C -3.983476 -1.266691 -1.127102
H -3.274534 -2.102871 -1.122322
H -4.656063 -1.410254 -1.984359
H -4.591673 -1.329888 -0.221023
C -2.604169 0.129355 -2.658095
H -1.980883 1.021148 -2.780154
H -3.387429 0.159078 -3.427847
H -1.997026 -0.761071 -2.845714
C -0.370756 -2.427506 -0.670045
C 0.342375 -0.171499 -2.162167
N 1.749739 -0.016678 2.693440
N 1.366358 -1.196377 2.592106
O 0.503600 -1.533672 1.632812

57
Complex-3 el energy= -1361.75728715
Ru 0.289449 -0.498644 -0.444169
H 1.661964 -1.676131 3.389509
P -1.916740 0.304226 0.067522
O -0.562964 -3.374299 -1.088230
O 0.405896 0.396270 -3.343739
N 2.461643 -0.515951 -0.506376
N 0.788976 1.472766 0.063342
C 3.223244 -1.594953 -0.732767
H 2.695706 -2.490727 -1.040644
C 4.603162 -1.580845 -0.563480
H 5.181431 -2.479475 -0.754035
C 5.202830 -0.398760 -0.126590
H 6.277193 -0.348316 0.031774
C 4.409430 0.717332 0.117416
H 4.854089 1.637955 0.478159
C 3.025488 0.644083 -0.081410
C 2.106999 1.778395 0.155247
C 2.541163 3.065528 0.420595
H 3.594883 3.310341 0.475415
C 1.555354 4.070907 0.587830
H 1.864826 5.092551 0.798162
C 0.223355 3.768981 0.482378
H -0.535671 4.536439 0.606882
C -0.209018 2.423213 0.204896
C -1.543742 2.046913 0.081733
H -2.316827 2.786280 0.269892
C -2.508111 -0.188098 1.831443
C -3.944083 0.272311 2.135495
H -4.072248 1.348123 1.964777
H -4.150553 0.084826 3.198665
H -4.702376 -0.267338 1.560376
C -1.573051 0.536823 2.821498
H -0.525583 0.281801 2.651288
H -1.839736 0.222665 3.841030
H -1.692810 1.623134 2.755366
C -2.383005 -1.708881 2.029549
H -3.013038 -2.278501 1.339230
H -2.699169 -1.966879 3.050337
H -1.346530 -2.028777 1.907421
C -3.331888 0.019793 -1.188269
C -4.416639 1.106750 -1.048294
H -4.916532 1.096307 -0.078454
H -5.183814 0.942811 -1.817846
H -3.992657 2.103974 -1.209698
C -3.942534 -1.383489 -1.037788
H -3.177709 -2.166997 -1.093206

H -4.652123 -1.556731 -1.858943
H -4.491326 -1.507732 -0.100437
C -2.751641 0.141315 -2.606634
H -2.202253 1.079052 -2.739099
H -3.576545 0.128743 -3.332177
H -2.091284 -0.696826 -2.847753
C -0.220287 -2.306659 -0.840202
C 0.248261 0.055765 -2.257355
N 1.803018 -2.497300 2.760763
N 1.309431 -2.231510 1.652178
O 0.735925 -1.015498 1.554908

55
Complex-4 el energy= -1252.30547181
Ru -0.344475 -0.710485 0.060603
H -1.093134 0.038369 -2.216579
P 1.821744 0.303763 -0.027872
O 0.665711 -3.590919 -0.132529
O -0.797202 -0.689247 3.075331
N -2.528451 -0.839558 -0.054275
N -0.969450 1.302061 0.092918
C -3.228232 -1.971363 -0.206143
H -2.649515 -2.889139 -0.182373
C -4.606206 -1.979014 -0.391101
H -5.133617 -2.920628 -0.509465
C -5.273878 -0.752703 -0.427334
H -6.350054 -0.711837 -0.576235
C -4.545513 0.422358 -0.279887
H -5.043273 1.384510 -0.324618
C -3.158228 0.362368 -0.089844
C -2.301290 1.559618 0.059227
C -2.804208 2.845370 0.159924
H -3.868922 3.043998 0.144277
C -1.872655 3.905031 0.309020
H -2.235152 4.927953 0.387073
C -0.528080 3.651274 0.359410
H 0.188727 4.459385 0.477537
C -0.023638 2.303535 0.263583
C 1.325895 1.979956 0.332029
H 2.055235 2.782776 0.392420
C 2.625645 0.271384 -1.778352
C 4.072815 0.791328 -1.805144
H 4.152142 1.804172 -1.391632
H 4.399748 0.842651 -2.853294
H 4.779216 0.141900 -1.280242
C 1.783874 1.204936 -2.669388
H 0.751804 0.854128 -2.702642
H 2.194469 1.177591 -3.689147
H 1.812779 2.239515 -2.311350
C 2.550699 -1.158357 -2.345818
H 3.060716 -1.892745 -1.713018
H 3.039266 -1.179775 -3.331108
H 1.503184 -1.446981 -2.473322
C 3.132288 -0.196180 1.278212
C 4.161260 0.932760 1.490196
H 4.751873 1.155357 0.600825
H 4.859363 0.631424 2.283742
H 3.666119 1.853881 1.817321
C 3.829834 -1.511222 0.891921
H 3.104835 -2.314365 0.715159
H 4.481313 -1.830432 1.717728
H 4.454450 -1.415753 -0.000153
C 2.420633 -0.409527 2.624063
H 1.784513 0.442894 2.884851
H 3.176257 -0.521933 3.413859
H 1.813373 -1.318563 2.621082
C 0.273958 -2.511606 -0.057196
C -0.502594 -0.714513 1.962227
O -0.535255 -0.722783 -2.004965

57
Complex-4 + N2 el energy= -1361.83609049
Ru 0.160060 -0.599401 -0.362178
H 1.077768 -0.151889 1.924012
P -2.021739 0.244300 0.145512
O -0.689684 -3.530328 -0.575021
O 0.269959 -0.047325 -3.358442
N 2.345421 -0.612104 -0.533333
N 0.695051 1.419457 -0.094160
C 3.103398 -1.702639 -0.704058
H 2.564459 -2.637757 -0.817909
C 4.492873 -1.651792 -0.724572
H 5.067989 -2.562038 -0.863126
C 5.110008 -0.410656 -0.552948
H 6.193806 -0.325596 -0.556469
C 4.322788 0.719072 -0.363625
H 4.784338 1.687829 -0.209597
C 2.925716 0.602358 -0.358064
C 2.010436 1.747867 -0.159222

C	2.446250	3.057286	-0.053066
H	3.496443	3.315597	-0.112238
C	1.462984	4.065271	0.120083
H	1.773325	5.104201	0.210254
C	0.133304	3.742856	0.170532
H	-0.623404	4.512033	0.299225
C	-0.302697	2.373225	0.051516
C	-1.636662	1.985466	0.078216
H	-2.398239	2.738483	0.260269
C	-2.631148	-0.177911	1.925707
C	-4.093984	0.215819	2.192662
H	-4.272851	1.281068	2.002392
H	-4.308396	0.036312	3.255623
H	-4.816334	-0.369512	1.616868
C	-1.755064	0.628890	2.903132
H	-0.708106	0.350955	2.780952
H	-2.062381	0.384201	3.930244
H	-1.871445	1.707660	2.754487
C	-2.416693	-1.679953	2.189312
H	-2.947353	-2.316011	1.472331
H	-2.797328	-1.927520	3.191150
H	-1.346917	-1.906720	2.159910
C	-3.446152	-0.073693	-1.097694
C	-4.542739	1.003303	-0.971582
H	-5.044313	1.003139	-0.003365
H	-5.307474	0.821830	-1.739738
H	-4.127975	2.002227	-1.147442
C	-4.033411	-1.484035	-0.921232
H	-3.256102	-2.254245	-0.989612
H	-4.759862	-1.676222	-1.723496
H	-4.554786	-1.612726	0.030843
C	-2.879576	0.033049	-2.522843
H	-2.306045	0.955600	-2.662680
H	-3.712717	0.040540	-3.239165
H	-2.244622	-0.821512	-2.770017
C	-0.360240	-2.430424	-0.498557
C	0.100321	-0.275076	-2.242180
N	3.409264	-0.643711	2.660078
N	3.887557	-1.634276	2.583578
O	0.591307	-0.935600	1.635614

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ts-1-2 el energy= -1361.71437712

Ru	-0.278734	-0.454059	0.441434
H	-0.538781	-0.742093	-1.302763
P	1.921687	0.318405	-0.068183
O	0.589935	-3.327878	1.048911
O	-0.472287	0.369568	3.388513
N	-2.444076	-0.469164	0.404532
N	-0.764090	1.521788	-0.090099
C	-3.221363	-1.539337	0.637662
H	-2.699571	-2.451911	0.899526
C	-4.605056	-1.494162	0.520728
H	-5.192333	-2.386741	0.712788
C	-5.200245	-0.288853	0.142198
H	-6.279050	-0.213747	0.030822
C	-4.395769	0.819008	-0.096913
H	-4.837410	1.760832	-0.401896
C	-3.005787	0.715599	0.041895
C	-2.077950	1.841729	-0.189553
C	-2.498406	3.131568	-0.469482
H	-3.548973	3.385830	-0.538625
C	-1.502305	4.123867	-0.645541
H	-1.800146	5.146892	-0.865678
C	-0.173277	3.806559	-0.540761
H	0.594347	4.563846	-0.675035
C	0.244049	2.458616	-0.253439
C	1.574684	2.064672	-0.142075
H	2.357425	2.791270	-0.339747
C	2.522533	-0.233891	-1.817345
C	3.975949	0.173979	-2.116262
H	4.133470	1.249714	-1.973660
H	4.193455	-0.049899	-3.170161
H	4.708250	-0.370643	-1.513525
C	1.632142	0.496870	-2.841610
H	0.567191	0.326065	-2.678932
H	1.877891	0.128196	-3.847271
H	1.809145	1.576800	-2.816183
C	2.362594	-1.754811	-1.984293
H	2.975446	-2.320995	-1.275671
H	2.675810	-2.044505	-2.997170
H	1.323291	-2.067779	-1.855119
C	3.329958	0.060022	1.200885
C	4.435907	1.120705	1.032154
H	4.947882	1.063334	0.070242
H	5.190840	0.974164	1.817227
H	4.028551	2.131116	1.148769
C	3.913235	-1.359990	1.108973
H	3.131286	-2.124295	1.185480
H	4.611810	-1.517532	1.942738

H	4.468640	-1.530511	0.182458
C	2.734776	0.245658	2.606592
H	2.180099	1.186635	2.688277
H	3.551320	0.269313	3.341269
H	2.073564	-0.582350	2.876732
C	0.214197	-2.273830	0.778719
C	-0.294900	0.049730	2.299487
N	-1.286517	-1.169809	-2.376351
N	-1.567630	-2.303007	-2.174563
O	-1.419902	-3.165365	-1.315174

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ts-2-3 el energy= -1361.74460491

Ru	0.253554	-0.691333	-0.226095
H	1.424015	1.051975	2.242883
P	-1.927662	0.307576	-0.003203
O	-0.722365	-3.594514	-0.110960
O	0.555215	-0.551349	-3.232696
N	2.424335	-0.820696	-0.255995
N	0.860870	1.322686	-0.221446
C	3.133071	-1.956700	-0.182970
H	2.555200	-2.874729	-0.175748
C	4.519410	-1.965603	-0.104685
H	5.052585	-2.908912	-0.040236
C	5.188956	-0.739834	-0.096309
H	6.273031	-0.701525	-0.026444
C	4.453518	0.436673	-0.163714
H	4.953120	1.397950	-0.132342
C	3.056673	0.380753	-0.240710
C	2.194177	1.580121	-0.288968
C	2.683999	2.869227	-0.387378
H	3.746521	3.071298	-0.442231
C	1.743140	3.930259	-0.423042
H	2.098428	4.956459	-0.487657
C	0.398398	3.674650	-0.382871
H	-0.325660	4.484018	-0.417647
C	-0.095935	2.323071	-0.303685
C	-1.447757	1.996584	-0.306375
H	-2.180950	2.797912	-0.301604
C	-2.673846	0.193619	1.770977
C	-4.110097	0.739451	1.855443
H	-4.179793	1.768335	1.482189
H	-4.408413	0.757142	2.912941
H	-4.841463	0.122786	1.325669
C	-1.798901	1.073278	2.684117
H	-0.764878	0.728494	2.677184
H	-2.180950	0.996669	3.711921
H	-1.833410	2.124951	2.380265
C	-2.624385	-1.262894	2.269029
H	-3.190110	-1.947617	1.628625
H	-3.070110	-1.311705	3.273020
H	-1.589523	-1.608433	2.342255
C	-3.280683	-0.145662	-1.284648
C	-4.310363	0.993939	-1.425629
H	-4.874598	1.185943	-0.512434
H	-5.031761	0.723186	-2.209072
H	-3.820887	1.924597	-1.733414
C	-3.972294	-1.471414	-0.926027
H	-3.246214	-2.281787	-0.789995
H	-4.641134	-1.762707	-1.748043
H	-4.578958	-1.402957	-0.019384
C	-2.611112	-0.312377	-2.657888
H	-1.983508	0.549076	-2.909266
H	-3.390239	-0.396984	-3.427748
H	-2.007338	-1.222800	-2.705943
C	-0.345478	-2.511336	-0.163502
C	0.320429	-0.611078	-2.108216
N	2.085193	0.369218	2.666738
N	1.644190	-0.781956	2.506306
O	0.438139	-0.895234	1.897599

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ts-3-4 el energy= -1361.70294466

Ru	0.256350	-0.538708	-0.415806
H	1.777226	-0.657523	2.419815
P	-1.938717	0.288676	0.073309
O	-0.613068	-3.448420	-0.816874
O	0.379279	0.177584	-3.378925
N	2.443894	-0.550537	-0.508360
N	0.768450	1.461065	-0.025892
C	3.212339	-1.628559	-0.713633
H	2.687065	-2.537157	-0.989647
C	4.594270	-1.600881	-0.565440
H	5.176881	-2.501047	-0.734852
C	5.191373	-0.399956	-0.177863
H	6.267183	-0.336724	-0.035065
C	4.393524	0.719282	0.032512
H	4.837583	1.656530	0.348291
C	3.006647	0.630293	-0.144966
C	2.085711	1.771568	0.048043

C 2.520997 3.069277 0.257686
H 3.574668 3.317217 0.296655
C 1.535214 4.080274 0.386773
H 1.844751 5.110422 0.550413
C 0.203025 3.772232 0.304743
H -0.556136 4.543349 0.403503
C -0.230193 2.414553 0.091770
C -1.565200 2.031058 0.009193
H -2.336375 2.777664 0.176129
C -2.531642 -0.128190 1.857038
C -3.976312 0.318159 2.139477
H -4.124015 1.383864 1.926190
H -4.180778 0.169624 3.209192
H -4.724391 -0.257441 1.586406
C -1.612414 0.654779 2.815784
H -0.564574 0.399892 2.648589
H -1.873286 0.380422 3.848193
H -1.745230 1.735725 2.702244
C -2.371215 -1.635739 2.122308
H -2.958051 -2.252240 1.433429
H -2.718057 -1.861304 3.141179
H -1.317163 -1.914782 2.049146
C -3.358541 -0.046042 -1.166405
C -4.447561 1.040596 -1.061191
H -4.945702 1.061897 -0.090882
H -5.215513 0.847471 -1.823228
H -4.027700 2.033267 -1.257881
C -3.961168 -1.446114 -0.963061
H -3.193378 -2.227385 -1.006443
H -4.682763 -1.647868 -1.767206
H -4.493505 -1.544487 -0.013350
C -2.785638 0.027938 -2.590965
H -2.231637 0.957976 -2.755496
H -3.614526 -0.003589 -3.311496
H -2.130301 -0.820174 -2.808324
C -0.267019 -2.361740 -0.668819
C 0.218296 -0.102355 -2.274998
N 2.372909 -1.707814 2.725268
N 1.629149 -2.316664 2.046707
O 0.688953 -0.944856 1.565593

60
ts-3-4-oh2 el energy= -1438.15916514
Ru 0.161841 -0.601308 -0.418374
P -2.022165 0.296616 0.029330
O -0.710945 -3.538194 -0.426807
O 0.269398 -0.313575 -3.447103
N 2.335333 -0.651073 -0.600702
N 0.705872 1.424924 -0.296339
C 3.082961 -1.754668 -0.745017
H 2.535411 -2.686966 -0.832112
C 4.472027 -1.719481 -0.761072
H 5.036768 -2.639796 -0.872080
C 5.102152 -0.481914 -0.617096
H 6.186737 -0.408662 -0.616293
C 4.326449 0.662972 -0.472375
H 4.799592 1.631635 -0.357410
C 2.928679 0.562985 -0.468614
C 2.026688 1.727386 -0.320642
C 2.483598 3.030504 -0.210813
H 3.539327 3.270859 -0.242612
C 1.511802 4.059431 -0.093549
H 1.837497 5.093968 -0.009455
C 0.176538 3.760432 -0.085700
H -0.570419 4.543907 0.007928
C -0.278911 2.394701 -0.180895
C -1.617117 2.025432 -0.152051
H -2.369580 2.795055 -0.004995
C -2.646256 0.008294 1.830813
C -4.111605 0.421795 2.052377
H -4.286326 1.470877 1.785233
H -4.335652 0.319442 3.123406
H -4.829474 -0.202745 1.513650
C -1.785396 0.889027 2.756935
H -0.727061 0.648758 2.666135
H -2.090344 0.698904 3.796081
H -1.931242 1.953855 2.546282
C -2.444992 -1.471749 2.203522
H -2.987043 -2.152230 1.537476
H -2.820778 -1.641113 3.222897
H -1.379438 -1.714642 2.183027
C -3.441322 -0.092079 -1.199636
C -4.529485 0.999883 -1.153217
H -5.040771 1.065562 -0.192590
H -5.288029 0.775622 -1.916066
H -4.104555 1.982224 -1.388441
C -4.040277 -1.483686 -0.934757
H -3.267630 -2.261597 -0.944600
H -4.760783 -1.724283 -1.729180

H -4.571180 -1.545849 0.018685
C -2.865231 -0.084131 -2.624939
H -2.276884 0.819066 -2.819633
H -3.693855 -0.108948 -3.345895
H -2.244128 -0.963292 -2.813975
C -0.367317 -2.441501 -0.419794
C 0.101816 -0.428255 -2.314311
N 2.528133 -1.717728 2.630230
H 2.586913 -0.575414 2.844081
N 1.610300 -2.045007 1.976785
O 0.560396 -0.706490 1.613285
H 1.265755 0.250201 2.130437
O 2.086929 0.727388 2.753253
H 2.586165 1.370796 2.232678

70
ts-3-4-thf el energy= -
1594.18244069
Ru 0.475343 -0.973592 -0.320607
P 2.276975 0.511373 0.223342
O 1.689159 -1.929702 -2.965115
O 1.348493 -3.401524 1.304313
N -1.521655 -1.866496 -0.213260
N -0.304902 -0.207855 1.475670
C -2.079586 -2.647100 -1.150102
H -1.423695 -2.959333 -1.956396
C -3.416206 -3.022509 -1.108563
H -3.828503 -3.650784 -1.892078
C -4.200582 -2.552617 -0.051900
H -5.256057 -2.806188 0.009077
C -3.621234 -1.744791 0.917965
H -4.218351 -1.340730 1.726253
C -2.263406 -1.413295 0.827505
C -1.569140 -0.560273 1.814526
C -2.147422 -0.150469 3.003378
H -3.156286 -0.437307 3.271538
C -1.371992 0.662948 3.865465
H -1.802067 1.009950 4.802856
C -0.090434 1.015902 3.530607
H 0.508071 1.639975 4.188705
C 0.499804 0.566785 2.295988
C 1.799036 0.874919 1.901115
H 2.390314 1.542173 2.521849
C 2.245314 2.156587 -0.775799
C 3.449714 3.070403 -0.494947
H 3.564262 3.277209 0.576098
H 3.276637 4.033833 -0.995193
H 4.394399 2.673942 -0.878664
C 0.976439 2.905672 -0.325625
H 0.094891 2.282570 -0.486438
H 0.875078 3.818627 -0.930621
H 1.033896 3.194845 0.729097
C 2.138276 1.852716 -2.280563
H 2.116477 2.799594 -2.839443
H 1.211607 1.313258 -2.489480
H 2.985223 1.270276 -2.657431
C 4.066732 -0.168660 0.264678
C 4.947265 0.660632 1.221177
H 5.068168 1.698776 0.908206
H 5.948336 0.208984 1.262741
H 4.536046 0.649855 2.236645
C 4.682463 -0.214616 -1.143741
H 4.049853 -0.772725 -1.843761
H 5.653528 -0.727376 -1.095959
H 4.858273 0.779962 -1.562275
C 4.028402 -1.602085 0.818552
H 3.483905 -1.653992 1.767116
H 5.057142 -1.942620 1.000386
H 3.573736 -2.298483 0.108386
C 1.211171 -1.575496 -1.980458
C 1.134927 -2.458528 0.680789
N -2.393814 0.393771 -2.570741
H -2.033616 0.608434 -1.390695
N -1.278987 0.183663 -2.878190
O -0.614371 0.486683 -1.302462
C -4.568757 1.744885 -0.509067
O -3.468203 1.307271 0.285552
C -2.756815 2.480195 0.678834
C -2.759201 3.376183 -0.567518
C -4.088365 3.001471 -1.274842
H -4.846567 0.912093 -1.162036
H -5.423921 1.985026 0.145412
H -3.273803 2.965481 1.524934
H -1.762502 2.167090 1.004162
H -2.692756 4.440286 -0.316039
H -1.903884 3.123931 -1.201123
H -4.829556 3.806123 -1.213856
H -3.921549 2.778160 -2.332752

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ts-1b-2b el energy= -1361.70882074

Ru	0.211037	-0.677237	-0.387224
H	0.449388	-1.055942	1.386021
P	-1.927019	0.306924	0.025700
O	-0.766361	-3.573891	-0.325528
O	0.293567	-0.440964	-3.442735
N	2.372757	-0.791586	-0.376347
N	0.803537	1.341634	-0.303528
C	3.091092	-1.925335	-0.341485
H	2.519663	-2.846709	-0.379825
C	4.476561	-1.929251	-0.248207
H	5.014762	-2.871534	-0.217475
C	5.138612	-0.700475	-0.186546
H	6.221798	-0.657963	-0.105295
C	4.395446	0.472668	-0.220022
H	4.888503	1.435370	-0.150842
C	2.999515	0.413676	-0.312838
C	2.132702	1.606877	-0.329842
C	2.618810	2.901908	-0.372692
H	3.681456	3.109506	-0.398882
C	1.676370	3.959531	-0.390344
H	2.027665	4.988771	-0.419443
C	0.331959	3.695533	-0.371691
H	-0.396882	4.501319	-0.385427
C	-0.153120	2.340933	-0.330539
C	-1.504335	2.001880	-0.314446
H	-2.246344	2.792777	-0.259179
C	-2.433694	0.197851	1.880928
C	-3.814267	0.823244	2.146865
H	-3.884654	1.840398	1.743224
H	-3.966240	0.891704	3.233237
H	-4.637358	0.226290	1.742058
C	-1.394129	1.029754	2.658663
H	-0.362250	0.770930	2.411414
H	-1.537208	0.859531	3.734628
H	-1.519243	2.098726	2.458734
C	-2.414882	-1.255967	2.383903
H	-3.101510	-1.903377	1.830401
H	-2.724670	-1.273598	3.438418
H	-1.413826	-1.690149	2.332810
C	-3.413622	-0.153583	-1.085607
C	-4.449063	0.987642	-1.127888
H	-4.905866	1.190816	-0.157538
H	-5.255056	0.709836	-1.821367
H	-3.995992	1.913314	-1.499067
C	-4.073146	-1.466646	-0.633468
H	-3.343644	-2.280906	-0.550398
H	-4.821657	-1.769190	-1.379187
H	-4.589503	-1.369356	0.325799
C	-2.885103	-0.344627	-2.516911
H	-2.302757	0.521343	-2.849057
H	-3.736449	-0.462402	-3.201332
H	-2.266503	-1.242917	-2.601929
C	-0.379484	-2.489370	-0.356928
C	0.172963	-0.507422	-2.302902
N	1.043661	-1.574700	2.419940
N	1.781192	-0.738388	2.858067
O	2.110404	0.409395	2.572877

57

Complex-2b el energy= -1361.75085656

Ru	0.301039	-0.562976	-0.341592
H	1.076263	-2.750884	1.065068
P	-1.905357	0.327401	0.034302
O	-0.740408	-3.406816	-0.802073
O	0.466034	-0.031903	-3.328244
N	2.480820	-0.601086	-0.382138
N	0.813641	1.457705	-0.097765
C	3.250909	-1.690921	-0.515337
H	2.733285	-2.609213	-0.771268
C	4.627590	-1.661675	-0.329405
H	5.208280	-2.572131	-0.438253
C	5.219646	-0.446416	0.018050
H	6.291014	-0.381194	0.190044
C	4.423195	0.685957	0.145707
H	4.863811	1.636759	0.422789
C	3.042011	0.595866	-0.065865
C	2.130462	1.755834	0.018138
C	2.572822	3.060391	0.154125
H	3.626665	3.299658	0.226117
C	1.597014	4.088386	0.163732
H	1.913476	5.124105	0.267422
C	0.265378	3.789919	0.042523
H	-0.486966	4.573734	0.052665
C	-0.175492	2.425450	-0.087901
C	-1.512383	2.048570	-0.193213
H	-2.280040	2.812551	-0.111326
C	-2.524403	0.080540	1.840824
C	-3.978823	0.537551	2.050244

H	-4.126709	1.578752	1.739705
H	-4.203909	0.484776	3.124641
H	-4.712354	-0.089949	1.536115
C	-1.635940	0.966508	2.738450
H	-0.576262	0.735773	2.617968
H	-1.911044	0.779494	3.786386
H	-1.798365	2.028489	2.526070
C	-2.368833	-1.394848	2.248388
H	-2.958126	-2.070162	1.619110
H	-2.714816	-1.523568	3.283499
H	-1.321805	-1.701389	2.207465
C	-3.305457	-0.119941	-1.191989
C	-4.382364	0.984017	-1.213117
H	-4.897911	1.103614	-0.259049
H	-5.138406	0.725084	-1.967343
H	-3.947697	1.948698	-1.496968
C	-3.932706	-1.486389	-0.866973
H	-3.179879	-2.281258	-0.829460
H	-4.648143	-1.748600	-1.658967
H	-4.479231	-1.488926	0.079565
C	-2.706779	-0.191113	-2.606134
H	-2.150365	0.718592	-2.854192
H	-3.522681	-0.295807	-3.334288
H	-2.050041	-1.057743	-2.726196
C	-0.297698	-2.366628	-0.574389
C	0.287533	-0.238193	-2.212789
N	1.506658	-2.682280	2.013293
N	1.372555	-1.526590	2.451161
O	0.766468	-0.585125	1.748810

57

Complex-1 + N2O-b el energy= -1361.74648110

Ru	0.114708	-0.747780	-0.320909
H	0.337398	-0.576810	1.296983
P	-1.993094	0.276571	0.069115
O	-0.764608	-3.578740	0.379813
O	0.121190	-1.028795	-3.436617
N	2.278773	-0.852058	-0.402324
N	0.703320	1.271707	-0.540766
C	3.009755	-1.972018	-0.284618
H	2.444537	-2.892451	-0.182707
C	4.398883	-1.964947	-0.275772
H	4.944618	-2.897556	-0.170938
C	5.054734	-0.736824	-0.388242
H	6.140506	-0.683735	-0.375043
C	4.300444	0.423604	-0.514164
H	4.788835	1.388172	-0.593073
C	2.900315	0.352147	-0.526856
C	2.025666	1.535910	-0.648360
C	2.507083	2.819151	-0.859744
H	3.566393	3.022947	-0.957478
C	1.558006	3.865242	-0.957916
H	1.900338	4.884625	-1.124455
C	0.217056	3.604905	-0.840928
H	-0.515105	4.405110	-0.909182
C	-0.258749	2.264216	-0.617420
C	-1.602311	1.929375	-0.472384
H	-2.344867	2.722151	-0.461541
C	-2.448944	0.382809	1.941545
C	-3.832923	1.008254	2.186059
H	-3.933780	1.978167	1.684219
H	-3.959128	1.183595	3.263914
H	-4.655328	0.361412	1.866122
C	-1.404599	1.309547	2.593682
H	-0.381645	0.975930	2.401045
H	-1.566238	1.316676	3.681079
H	-1.497607	2.335328	2.222935
C	-2.372401	-1.002407	2.605160
H	-3.075069	-1.720415	2.170995
H	-2.614962	-0.907850	3.673434
H	-1.364361	-1.419327	2.524271
C	-3.523589	-0.299720	-0.926027
C	-4.572126	0.822703	-1.053756
H	-4.996350	1.129214	-0.095960
H	-5.400137	0.467127	-1.683185
H	-4.141038	1.704875	-1.539724
C	-4.148758	-1.562137	-0.310176
H	-3.402913	-2.352926	-0.165429
H	-4.919122	-1.954108	-0.989336
H	-4.631394	-1.366437	0.651922
C	-3.047220	-0.640920	-2.347822
H	-2.469915	0.180771	-2.785513
H	-3.922675	-0.820055	-2.987390
H	-2.435407	-1.547121	-2.359651
C	-0.422561	-2.514512	0.086954
C	0.028400	-0.915347	-2.298478
N	2.876651	-1.091105	2.850644
N	2.605573	-0.001050	2.714655
O	2.331734	1.143761	2.572684

57
ts-2b-3b el energy= -1361.74443665
Ru 0.291330 -0.556289 -0.344061
H 1.159616 -2.999820 1.735060
P -1.936096 0.293456 0.034588
O -0.570993 -3.476223 -0.682725
O 0.459876 0.041858 -3.306122
N 2.462954 -0.551147 -0.411168
N 0.772207 1.465771 -0.044837
C 3.241983 -1.628742 -0.581356
H 2.727551 -2.552673 -0.822359
C 4.623106 -1.580915 -0.441621
H 5.213074 -2.481148 -0.580912
C 5.208382 -0.362695 -0.094129
H 6.283584 -0.284633 0.045431
C 4.400468 0.755377 0.079476
H 4.835533 1.706988 0.362557
C 3.015664 0.648310 -0.091832
C 2.086399 1.788153 0.044845
C 2.507319 3.097159 0.201773
H 3.557981 3.353787 0.259042
C 1.513239 4.106259 0.254933
H 1.812416 5.144688 0.380648
C 0.185910 3.786449 0.142980
H -0.580054 4.556253 0.178235
C -0.232391 2.418004 -0.019202
C -1.562673 2.025094 -0.143524
H -2.341321 2.775947 -0.044354
C -2.575366 0.012244 1.828615
C -4.019525 0.504136 2.027778
H -4.141532 1.550216 1.721781
H -4.256127 0.449506 3.099648
H -4.761224 -0.104954 1.502519
C -1.670035 0.856307 2.750165
H -0.616213 0.598670 2.625521
H -1.954050 0.650954 3.792320
H -1.805689 1.926664 2.562658
C -2.461682 -1.473936 2.212300
H -3.060826 -2.123982 1.566251
H -2.827765 -1.607061 3.240425
H -1.417479 -1.794761 2.179405
C -3.316768 -0.141903 -1.217631
C -4.401717 0.953868 -1.238443
H -4.932146 1.055281 -0.290449
H -5.144439 0.701338 -2.007989
H -3.969497 1.925783 -1.500610
C -3.935918 -1.517132 -0.917908
H -3.173347 -2.303010 -0.865822
H -4.628851 -1.783515 -1.728286
H -4.503967 -1.530856 0.015900
C -2.699162 -0.189284 -2.624223
H -2.152614 0.730689 -2.855365
H -3.503824 -0.297474 -3.364347
H -2.028006 -1.044945 -2.744513
C -0.224121 -2.386737 -0.555284
C 0.285683 -0.190694 -2.194017
N 1.986111 -2.529486 2.169156
N 1.771374 -1.306830 2.212190
O 0.569971 -0.886527 1.756088

57
ts-3b-4b el energy= -1361.70194217
Ru 0.229133 -0.636967 -0.383398
H 1.301849 -1.887998 2.507985
P -1.934035 0.293135 0.058320
O -0.717141 -3.541438 -0.518701
O 0.328994 -0.155518 -3.398223
N 2.419383 -0.706257 -0.490011
N 0.800652 1.382121 -0.183951
C 3.156952 -1.822403 -0.556406
H 2.606502 -2.742303 -0.727749
C 4.538665 -1.816164 -0.406050
H 5.096421 -2.745891 -0.463027
C 5.170301 -0.592449 -0.171396
H 6.247711 -0.542391 -0.035352
C 4.404359 0.564888 -0.101743
H 4.872562 1.520615 0.104381
C 3.014793 0.492396 -0.266825
C 2.124700 1.669452 -0.189334
C 2.592614 2.971463 -0.143065
H 3.651901 3.196530 -0.165303
C 1.632524 4.013040 -0.092162
H 1.967415 5.047470 -0.051715
C 0.292554 3.728275 -0.097358
H -0.448050 4.522557 -0.060585
C -0.173218 2.366214 -0.153052
C -1.518798 2.009967 -0.174948
H -2.269239 2.788176 -0.069447
C -2.508195 0.064608 1.880319

C	-3.927525	0.597328	2.140022
H	-4.035361	1.642519	1.825572
H	-4.117487	0.562472	3.222111
H	-4.708648	0.002905	1.656485
C	-1.534799	0.889845	2.745693
H	-0.504231	0.573943	2.576676
H	-1.783119	0.722961	3.803969
H	-1.625127	1.960615	2.535468
C	-2.410168	-1.417067	2.284256
H	-3.042583	-2.067814	1.671741
H	-2.737532	-1.528536	3.328175
H	-1.372772	-1.753738	2.214531
C	-3.382343	-0.116926	-1.124928
C	-4.435381	1.009492	-1.114822
H	-4.915810	1.143851	-0.144479
H	-5.221894	0.765990	-1.842779
H	-3.988349	1.963286	-1.415777
C	-4.027247	-1.469048	-0.777609
H	-3.285200	-2.275488	-0.746236
H	-4.762043	-1.727301	-1.553151
H	-4.554729	-1.453087	0.179972
C	-2.828996	-0.202724	-2.556505
H	-2.254791	0.691236	-2.820638
H	-3.669068	-0.284864	-3.259963
H	-2.197768	-1.085308	-2.695112
C	-0.347094	-2.451748	-0.481701
C	0.178777	-0.338341	-2.272774
N	2.223676	-1.346340	3.096348
N	2.044163	-0.336466	2.527252
O	0.661663	-0.957153	1.611148

57

Complex-3b el energy= -1361.75511747

Ru	0.261041	-0.696900	-0.257899
H	1.136880	-0.791280	3.920382
P	-1.917996	0.302484	-0.029274
O	-0.709837	-3.594869	-0.032695
O	0.446507	-0.640813	-3.286131
N	2.428878	-0.816642	-0.332986
N	0.843139	1.316231	-0.341447
C	3.148098	-1.944459	-0.260549
H	2.581452	-2.869583	-0.293039
C	4.532381	-1.940118	-0.138851
H	5.075427	-2.878152	-0.078042
C	5.185315	-0.706594	-0.088457
H	6.266254	-0.656341	0.015544
C	4.437821	0.462552	-0.163530
H	4.925233	1.428840	-0.104350
C	3.045010	0.392423	-0.282561
C	2.173230	1.582301	-0.360889
C	2.656234	2.873082	-0.476177
H	3.718489	3.082642	-0.502163
C	1.710034	3.923616	-0.578178
H	2.059123	4.950624	-0.662307
C	0.366370	3.656884	-0.577353
H	-0.363213	4.457784	-0.659922
C	-0.117255	2.305004	-0.466829
C	-1.468306	1.964527	-0.479909
H	-2.208689	2.758960	-0.503685
C	-2.567012	0.330140	1.782854
C	-3.997906	0.881097	1.907541
H	-4.097386	1.869141	1.442335
H	-4.229802	1.000392	2.975341
H	-4.756929	0.215715	1.485797
C	-1.642153	1.288431	2.559345
H	-0.593752	1.014781	2.454250
H	-1.903950	1.240300	3.625895
H	-1.768671	2.321714	2.220427
C	-2.485177	-1.079354	2.396884
H	-3.079614	-1.814505	1.844722
H	-2.877911	-1.046586	3.423641
H	-1.447133	-1.417829	2.442694
C	-3.324137	-0.264030	-1.199800
C	-4.369518	0.854962	-1.382292
H	-4.894007	1.111789	-0.460878
H	-5.122856	0.520821	-2.109262
H	-3.903106	1.762502	-1.781301
C	-3.988613	-1.556942	-0.698171
H	-3.252940	-2.353083	-0.534049
H	-4.697644	-1.915249	-1.457672
H	-4.548628	-1.413887	0.229711
C	-2.719182	-0.542824	-2.585066
H	-2.128897	0.305848	-2.945705
H	-3.533126	-0.716182	-3.302323
H	-2.092221	-1.439281	-2.580757
C	-0.329685	-2.513338	-0.120904
C	0.255618	-0.674567	-2.153436
N	1.864053	-0.171946	3.499425
N	1.647346	-0.083700	2.278130

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O      0.579685 -0.772805  1.838515

57
Complex-4b + N2     el energy= -
1361.83525028
Ru     0.159852 -0.671617 -0.298245
H      0.798570 -1.435941  2.072139
P     -2.011530  0.274748  0.095374
O     -0.742914 -3.577375 -0.016121
O      0.154938 -0.643476 -3.348514
N      2.335907 -0.728300 -0.492282
N      0.691010  1.360659 -0.367931
C      3.093584 -1.832043 -0.535465
H      2.553751 -2.772785 -0.585496
C      4.483045 -1.789550 -0.515519
H      5.056114 -2.711034 -0.550835
C      5.101438 -0.539863 -0.440703
H      6.185127 -0.457827 -0.413645
C      4.314772  0.604780 -0.391924
H      4.777257  1.582187 -0.318167
C      2.917352  0.495635 -0.422748
C      2.010409  1.662463 -0.401853
C      2.460915  2.971104 -0.460657
H      3.516491  3.210040 -0.501065
C      1.487284  4.000228 -0.494003
H      1.808581  5.038758 -0.540412
C      0.151098  3.698501 -0.471148
H     -0.600035  4.483336 -0.496002
C     -0.295595  2.330920 -0.400371
C     -1.635746  1.955921 -0.357998
H     -2.395153  2.731261 -0.310327
C     -2.532611  0.268218  1.949243
C     -3.957304  0.799486  2.180053
H     -4.095390  1.796492  1.744484
H     -4.119275  0.893452  3.263208
H     -4.737394  0.136506  1.793620
C     -1.555356  1.211932  2.680257
H     -0.523005  0.878386  2.541298
H     -1.794114  1.189325  3.754148
H     -1.661910  2.243505  2.328138
C     -2.389099 -1.148944  2.530255
H     -3.013454 -1.888187  2.017982
H     -2.688186 -1.139809  3.588330
H     -1.343406 -1.459266  2.473603
C     -3.486028 -0.298659 -0.983445
C     -4.560330  0.803593 -1.078785
H     -5.018605  1.046244 -0.118898
H     -5.360310  0.461858 -1.750505
H     -4.139203  1.721176 -1.504212
C     -4.093165 -1.608701 -0.454666
H     -3.334292 -2.393233 -0.351241
H     -4.846741 -1.971049 -1.168156
H     -4.590211 -1.485365  0.511301
C     -2.973276 -0.549145 -2.410911
H     -2.418243  0.312457 -2.796201
H     -3.832198 -0.722186 -3.074051
H     -2.335027 -1.435707 -2.462825
C     -0.384234 -2.487807 -0.134007
C      0.042400 -0.650678 -2.203131
O      0.682881 -0.549919  1.706891
N      3.335850 -1.069635  2.756125
N      3.827686 -0.082847  2.777382

60
ts-3-4-oh2-b     el energy= -
1438.15397275
Ru     0.174770 -0.426276 -0.555545
H      2.554691 -2.246577  2.241835
P     -2.021639  0.267037  0.124460
O     -0.676026 -3.237949 -1.414721
O      0.169899  0.746175 -3.362001
N      2.353052 -0.357475 -0.731788
N      0.658551  1.521650  0.081328
C      3.138914 -1.386279 -1.080126
H      2.622875 -2.269312 -1.445192
C      4.524124 -1.335300 -0.990003
H      5.121417 -2.194719 -1.278938
C      5.109910 -0.157189 -0.517391
H      6.189489 -0.076641 -0.419630
C      4.296557  0.912417 -0.166370
H      4.730988  1.826826  0.220891
C      2.903971  0.798716 -0.279571
C      1.965901  1.877304  0.091984
C      2.375166  3.159041  0.414266
H      3.420786  3.441628  0.409080
C      1.371197  4.107732  0.735252
H      1.659623  5.122907  0.999456
C      0.047585  3.757459  0.710300
H     -0.726615  4.480905  0.950914
C     -0.357695  2.419411  0.359797
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C	-1.685326	2.009214	0.290247
H	-2.465516	2.704140	0.587094
C	-2.544765	-0.407087	1.847695
C	-3.983806	-0.023174	2.232172
H	-4.149615	1.059178	2.168943
H	-4.149536	-0.316438	3.278350
H	-4.743769	-0.531356	1.631178
C	-1.600359	0.250347	2.873385
H	-0.556366	0.056767	2.628164
H	-1.809200	-0.181568	3.862747
H	-1.763878	1.331760	2.928498
C	-2.365213	-1.934901	1.895453
H	-2.967819	-2.456665	1.144791
H	-2.680405	-2.302642	2.882577
H	-1.311688	-2.190821	1.757599
C	-3.474373	0.073763	-1.108544
C	-4.577388	1.113486	-0.823857
H	-5.046478	0.990247	0.153364
H	-5.364513	1.011047	-1.583888
H	-4.180340	2.132264	-0.892738
C	-4.049947	-1.352140	-1.081805
H	-3.272553	-2.106688	-1.248959
H	-4.789326	-1.456438	-1.888335
H	-4.556197	-1.587324	-0.141855
C	-2.949966	0.353175	-2.526026
H	-2.424962	1.312431	-2.579628
H	-3.800736	0.395198	-3.219964
H	-2.282334	-0.439819	-2.875371
C	-0.338165	-2.186600	-1.091556
C	0.055714	0.298202	-2.308910
N	2.683012	-1.169038	2.598314
N	1.857149	-0.422944	2.218670
O	0.625149	-1.232182	1.324612
O	1.863529	-3.266352	1.490955
H	2.343115	-3.526660	0.693684
H	1.138566	-2.399496	1.277607

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ts-3-4-thf-b el energy= -1594.17835734

Ru	-0.194024	0.182889	-0.645552
P	-2.292496	-0.610484	0.193471
O	0.511700	-2.414814	-2.097307
O	-1.202943	1.622161	-3.142285
N	1.556407	1.486357	-0.803284
N	-0.779775	1.920137	0.393366
C	2.735739	1.132231	-1.331771
H	2.774994	0.153628	-1.795283
C	3.862667	1.942848	-1.239717
H	4.800439	1.615446	-1.678139
C	3.751366	3.160207	-0.565214
H	4.610702	3.818326	-0.462574
C	2.529630	3.517663	-0.006608
H	2.430407	4.443151	0.549089
C	1.429083	2.660581	-0.134013
C	0.104964	2.944524	0.459475
C	-0.223061	4.159455	1.036516
H	0.482798	4.980173	1.074629
C	-1.531154	4.305291	1.562374
H	-1.818371	5.245798	2.028112
C	-2.433705	3.277618	1.484866
H	-3.439196	3.385229	1.882606
C	-2.076733	2.026013	0.867405
C	-2.954495	0.953951	0.730954
H	-3.941147	1.023472	1.180023
C	-2.120174	-1.745717	1.737471
C	-3.460200	-2.324130	2.222111
H	-4.203679	-1.537628	2.400176
H	-3.290573	-2.833751	3.181271
H	-3.887584	-3.062097	1.536530
C	-1.563912	-0.855225	2.866143
H	-0.626670	-0.383886	2.569325
H	-1.370052	-1.487565	3.744897
H	-2.281862	-0.079348	3.151661
C	-1.115935	-2.876091	1.448802
H	-1.417088	-3.508486	0.607022
H	-1.036218	-3.523022	2.334871
H	-0.132586	-2.442256	1.246533
C	-3.550761	-1.381512	-1.027031
C	-4.993184	-1.219175	-0.506973
H	-5.178046	-1.750777	0.427815
H	-5.688636	-1.619010	-1.258265
H	-5.236916	-0.161396	-0.358779
C	-3.234108	-2.861185	-1.301457
H	-2.202070	-2.997332	-1.644745
H	-3.897398	-3.230039	-2.096620
H	-3.388844	-3.496802	-0.425424
C	-3.462772	-0.616936	-2.357759
H	-3.563698	0.463098	-2.209109
H	-4.280253	-0.945890	-3.014239

H	-2.522243	-0.817532	-2.878867
C	0.277259	-1.429896	-1.548647
C	-0.912898	1.014505	-2.209522
N	2.764613	0.093466	1.944828
H	2.320720	-0.658926	1.089302
N	1.704344	0.561866	2.136222
O	0.882603	-0.493757	0.986421
C	3.028529	-3.080569	-0.148084
O	3.514496	-1.781263	-0.541531
C	4.832391	-1.577683	-0.020877
C	4.956947	-2.530915	1.167828
C	4.148615	-3.741153	0.671994
H	2.117804	-2.926583	0.444407
H	2.763166	-3.647598	-1.048020
H	5.580565	-1.809893	-0.797935
H	4.922114	-0.521089	0.253544
H	5.996710	-2.773552	1.412836
H	4.486625	-2.083600	2.051371
H	4.772413	-4.376549	0.030228
H	3.757643	-4.363175	1.484067

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ts-1b-5b el energy= -1361.67046206

Ru	0.241409	-0.516860	-0.474184
H	0.658562	-1.919139	1.256980
P	-1.952110	0.289997	0.074725
O	-0.585645	-3.443746	-0.898218
O	0.239588	0.162403	-3.402523
N	2.419560	-0.527834	-0.541233
N	0.739692	1.472641	-0.025934
C	3.189984	-1.603615	-0.761477
H	2.667012	-2.515013	-1.031893
C	4.573088	-1.568220	-0.634942
H	5.155640	-2.467450	-0.808021
C	5.170428	-0.362737	-0.264424
H	6.248330	-0.293404	-0.142608
C	4.371343	0.753708	-0.043194
H	4.817649	1.693395	0.261079
C	2.983245	0.656998	-0.182874
C	2.060370	1.786629	0.042872
C	2.485746	3.080092	0.283804
H	3.538314	3.330616	0.331933
C	1.498902	4.083389	0.451658
H	1.806860	5.109068	0.642667
C	0.167206	3.772110	0.373378
H	-0.595293	4.535468	0.501166
C	-0.259144	2.419822	0.129701
C	-1.595758	2.032230	0.052205
H	-2.371655	2.768911	0.235727
C	-2.442888	-0.197034	1.873878
C	-3.842082	0.325885	2.241929
H	-3.935794	1.401817	2.051884
H	-4.000500	0.169791	3.318001
H	-4.647753	-0.196348	1.716617
C	-1.420581	0.486192	2.801903
H	-0.387462	0.191753	2.589052
H	-1.646085	0.195021	3.837597
H	-1.491018	1.576547	2.730965
C	-2.378141	-1.718885	2.085194
H	-1.368695	-2.104539	1.913299
H	-3.069441	-2.271770	1.442799
H	-2.640335	-1.947229	3.127284
C	-3.412941	-0.026261	-1.115316
C	-4.491014	1.064605	-0.956474
H	-4.944587	1.081632	0.036200
H	-5.292624	0.877404	-1.684265
H	-4.077175	2.056820	-1.166249
C	-4.019464	-1.423542	-0.909710
H	-3.257644	-2.210319	-0.964409
H	-4.751358	-1.617798	-1.705968
H	-4.543543	-1.518260	0.045340
C	-2.879637	0.063806	-2.554460
H	-2.323482	0.992307	-2.721075
H	-3.727699	0.049362	-3.252524
H	-2.238075	-0.787136	-2.801414
C	-0.254429	-2.353925	-0.729312
C	0.150709	-0.075848	-2.280374
O	1.590809	-0.489594	2.189555
N	1.498810	-1.774833	2.030454
N	2.083343	-2.712047	2.457963

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Complex-5b el energy= -1361.71453574

Ru	0.276730	-0.555717	-0.364865
H	0.779071	-2.709783	1.832382
P	-1.935968	0.287909	0.056902
O	-0.626062	-3.459874	-0.742492
O	0.366429	0.007136	-3.352759
N	2.453602	-0.550144	-0.455707

N	0.752356	1.468569	-0.108181
C	3.238924	-1.622877	-0.619700
H	2.732098	-2.544361	-0.888311
C	4.616370	-1.575834	-0.443755
H	5.211459	-2.473622	-0.577520
C	5.189777	-0.361737	-0.065612
H	6.260411	-0.284180	0.105486
C	4.375616	0.753564	0.096656
H	4.801319	1.702795	0.401351
C	2.996328	0.646010	-0.112375
C	2.065353	1.788054	-0.000834
C	2.484818	3.098890	0.146887
H	3.535097	3.355021	0.212774
C	1.491606	4.109146	0.174278
H	1.790724	5.149188	0.286629
C	0.164176	3.789105	0.058270
H	-0.601639	4.559531	0.080503
C	-0.253061	2.418879	-0.082078
C	-1.584168	2.016820	-0.179618
H	-2.365172	2.765016	-0.078673
C	-2.508477	0.044891	1.878369
C	-3.948987	0.525215	2.123773
H	-4.092203	1.563498	1.800889
H	-4.146049	0.490893	3.204506
H	-4.703656	-0.100729	1.638168
C	-1.574951	0.911941	2.748712
H	-0.525449	0.644606	2.606232
H	-1.831518	0.741221	3.804331
H	-1.708781	1.976789	2.532046
C	-2.357071	-1.429187	2.290221
H	-1.304625	-1.715770	2.235520
H	-2.949982	-2.109735	1.670828
H	-2.690833	-1.552435	3.330328
C	-3.356462	-0.187966	-1.133215
C	-4.449242	0.900167	-1.141826
H	-4.943577	1.023661	-0.176933
H	-5.219181	0.622642	-1.875190
H	-4.034298	1.867313	-1.445899
C	-3.957140	-1.558839	-0.779346
H	-3.189821	-2.340534	-0.740485
H	-4.679424	-1.845556	-1.556501
H	-4.489931	-1.554356	0.175404
C	-2.787844	-0.266252	-2.559459
H	-2.256337	0.651278	-2.831545
H	-3.617453	-0.397703	-3.267642
H	-2.114172	-1.119499	-2.682648
C	-0.251724	-2.382408	-0.571665
C	0.221693	-0.215101	-2.234968
O	0.745071	-0.732985	1.678961
N	1.450529	-1.924093	2.010292
N	2.549316	-2.017384	2.436237

57

Complex-6b el energy= -1361.72788645

Ru	0.320352	-0.523107	-0.311229
H	1.385581	-1.898201	3.144021
P	-1.898157	0.337957	0.023092
O	-0.585676	-3.407528	-0.873253
O	0.546788	0.026454	-3.281865
N	2.492154	-0.556645	-0.312949
N	0.820116	1.490005	0.005363
C	3.258121	-1.648238	-0.454461
H	2.728411	-2.569436	-0.668229
C	4.640041	-1.610702	-0.303495
H	5.222286	-2.519034	-0.423835
C	5.237725	-0.389951	0.015814
H	6.314069	-0.318765	0.152326
C	4.440944	0.740337	0.162471
H	4.886138	1.694433	0.420947
C	3.054373	0.642935	-0.011801
C	2.136013	1.797004	0.102373
C	2.572849	3.102315	0.257756
H	3.626101	3.347609	0.318940
C	1.589906	4.122661	0.301487
H	1.900247	5.158471	0.422935
C	0.259059	3.817673	0.185956
H	-0.497494	4.597197	0.213896
C	-0.174712	2.453409	0.025360
C	-1.508251	2.073004	-0.101667
H	-2.280261	2.831969	-0.011738
C	-2.588786	0.020180	1.794146
C	-4.036454	0.504945	1.981131
H	-4.149145	1.562219	1.712549
H	-4.300487	0.409658	3.044034
H	-4.766051	-0.080592	1.414396
C	-1.706050	0.833775	2.762618
H	-0.653780	0.556743	2.676999
H	-2.036812	0.625235	3.790854
H	-1.808199	1.908714	2.581487
C	-2.482776	-1.475627	2.137253

H	-3.095270	-2.103539	1.482808
H	-2.829961	-1.638178	3.167919
H	-1.446803	-1.812545	2.071077
C	-3.264523	-0.046357	-1.262414
C	-4.339932	1.058450	-1.273585
H	-4.885476	1.142630	-0.332455
H	-5.072355	0.831966	-2.061051
H	-3.894882	2.032561	-1.504802
C	-3.897094	-1.425953	-1.013515
H	-3.138389	-2.215605	-0.964559
H	-4.571625	-1.667628	-1.846983
H	-4.488872	-1.461503	-0.094917
C	-2.621578	-0.061822	-2.658529
H	-2.049902	0.852192	-2.849626
H	-3.414722	-0.127698	-3.416061
H	-1.967855	-0.928118	-2.793359
C	-0.175495	-2.378332	-0.563532
C	0.346611	-0.183850	-2.168373
O	0.688320	-0.764352	1.757681
N	1.146335	-2.018327	2.139138
N	1.259532	-3.025766	1.509830

57

ts-5b-6b el energy= -1361.71381697

Ru	0.297889	-0.550014	-0.335984
H	0.542447	-2.518699	2.596301
P	-1.935318	0.289238	0.023011
O	-0.533264	-3.483267	-0.634420
O	0.468993	-0.008706	-3.319610
N	2.468027	-0.531438	-0.414450
N	0.760217	1.475347	-0.061312
C	3.256534	-1.595297	-0.609196
H	2.751352	-2.519077	-0.870565
C	4.638548	-1.535470	-0.479421
H	5.237507	-2.425086	-0.646091
C	5.210485	-0.323892	-0.093793
H	6.285133	-0.237602	0.046122
C	4.390307	0.780028	0.113874
H	4.815778	1.728994	0.419962
C	3.007814	0.663874	-0.068327
C	2.070824	1.799579	0.061771
C	2.482713	3.110174	0.232280
H	3.530987	3.369987	0.313813
C	1.485021	4.115804	0.260671
H	1.778120	5.155401	0.392009
C	0.160925	3.792492	0.118401
H	-0.608066	4.559891	0.136450
C	-0.248362	2.422709	-0.047380
C	-1.576376	2.020217	-0.181544
H	-2.359947	2.767286	-0.091397
C	-2.587316	0.040036	1.819020
C	-4.033633	0.528107	2.007505
H	-4.156698	1.569125	1.685513
H	-4.275868	0.488562	3.078941
H	-4.771084	-0.090067	1.487020
C	-1.686617	0.896720	2.733099
H	-0.634853	0.619366	2.634332
H	-1.992412	0.727068	3.775955
H	-1.800734	1.962931	2.512456
C	-2.466387	-1.436931	2.228846
H	-3.059913	-2.106423	1.598483
H	-2.816661	-1.558841	3.263757
H	-1.418312	-1.740741	2.184026
C	-3.313978	-0.176031	-1.221811
C	-4.404489	0.913386	-1.266783
H	-4.938718	1.030848	-0.322734
H	-5.143750	0.643008	-2.033684
H	-3.975593	1.882054	-1.545857
C	-3.926613	-1.548760	-0.897684
H	-3.159154	-2.328641	-0.827539
H	-4.614438	-1.835753	-1.705402
H	-4.499563	-1.547700	0.033484
C	-2.694330	-0.248069	-2.626633
H	-2.151770	0.669742	-2.874764
H	-3.497816	-0.374497	-3.365245
H	-2.018300	-1.102017	-2.729057
C	-0.196106	-2.388234	-0.519404
C	0.292192	-0.221608	-2.204059
O	0.660323	-0.752224	1.736755
N	1.306763	-1.947321	2.171562
N	2.456372	-2.228943	2.143263

57

ts-4-6b el energy= -1361.68606314

Ru	-0.285697	-0.491769	0.385338
H	-1.690001	-1.295328	-2.644332
P	1.934438	0.290094	-0.058907
O	0.542484	-3.402654	0.852008
O	-0.461134	0.244627	3.347442
N	-2.473548	-0.451435	0.434270

N	-0.744818	1.520325	-0.022906
C	-3.275309	-1.497171	0.679574
H	-2.778404	-2.406876	0.999649
C	-4.655137	-1.436053	0.518339
H	-5.264901	-2.311364	0.720045
C	-5.214792	-0.231849	0.085442
H	-6.288120	-0.141093	-0.062574
C	-4.383936	0.857397	-0.152535
H	-4.800836	1.799805	-0.489319
C	-3.000062	0.734453	0.034531
C	-2.049639	1.851006	-0.160033
C	-2.453979	3.151716	-0.416015
H	-3.500301	3.417699	-0.504154
C	-1.445913	4.142390	-0.523576
H	-1.729563	5.174584	-0.718966
C	-0.123676	3.812232	-0.382577
H	0.653046	4.567512	-0.467141
C	0.275231	2.450600	-0.131250
C	1.599289	2.040769	-0.005675
H	2.389957	2.768908	-0.163610
C	2.555677	-0.140145	-1.829828
C	4.016725	0.265056	-2.086142
H	4.189455	1.327046	-1.872981
H	4.236814	0.107861	-3.151714
H	4.738967	-0.328585	-1.517696
C	1.671990	0.665069	-2.804192
H	0.615377	0.436783	-2.641900
H	1.940527	0.378594	-3.832089
H	1.835872	1.742252	-2.693675
C	2.354751	-1.642883	-2.095055
H	2.904642	-2.276338	-1.390937
H	2.716880	-1.883479	-3.105585
H	1.287823	-1.877065	-2.040449
C	3.323150	-0.070129	1.208376
C	4.437016	0.992500	1.121772
H	4.953958	1.000346	0.161051
H	5.186066	0.785626	1.899037
H	4.034399	1.994396	1.307558
C	3.899883	-1.483211	1.020145
H	3.115088	-2.247685	1.053714
H	4.604156	-1.696985	1.836622
H	4.445156	-1.596361	0.079359
C	2.724249	0.020025	2.621361
H	2.186911	0.962110	2.772037
H	3.538027	-0.027370	3.358304
H	2.045599	-0.812371	2.827398
C	0.199767	-2.318915	0.668547
C	-0.281758	-0.048666	2.248383
O	-0.643857	-0.855148	-1.594808
N	-1.691872	-2.248313	-2.179338
N	-2.025990	-3.228568	-1.709688

57

ts-1-5 el energy= -1361.67649535

Ru	0.231762	-0.500610	-0.502253
H	0.909542	-0.611355	1.628500
P	-1.933543	0.318731	0.091177
O	-0.591296	-3.416018	-1.049528
O	0.227537	0.358895	-3.380436
N	2.428189	-0.544313	-0.508492
N	0.776905	1.467558	0.030173
C	3.176071	-1.646286	-0.679184
H	2.631035	-2.558615	-0.890243
C	4.558394	-1.629186	-0.549311
H	5.125257	-2.544460	-0.687368
C	5.179975	-0.423194	-0.217380
H	6.258688	-0.372273	-0.093525
C	4.402863	0.712902	-0.024671
H	4.863805	1.649892	0.266423
C	3.012702	0.636175	-0.171929
C	2.103213	1.779724	0.052214
C	2.543231	3.072136	0.267593
H	3.598313	3.316914	0.274466
C	1.566619	4.082375	0.461484
H	1.886276	5.107161	0.637338
C	0.231761	3.779324	0.425145
H	-0.521089	4.549641	0.567702
C	-0.213168	2.430418	0.189828
C	-1.553062	2.059895	0.121720
H	-2.318843	2.805544	0.312348
C	-2.404597	-0.216732	1.884836
C	-3.830926	0.210953	2.272525
H	-3.991347	1.285498	2.123349
H	-3.977153	0.004370	3.341943
H	-4.604522	-0.339449	1.729718
C	-1.443496	0.521487	2.837451
H	-0.390488	0.367722	2.589754
H	-1.598358	0.144514	3.857075
H	-1.629565	1.599898	2.831963
C	-2.244208	-1.738132	2.054311

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H    -2.899760 -2.301065  1.381835
H    -2.517694 -2.013473  3.082687
H    -1.215171 -2.071067  1.883098
C    -3.411028  0.050313 -1.085787
C    -4.503033  1.114516 -0.858675
H    -4.951859  1.068352  0.134863
H    -5.306113  0.958052 -1.592002
H    -4.105667  2.123671 -1.014396
C    -3.986111 -1.368079 -0.939406
H    -3.209868 -2.133515 -1.055069
H    -4.734661 -1.534970 -1.726296
H    -4.481309 -1.526672  0.022409
C    -2.899438  0.219219 -2.526435
H    -2.353578  1.160013 -2.654520
H    -3.758060  0.230859 -3.211397
H    -2.253646 -0.611462 -2.824754
C    -0.260814 -2.343432 -0.812325
C     0.137032  0.010333 -2.286355
N     2.239450 -1.370375  2.931041
N     1.444670 -1.492879  2.062989
O     1.008143 -2.544899  1.393931

57
Complex-5     el energy= -1361.71378481
Ru    0.239532 -0.686019 -0.209309
H     1.123297  0.945361  2.486351
P    -1.942546  0.301337  0.010795
O    -0.718172 -3.592059 -0.090207
O     0.569351 -0.583850 -3.223030
N     2.413227 -0.812255 -0.257498
N     0.848319  1.329706 -0.200976
C     3.122181 -1.947415 -0.199066
H     2.543502 -2.864251 -0.164219
C     4.510510 -1.957158 -0.169899
H     5.045176 -2.900312 -0.116313
C     5.180513 -0.732549 -0.192063
H     6.266416 -0.694716 -0.160994
C     4.444100  0.444849 -0.239742
H     4.946342  1.405392 -0.233245
C     3.045733  0.388948 -0.268809
C     2.180129  1.588428 -0.285162
C     2.666325  2.880941 -0.367918
H     3.727756  3.085831 -0.433016
C     1.723794  3.940443 -0.374093
H     2.076781  4.968058 -0.429769
C     0.379512  3.682854 -0.317810
H    -0.345780  4.491802 -0.331180
C    -0.111276  2.329822 -0.248782
C    -1.463207  2.001109 -0.227227
H    -2.197143  2.801560 -0.203664
C    -2.728540  0.118385  1.764111
C    -4.180705  0.619407  1.846333
H    -4.272049  1.663112  1.522263
H    -4.499472  0.577175  2.897230
H    -4.885192  0.010935  1.273154
C    -1.894405  0.984121  2.725142
H    -0.869793  0.616710  2.756801
H    -2.319637  0.901217  3.735277
H    -1.899625  2.038586  2.430071
C    -2.638450 -1.351031  2.216434
H    -3.154526 -2.036672  1.536169
H    -3.109877 -1.453187  3.204562
H    -1.591865 -1.655577  2.308779
C    -3.276783 -0.107742 -1.307059
C    -4.316293  1.026997 -1.411036
H    -4.895071  1.174485 -0.498969
H    -5.024419  0.784701 -2.215608
H    -3.831450  1.974541 -1.671302
C    -3.955661 -1.456855 -1.017256
H    -3.219782 -2.263644 -0.916283
H    -4.615737 -1.716557 -1.856819
H    -4.568668 -1.441334 -0.112402
C    -2.590113 -0.205347 -2.678659
H    -1.949501  0.661270 -2.874085
H    -3.359445 -0.239106 -3.462155
H    -1.995982 -1.118276 -2.768834
C    -0.349039 -2.504997 -0.137561
C     0.314525 -0.626143 -2.101996
O     0.515998 -0.843889  1.885383
N     1.545996 -0.003242  2.408464
N     2.643886 -0.313687  2.724496

57
ts-5-6     el energy= -1361.71337133
Ru    0.261376 -0.681876 -0.164862
H     1.200487  0.680225  3.146600
P    -1.948906  0.286391 -0.038726
O    -0.637782 -3.592700  0.153782
O     0.603981 -0.744648 -3.176135
N     2.429541 -0.773041 -0.227839
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N	0.827003	1.340041	-0.257832
C	3.159808	-1.896297	-0.212295
H	2.598570	-2.823758	-0.177003
C	4.547331	-1.882623	-0.218126
H	5.098873	-2.817379	-0.198777
C	5.196032	-0.646152	-0.227238
H	6.281582	-0.589690	-0.219136
C	4.438297	0.518007	-0.243307
H	4.923958	1.487087	-0.245341
C	3.040447	0.438538	-0.248836
C	2.154737	1.622080	-0.284245
C	2.621832	2.922283	-0.369506
H	3.681248	3.146282	-0.387276
C	1.662104	3.962367	-0.452643
H	1.998352	4.995325	-0.514568
C	0.321926	3.678790	-0.466603
H	-0.416786	4.471993	-0.542924
C	-0.146311	2.318765	-0.382472
C	-1.492130	1.964949	-0.420382
H	-2.238617	2.753667	-0.453524
C	-2.747601	0.274551	1.718621
C	-4.210092	0.751924	1.739300
H	-4.322533	1.747874	1.294719
H	-4.529968	0.827604	2.788214
H	-4.900504	0.064922	1.242365
C	-1.940693	1.268205	2.576699
H	-0.882093	1.010695	2.556349
H	-2.298814	1.207622	3.614464
H	-2.068838	2.296755	2.224058
C	-2.641237	-1.136765	2.325591
H	-3.145932	-1.893930	1.715916
H	-3.121476	-1.140528	3.315045
H	-1.592456	-1.418107	2.453460
C	-3.264605	-0.269434	-1.319198
C	-4.320155	0.832505	-1.542518
H	-4.918240	1.048808	-0.656962
H	-5.009241	0.507431	-2.334424
H	-3.845974	1.762052	-1.877096
C	-3.925409	-1.593700	-0.900699
H	-3.178101	-2.373891	-0.712282
H	-4.573205	-1.947554	-1.715075
H	-4.547237	-1.497088	-0.006932
C	-2.565381	-0.493103	-2.669366
H	-1.949658	0.366619	-2.953998
H	-3.327584	-0.633957	-3.447958
H	-1.943567	-1.392216	-2.658281
C	-0.289481	-2.505355	0.024750
C	0.349166	-0.730293	-2.054489
O	0.384912	-0.625859	1.950647
N	1.551005	-0.132739	2.595380
N	2.658220	-0.552829	2.593234

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ts-4b-6 el energy= -1361.68522375

Ru	0.202445	-0.663399	-0.332479
H	1.149902	-1.169819	3.085875
P	-1.961584	0.287431	0.056235
O	-0.704096	-3.578543	-0.255679
O	0.303612	-0.366415	-3.375844
N	2.389605	-0.726919	-0.448144
N	0.771079	1.371145	-0.242885
C	3.131175	-1.841210	-0.490654
H	2.578757	-2.771041	-0.584222
C	4.518742	-1.820233	-0.412896
H	5.079676	-2.749218	-0.448968
C	5.152742	-0.582654	-0.283173
H	6.235640	-0.519315	-0.211278
C	4.382250	0.572346	-0.236414
H	4.854760	1.540076	-0.113408
C	2.986211	0.484647	-0.320898
C	2.092713	1.661233	-0.267886
C	2.559176	2.966464	-0.270732
H	3.617511	3.194179	-0.306344
C	1.596892	4.006380	-0.255067
H	1.929167	5.042590	-0.254260
C	0.257204	3.718250	-0.246315
H	-0.485154	4.511866	-0.238027
C	-0.204748	2.353690	-0.247238
C	-1.549654	1.993742	-0.249642
H	-2.301230	2.774634	-0.175117
C	-2.543833	0.144407	1.884878
C	-3.964851	0.681663	2.122477
H	-4.078683	1.710493	1.759872
H	-4.153485	0.696094	3.205526
H	-4.743621	0.061406	1.668225
C	-1.571913	1.014835	2.707785
H	-0.538531	0.708654	2.524108
H	-1.801484	0.879060	3.775521
H	-1.686031	2.076287	2.463943
C	-2.439165	-1.317593	2.354393

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H    -3.078030 -1.993988  1.777353
H    -2.758455 -1.382708  3.405378
H    -1.401320 -1.655616  2.285557
C    -3.409749 -0.172950 -1.108349
C    -4.467005  0.948670 -1.146213
H    -4.951997  1.119067 -0.183771
H    -5.249871  0.674429 -1.867306
H    -4.021938  1.891646 -1.482399
C    -4.049182 -1.512237 -0.705739
H    -3.301878 -2.311543 -0.635406
H    -4.778907 -1.808836 -1.472445
H    -4.581280 -1.457592  0.248034
C    -2.854329 -0.316386 -2.534425
H    -2.278634  0.565771 -2.833038
H    -3.693138 -0.426988 -3.235681
H    -2.222381 -1.203231 -2.634856
C    -0.352827 -2.482733 -0.306175
C     0.154238 -0.479311 -2.239498
O     0.593116 -0.855953  1.670703
N     2.088954 -0.794489  2.766600
N     3.191966 -0.540750  2.704422

57
Complex-6     el energy= -1361.71640790
Ru    0.252895 -0.701758 -0.251598
H     1.361880 -1.178452  3.512373
P    -1.916942  0.305386 -0.003373
O    -0.748689 -3.595918 -0.299617
O     0.467107 -0.384993 -3.261636
N     2.425581 -0.820105 -0.281635
N     0.852082  1.322399 -0.231236
C     3.139325 -1.951714 -0.218034
H     2.567146 -2.873339 -0.253574
C     4.524822 -1.955233 -0.106456
H     5.063953 -2.896369 -0.058255
C     5.184167 -0.724946 -0.055098
H     6.266355 -0.680393  0.039266
C     4.441636  0.447946 -0.115423
H     4.932302  1.411821 -0.046718
C     3.047157  0.385890 -0.223771
C     2.181291  1.580529 -0.282842
C     2.670914  2.867809 -0.405353
H     3.733870  3.069117 -0.456772
C     1.730766  3.926026 -0.472480
H     2.084530  4.951908 -0.551679
C     0.385798  3.666358 -0.449035
H    -0.341320  4.471320 -0.512732
C    -0.101804  2.314771 -0.355602
C    -1.454781  1.979043 -0.391301
H    -2.192634  2.776003 -0.403808
C    -2.569081  0.286460  1.804703
C    -3.960082  0.928223  1.942462
H    -3.996691  1.928107  1.493111
H    -4.185612  1.043264  3.012271
H    -4.758293  0.317978  1.508617
C    -1.578894  1.151484  2.610305
H    -0.546578  0.839634  2.455077
H    -1.812247  1.050881  3.679944
H    -1.663387  2.207963  2.336718
C    -2.584623 -1.144126  2.372188
H    -3.244101 -1.813613  1.811403
H    -2.956444 -1.112743  3.407149
H    -1.572836 -1.557761  2.382867
C    -3.324488 -0.203790 -1.197520
C    -4.342177  0.942066 -1.366908
H    -4.864088  1.195231 -0.442445
H    -5.100139  0.637575 -2.102208
H    -3.852956  1.845062 -1.748047
C    -4.027894 -1.487456 -0.726956
H    -3.315058 -2.302775 -0.556124
H    -4.728767 -1.819702 -1.505701
H    -4.604762 -1.339530  0.190018
C    -2.711502 -0.470927 -2.581509
H    -2.120977  0.381805 -2.931042
H    -3.521294 -0.639044 -3.304860
H    -2.081274 -1.365589 -2.581230
C    -0.356627 -2.515213 -0.284960
C     0.279393 -0.506986 -2.134131
O     0.454591 -1.156897  1.824165
N     1.442110 -0.584326  2.657561
N     2.173399  0.332516  2.493924

57
ts-1b-2c      el energy= -1361.69121343
Ru   -0.283607 -0.519430  0.413688
H    -0.624867 -0.455517 -1.412996
P     1.903740  0.327903 -0.053389
O     0.653548 -3.374208  0.997989
O    -0.616669  0.313924  3.340233
N    -2.446347 -0.592832  0.375300
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N	-0.833563	1.458380	-0.074506
C	-3.190575	-1.691230	0.585039
H	-2.638458	-2.596102	0.813540
C	-4.576499	-1.681564	0.497611
H	-5.135555	-2.595908	0.670840
C	-5.212318	-0.479454	0.176664
H	-6.294990	-0.429967	0.092102
C	-4.443270	0.657549	-0.037770
H	-4.916458	1.597820	-0.296739
C	-3.047667	0.588417	0.067611
C	-2.156054	1.745437	-0.147321
C	-2.613862	3.029243	-0.398257
H	-3.671498	3.257696	-0.447167
C	-1.645604	4.047574	-0.575553
H	-1.971579	5.066475	-0.773811
C	-0.307035	3.760893	-0.500716
H	0.438987	4.539007	-0.637789
C	0.149081	2.419853	-0.242410
C	1.491085	2.058124	-0.160777
H	2.250724	2.810025	-0.354713
C	2.640017	-0.221843	-1.755827
C	4.094840	0.234940	-1.965912
H	4.200772	1.319774	-1.846474
H	4.392818	-0.009288	-2.995248
H	4.804747	-0.262198	-1.299723
C	1.801274	0.453225	-2.856662
H	0.749152	0.169868	-2.819542
H	2.192695	0.141281	-3.835289
H	1.863318	1.544326	-2.791573
C	2.541160	-1.749127	-1.904900
H	3.126199	-2.284460	-1.150295
H	2.924371	-2.044999	-2.891774
H	1.504701	-2.090384	-1.831897
C	3.262882	0.145777	1.290677
C	4.329985	1.251238	1.160625
H	4.891520	1.207614	0.226806
H	5.050630	1.147147	1.983802
H	3.873005	2.243607	1.243923
C	3.906059	-1.250737	1.254148
H	3.151016	-2.043608	1.310035
H	4.569776	-1.365294	2.122789
H	4.510791	-1.417750	0.358691
C	2.600018	0.328314	2.665668
H	1.997734	1.242315	2.705352
H	3.382847	0.406360	3.432617
H	1.970372	-0.526552	2.926457
C	0.267336	-2.320594	0.733560
C	-0.364982	-0.015615	2.268429
N	-1.020882	-2.779768	-1.543789
N	-1.379436	-2.046118	-2.384048
O	-1.294855	-0.786600	-2.517927

57

Complex-2c el energy= -1361.74167741

Ru	0.254605	-0.728735	-0.241612
H	1.314345	1.094749	1.849605
P	-1.904521	0.303112	0.013998
O	-0.811193	-3.597783	-0.423043
O	0.547195	-0.320297	-3.252810
N	2.425139	-0.872600	-0.233246
N	0.880619	1.290570	-0.225163
C	3.122274	-2.011400	-0.104097
H	2.538698	-2.926099	-0.110582
C	4.502933	-2.026482	0.042691
H	5.026531	-2.971631	0.147052
C	5.179161	-0.803987	0.065970
H	6.258237	-0.770811	0.192599
C	4.455734	0.374973	-0.058306
H	4.955101	1.335614	-0.007381
C	3.064575	0.325071	-0.206877
C	2.218453	1.527737	-0.334269
C	2.717621	2.799178	-0.530213
H	3.781141	2.982185	-0.622489
C	1.787716	3.868850	-0.612546
H	2.153747	4.884488	-0.745667
C	0.441774	3.633249	-0.532381
H	-0.274146	4.447289	-0.604234
C	-0.065812	2.294036	-0.371851
C	-1.419402	1.977504	-0.359623
H	-2.147772	2.782785	-0.379290
C	-2.596298	0.265745	1.809062
C	-4.008096	0.870214	1.916604
H	-4.052811	1.882011	1.496178
H	-4.270140	0.948872	2.980871
H	-4.777536	0.256294	1.439854
C	-1.666870	1.152104	2.661226
H	-0.616327	0.866305	2.622066
H	-1.981923	1.076940	3.711145
H	-1.741245	2.201704	2.357747

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C    -2.601714 -1.173077  2.355765
H    -3.264619 -1.833386  1.787647
H    -2.962970 -1.159348  3.393670
H    -1.598149 -1.605882  2.359488
C    -3.294246 -0.179365 -1.216315
C    -4.307627  0.971412 -1.381928
H    -4.845305  1.210736 -0.463435
H    -5.053206  0.680031 -2.134731
H    -3.811758  1.879897 -1.740871
C    -4.004985 -1.472767 -0.784190
H    -3.295715 -2.292526 -0.621645
H    -4.694201 -1.786845 -1.580445
H    -4.595786 -1.346358  0.126754
C    -2.660807 -0.418211 -2.596300
H    -2.060646  0.439032 -2.917732
H    -3.460623 -0.563443 -3.335248
H    -2.037625 -1.317555 -2.608930
C    -0.392930 -2.530743 -0.343172
C     0.314051 -0.501070 -2.144275
N     0.578877 -1.208020  1.832289
N     1.222829 -0.813195  2.728773
O     1.815826  0.754013  2.608422

57
ts-1-2d      el energy= -1361.68649914
Ru    0.286248 -0.582112 -0.390439
H     0.227655 -1.770623  1.081263
P    -1.897481  0.320578  0.030666
O    -0.679812 -3.416825 -0.974536
O     0.601111  0.156622 -3.351195
N     2.447088 -0.670744 -0.365417
N     0.854406  1.412215  0.032623
C     3.180258 -1.785001 -0.517186
H     2.620881 -2.693235 -0.715826
C     4.565194 -1.788219 -0.414543
H     5.115042 -2.716024 -0.538816
C     5.211749 -0.579573 -0.142986
H     6.293927 -0.538643 -0.048383
C     4.453599  0.573985  0.012756
H     4.934201  1.518889  0.239206
C     3.058266  0.516547 -0.100208
C     2.179025  1.690709  0.060443
C     2.652413  2.985264  0.210956
H     3.712710  3.206742  0.219011
C     1.696694  4.020594  0.340827
H     2.033724  5.046789  0.471796
C     0.354065  3.742318  0.297554
H    -0.383801  4.534457  0.391991
C    -0.114756  2.394228  0.116905
C    -1.461296  2.045862  0.021328
H    -2.214078  2.815090  0.168257
C    -2.630444 -0.079724  1.768972
C    -4.041456  0.502325  1.966203
H    -4.078755  1.571947  1.727870
H    -4.318449  0.394721  3.024454
H    -4.805001 -0.015893  1.378701
C    -1.705433  0.611244  2.787624
H    -0.655775  0.355886  2.634544
H    -1.991314  0.295113  3.800714
H    -1.792965  1.700718  2.725959
C    -2.648267 -1.592933  2.042430
H    -3.233973 -2.151592  1.306346
H    -3.100811 -1.773356  3.027903
H    -1.638080 -2.008489  2.065977
C    -3.264499  0.061872 -1.292044
C    -4.294309  1.209033 -1.256846
H    -4.856696  1.258265 -0.323272
H    -5.018049  1.060804 -2.070505
H    -3.805329  2.175871 -1.418821
C    -3.960064 -1.299717 -1.128197
H    -3.238253 -2.124809 -1.109683
H    -4.629724 -1.467345 -1.983528
H    -4.569323 -1.356961 -0.222037
C    -2.604478  0.097443 -2.679367
H    -2.002538  1.001995 -2.814496
H    -3.388837  0.097223 -3.448744
H    -1.975498 -0.780631 -2.852278
C    -0.293541 -2.353501 -0.748482
C     0.378973 -0.057403 -2.245490
N     1.437112 -0.315680  2.206512
N     1.370201 -1.393377  2.664920
O     0.778028 -2.433753  2.279151

57
Complex-2d    el energy= -1361.83159111
Ru    0.346496 -0.562460 -0.107028
H     0.263597 -4.305714  0.382684
P    -1.851152  0.393484 -0.013412
O    -1.080921 -3.101400 -0.884056
O     0.631147 -0.546001 -3.107257
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N      2.529621 -0.624318 -0.069787
N      0.911168  1.497540 -0.052681
C      3.271095 -1.742803 -0.035793
H      2.705478 -2.669504 -0.055310
C      4.658879 -1.710366  0.047929
H      5.222212 -2.638326  0.071301
C      5.290233 -0.466166  0.109806
H      6.372824 -0.396695  0.183631
C      4.518923  0.690612  0.083724
H      4.991086  1.664503  0.146769
C      3.123807  0.599889 -0.012947
C      2.233560  1.783012 -0.068267
C      2.704711  3.083619 -0.166176
H      3.763726  3.310610 -0.190465
C      1.741556  4.119217 -0.271386
H      2.074782  5.152961 -0.338744
C      0.401976  3.830521 -0.307134
H     -0.336175  4.621732 -0.409829
C     -0.061549  2.466992 -0.232179
C     -1.399459  2.094357 -0.331757
H     -2.153696  2.872983 -0.403990
C     -2.600484  0.375158  1.765173
C     -3.997557  1.016902  1.841559
H     -4.001883  2.024375  1.409095
H     -4.287865  1.112818  2.898002
H     -4.768301  0.420519  1.346127
C     -1.672279  1.249245  2.635438
H     -0.613482  1.014448  2.515272
H     -1.932250  1.111079  3.694307
H     -1.791141  2.307370  2.384018
C     -2.665926 -1.059715  2.318499
H     -3.389638 -1.674414  1.776859
H     -2.974929 -1.034142  3.373414
H     -1.702613 -1.572250  2.263291
C     -3.214574 -0.094558 -1.264057
C     -4.187952  1.073808 -1.509679
H     -4.742452  1.370592 -0.616419
H     -4.922596  0.766456 -2.267206
H     -3.658879  1.951666 -1.896533
C     -3.970448 -1.355878 -0.812000
H     -3.275152 -2.174518 -0.602232
H     -4.631814 -1.680780 -1.627885
H     -4.602081 -1.180511  0.063710
C     -2.522572 -0.418733 -2.597622
H     -1.894718  0.411299 -2.938954
H     -3.291487 -0.591142 -3.363933
H     -1.924493 -1.329517 -2.510733
C     -0.197223 -2.567494 -0.238109
C      0.417630 -0.535356 -1.977512
N      0.641179 -0.884970  1.941365
N      0.989703 -1.159493  2.956767
O      0.610725 -3.404450  0.532496

3
N2O (SMD-BS2)    el energy= -
184.730064615
N      0.000000  0.000000 -1.195122
N      0.000000  0.000000 -0.073969
O      0.000000  0.000000  1.110454

3
H2O (SMD-BS2)   el energy= -
76.4681404508
O      0.000000  0.000000  0.118311
H      0.000000 -0.762618 -0.473245
H      0.000000  0.762618 -0.473245

54
Complex-1 (SMD-BS2)    el energy= -
1513.42208414
Ru    -0.362015 -0.716405 -0.003231
H     -0.344198 -0.561561 -1.635599
P      1.790265  0.271386 -0.057657
O      0.509984 -3.570043 -0.463172
O     -0.934770 -1.073552  3.011177
N     -2.493166 -0.820606 -0.241176
N     -0.962884  1.295070  0.098487
C     -3.195820 -1.944495 -0.437608
H     -2.629771 -2.864102 -0.463531
C     -4.568730 -1.941008 -0.603071
H     -5.092406 -2.873744 -0.760461
C     -5.240299 -0.724216 -0.564410
H     -6.313799 -0.681453 -0.694608
C     -4.516841  0.437987 -0.360051
H     -5.019172  1.393141 -0.330434
C     -3.133647  0.374408 -0.194213
C     -2.284885  1.560497  0.028892
C     -2.782285  2.842722  0.161983
H     -3.840102  3.047911  0.112285
C     -1.853557  3.885176  0.371921
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H	-2.211691	4.902150	0.480198
C	-0.514271	3.626402	0.435101
H	0.199365	4.425095	0.590209
C	-0.016845	2.286239	0.292410
C	1.324973	1.947305	0.331491
H	2.064117	2.730704	0.425916
C	2.579820	0.293947	-1.814880
C	3.986871	0.902273	-1.831412
H	4.004642	1.896181	-1.381691
H	4.307543	1.009399	-2.872248
H	4.724038	0.278087	-1.329936
C	1.687849	1.178229	-2.697264
H	0.649589	0.849039	-2.688549
H	2.052214	1.123493	-3.727498
H	1.719847	2.220180	-2.379016
C	2.614500	-1.119518	-2.407361
H	3.202727	-1.813775	-1.809459
H	3.065786	-1.076974	-3.403505
H	1.609767	-1.525428	-2.515616
C	3.109258	-0.249663	1.227028
C	4.115995	0.880364	1.488208
H	4.688963	1.157783	0.608229
H	4.824891	0.545886	2.251513
H	3.617652	1.771983	1.869928
C	3.835436	-1.526902	0.793139
H	3.133488	-2.330086	0.562965
H	4.471750	-1.870976	1.614028
H	4.476091	-1.371064	-0.072752
C	2.385401	-0.533711	2.547067
H	1.733552	0.290805	2.839282
H	3.130193	-0.667299	3.336751
H	1.798257	-1.448392	2.491001
C	0.183734	-2.479812	-0.274440
C	-0.609655	-0.909300	1.924871

57

ts-1-2 (SMD-BS2) el energy= -1698.12888977

Ru	0.284410	-0.430064	-0.436593
H	0.519304	-0.796976	1.276140
P	-1.921382	0.310845	0.063909
O	-0.492039	-3.268569	-1.176186
O	0.565600	0.408259	-3.340307
N	2.428098	-0.446935	-0.411933
N	0.761129	1.514538	0.157326
C	3.200324	-1.501943	-0.708015
H	2.685735	-2.401395	-1.010333
C	4.579160	-1.453501	-0.622548
H	5.162085	-2.330796	-0.866069
C	5.179531	-0.267366	-0.215191
H	6.255867	-0.195262	-0.129139
C	4.383848	0.825616	0.082114
H	4.832475	1.753887	0.402786
C	2.997904	0.723231	-0.027240
C	2.072210	1.836113	0.255616
C	2.486976	3.112152	0.574088
H	3.533128	3.364192	0.646421
C	1.491804	4.090992	0.792313
H	1.787934	5.102015	1.045248
C	0.168090	3.776652	0.688955
H	-0.595228	4.525386	0.855453
C	-0.248100	2.441859	0.358129
C	-1.570098	2.048130	0.243189
H	-2.354466	2.760991	0.456045
C	-2.567615	-0.324511	1.763202
C	-4.018876	0.081522	2.044278
H	-4.161831	1.159700	1.959682
H	-4.261173	-0.198907	3.073918
H	-4.734586	-0.418822	1.395184
C	-1.698850	0.325822	2.848584
H	-0.635631	0.173618	2.686893
H	-1.955430	-0.122048	3.813092
H	-1.882379	1.398028	2.911806
C	-2.429042	-1.848844	1.844275
H	-3.006855	-2.362593	1.077434
H	-2.793816	-2.190140	2.817694
H	-1.390666	-2.162956	1.751703
C	-3.297232	0.136756	-1.250372
C	-4.393990	1.193128	-1.050454
H	-4.922767	1.089840	-0.107709
H	-5.128157	1.086639	-1.854325
H	-3.985840	2.202628	-1.109903
C	-3.897945	-1.272654	-1.245877
H	-3.128840	-2.039385	-1.347455
H	-4.573672	-1.370334	-2.100618
H	-4.475469	-1.482342	-0.347961
C	-2.667878	0.382674	-2.624912
H	-2.107205	1.317683	-2.654943
H	-3.465870	0.447289	-3.369623
H	-2.015416	-0.437901	-2.917633

C -0.173771 -2.212898 -0.852723
C 0.336738 0.095564 -2.261558
N 1.292466 -1.220430 2.383860
N 1.527823 -2.359170 2.239721
O 1.356405 -3.284552 1.453961

57
ts-2-3 (SMD-BS2) el energy= -1698.16700359
Ru 0.263867 -0.704164 -0.113484
H 1.274656 1.472840 2.308293
P -1.928019 0.287278 -0.059632
O -0.631790 -3.578977 0.292641
O 0.648131 -1.017169 -3.058792
N 2.411505 -0.843339 -0.128857
N 0.860854 1.280843 -0.325695
C 3.115579 -1.974941 0.003412
H 2.546212 -2.885589 0.116793
C 4.497515 -1.985530 0.004433
H 5.026940 -2.920961 0.119175
C 5.171061 -0.777523 -0.137772
H 6.252828 -0.746789 -0.137903
C 4.443596 0.391644 -0.275795
H 4.950555 1.339103 -0.378792
C 3.051168 0.343421 -0.269076
C 2.191486 1.534433 -0.405231
C 2.677190 2.806725 -0.606310
H 3.735801 3.004821 -0.663554
C 1.738588 3.855901 -0.740780
H 2.093111 4.868974 -0.887743
C 0.399355 3.605563 -0.693171
H -0.320452 4.405742 -0.804544
C -0.094826 2.268989 -0.501197
C -1.438967 1.945274 -0.481164
H -2.171323 2.734813 -0.574862
C -2.748136 0.332264 1.684060
C -4.199974 0.825160 1.660858
H -4.288259 1.811829 1.204587
H -4.538587 0.915972 2.697412
H -4.882268 0.143341 1.158764
C -1.956383 1.326751 2.544055
H -0.905220 1.061782 2.592515
H -2.363121 1.302372 3.559611
H -2.051023 2.344234 2.164387
C -2.679422 -1.063801 2.316637
H -3.194294 -1.817353 1.721585
H -3.165327 -1.032273 3.296800
H -1.646746 -1.374895 2.464228
C -3.225475 -0.278282 -1.349091
C -4.249728 0.834879 -1.619515
H -4.840792 1.101727 -0.749561
H -4.940398 0.486836 -2.392802
H -3.761784 1.734903 -1.995365
C -3.921845 -1.569674 -0.906946
H -3.201044 -2.360401 -0.692566
H -4.562450 -1.921812 -1.720681
H -4.551645 -1.434854 -0.030801
C -2.505977 -0.555650 -2.671849
H -1.862791 0.273112 -2.969787
H -3.255354 -0.690789 -3.456369
H -1.921838 -1.472512 -2.626642
C -0.300361 -2.493343 0.139156
C 0.365285 -0.895852 -1.952938
N 1.980562 0.847412 2.737917
N 1.636576 -0.334981 2.597385
O 0.439898 -0.551121 2.009866

57
ts-3-4 (SMD-BS2) el energy= -1698.12498014
Ru 0.281705 -0.514283 -0.381776
H 1.746025 -0.818527 2.432729
P -1.930346 0.287789 0.055636
O -0.509386 -3.391684 -0.942588
O 0.524869 0.212602 -3.293342
N 2.439623 -0.536857 -0.449126
N 0.782200 1.459196 0.063554
C 3.199242 -1.610026 -0.697521
H 2.676146 -2.515531 -0.969053
C 4.578762 -1.574468 -0.602470
H 5.154714 -2.465909 -0.808074
C 5.186840 -0.381194 -0.230849
H 6.262908 -0.317665 -0.135063
C 4.400605 0.730553 0.022341
H 4.856858 1.662835 0.319858
C 3.014984 0.639070 -0.099691
C 2.097345 1.772885 0.130383
C 2.525486 3.062247 0.362668
H 3.574231 3.310077 0.405650
C 1.540065 4.062853 0.523916

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H      1.847275   5.084912   0.710684
C      0.213418   3.756604   0.444578
H     -0.541771   4.522173   0.565120
C     -0.217847   2.407547   0.199150
C     -1.544916   2.026441   0.103973
H     -2.317203   2.765001   0.268133
C     -2.614389  -0.201651   1.785496
C     -4.062551   0.248476   2.009618
H     -4.184387   1.319929   1.844479
H     -4.322348   0.048298   3.053745
H     -4.780339  -0.285227   1.390383
C     -1.750247   0.516797   2.832311
H     -0.696867   0.280453   2.712205
H     -2.065154   0.181184   3.825510
H     -1.883875   1.597520   2.782663
C     -2.495436  -1.718255   1.978280
H     -3.067129  -2.279599   1.240622
H     -2.883809  -1.983874   2.966601
H     -1.455148  -2.033026   1.930606
C     -3.293378   0.031260  -1.261207
C     -4.361486   1.130962  -1.163383
H     -4.896415   1.129846  -0.218745
H     -5.095094   0.971786  -1.958900
H     -3.923609   2.118481  -1.312575
C     -3.932578  -1.356747  -1.144484
H     -3.184424  -2.149909  -1.176053
H     -4.604359  -1.505909  -1.994740
H     -4.522004  -1.478321  -0.238578
C     -2.654365   0.142184  -2.648116
H     -2.086208   1.065584  -2.761779
H     -3.449471   0.146620  -3.398806
H     -2.009436  -0.707981  -2.863301
C     -0.205865  -2.307435  -0.722178
C      0.303243  -0.066105  -2.202203
N      2.199898  -1.966452   2.733634
N      1.356248  -2.398243   2.033714
O      0.659977  -0.961805   1.605202

57
ts-1-2b (SMD-BS2)    el energy= -
1698.12517972
Ru     0.215852  -0.663386  -0.336934
H      0.456350  -0.925524   1.428982
P     -1.937681   0.298839  -0.002983
O     -0.654637  -3.557553  -0.147986
O      0.424547  -0.686033  -3.361082
N      2.355946  -0.776298  -0.350131
N      0.796760   1.344969  -0.309445
C      3.070232  -1.910505  -0.338699
H      2.507123  -2.832048  -0.336755
C      4.452229  -1.911638  -0.324208
H      4.987872  -2.850499  -0.309577
C      5.117734  -0.690627  -0.327985
H      6.199208  -0.652222  -0.315802
C      4.381116   0.480923  -0.344440
H      4.881942   1.437330  -0.341563
C      2.988552   0.424151  -0.352984
C      2.121928   1.615246  -0.352254
C      2.599687   2.907560  -0.392930
H      3.657052   3.117975  -0.419319
C      1.655458   3.958571  -0.405321
H      2.002594   4.984421  -0.434542
C      0.317464   3.693737  -0.380098
H     -0.409229   4.495487  -0.390067
C     -0.163581   2.341175  -0.331559
C     -1.504763   1.999811  -0.296952
H     -2.249168   2.782732  -0.262891
C     -2.529481   0.165729   1.822208
C     -3.929442   0.752106   2.035559
H     -4.003773   1.774200   1.661432
H     -4.129569   0.782106   3.110979
H     -4.713329   0.152395   1.576321
C     -1.549483   0.995089   2.663842
H     -0.509820   0.747757   2.463298
H     -1.744178   0.799900   3.722134
H     -1.678385   2.061973   2.483269
C     -2.498999  -1.291762   2.296264
H     -3.140680  -1.940652   1.702626
H     -2.853540  -1.334670   3.330545
H     -1.489830  -1.697760   2.278757
C     -3.369464  -0.140203  -1.187661
C     -4.400777   0.995921  -1.248834
H     -4.886792   1.186639  -0.296450
H     -5.178278   0.719287  -1.966693
H     -3.945756   1.923500  -1.597253
C     -4.042120  -1.457566  -0.789767
H     -3.318545  -2.269856  -0.703943
H     -4.758717  -1.737128  -1.567518
H     -4.589557  -1.382452   0.147650
C     -2.783149  -0.306153  -2.593116
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H -2.173549 0.550206 -2.884205
H -3.605687 -0.386876 -3.309084
H -2.189777 -1.215281 -2.673563
C -0.327235 -2.458859 -0.230217
C 0.227223 -0.636772 -2.233234
N 1.046759 -1.455521 2.558021
N 1.775471 -0.646198 3.010606
O 2.182645 0.492486 2.794572

57
ts-2b-3b (SMD-BS2) el energy= -1698.16636626
Ru 0.295673 -0.545693 -0.302181
H 1.285202 -2.938353 1.864261
P -1.939565 0.289217 0.019755
O -0.511272 -3.448854 -0.685615
O 0.580224 -0.053674 -3.235171
N 2.439922 -0.562073 -0.369401
N 0.779713 1.455401 0.002575
C 3.202209 -1.641165 -0.586611
H 2.680783 -2.563141 -0.798332
C 4.582595 -1.589538 -0.533783
H 5.160396 -2.485535 -0.712003
C 5.189373 -0.375472 -0.234841
H 6.266931 -0.299444 -0.170797
C 4.401058 0.742394 -0.019235
H 4.856976 1.692372 0.216051
C 3.014277 0.636282 -0.099801
C 2.093963 1.776024 0.070356
C 2.515684 3.076695 0.237459
H 3.563139 3.328621 0.286958
C 1.526400 4.082641 0.324860
H 1.829008 5.113758 0.462502
C 0.202221 3.769883 0.233570
H -0.556380 4.539047 0.294951
C -0.222561 2.408167 0.056844
C -1.548094 2.023320 -0.047724
H -2.321872 2.771907 0.048905
C -2.667433 -0.075016 1.763006
C -4.126003 0.373228 1.909548
H -4.254085 1.428114 1.663801
H -4.413654 0.246600 2.957813
H -4.818979 -0.214390 1.311429
C -1.842404 0.735311 2.774613
H -0.778169 0.533690 2.688713
H -2.164153 0.451820 3.781722
H -2.014095 1.804987 2.654140
C -2.545895 -1.572326 2.073082
H -3.091049 -2.190307 1.360656
H -2.967462 -1.764755 3.064640
H -1.502715 -1.882482 2.085362
C -3.263070 -0.067680 -1.313792
C -4.334890 1.033025 -1.320617
H -4.899395 1.092377 -0.395146
H -5.042532 0.819459 -2.126661
H -3.893655 2.010125 -1.520315
C -3.901238 -1.447397 -1.119396
H -3.150383 -2.238158 -1.087665
H -4.556922 -1.652828 -1.970430
H -4.506911 -1.513440 -0.218617
C -2.586375 -0.049347 -2.687125
H -2.014275 0.864661 -2.847483
H -3.361109 -0.093141 -3.457392
H -1.939882 -0.913861 -2.829204
C -0.196131 -2.357201 -0.531629
C 0.341707 -0.238965 -2.128386
N 2.022942 -2.395630 2.354877
N 1.724630 -1.192905 2.354298
O 0.544331 -0.855749 1.804908

57
ts-1-2d (SMD-BS2) el energy= -1698.10247896
Ru 0.296029 -0.555965 -0.358006
H 0.223710 -1.738642 1.037091
P -1.900815 0.321524 0.017777
O -0.585793 -3.379049 -0.979017
O 0.686911 0.091023 -3.296649
N 2.440670 -0.637029 -0.360044
N 0.848490 1.421211 0.086331
C 3.171981 -1.740950 -0.564084
H 2.623429 -2.645591 -0.782031
C 4.552327 -1.734380 -0.492170
H 5.102261 -2.650176 -0.658471
C 5.197154 -0.537301 -0.201094
H 6.276234 -0.495473 -0.130706
C 4.442691 0.604744 0.003789
H 4.926733 1.540975 0.238546
C 3.052624 0.542499 -0.081966
C 2.169262 1.706007 0.117822

C 2.631324 2.994673 0.296573
H 3.685951 3.219588 0.313275
C 1.672428 4.018206 0.451095
H 2.003741 5.038066 0.606300
C 0.336599 3.737936 0.403273
H -0.399912 4.522665 0.516486
C -0.125927 2.395548 0.191558
C -1.463172 2.043954 0.091775
H -2.218782 2.803636 0.235849
C -2.680680 -0.141869 1.713894
C -4.084820 0.446670 1.896720
H -4.098856 1.523737 1.723691
H -4.395257 0.278626 2.932501
H -4.829678 -0.020727 1.256126
C -1.782135 0.479464 2.790053
H -0.737365 0.209344 2.666394
H -2.110380 0.123305 3.770891
H -1.847923 1.567372 2.781726
C -2.721292 -1.661877 1.903891
H -3.330238 -2.163808 1.154660
H -3.154506 -1.884558 2.883747
H -1.722951 -2.094527 1.881307
C -3.225360 0.115020 -1.351185
C -4.230482 1.275754 -1.315851
H -4.797222 1.327677 -0.390748
H -4.944602 1.141214 -2.133473
H -3.730673 2.232661 -1.468738
C -3.951921 -1.229192 -1.236807
H -3.253497 -2.066661 -1.210024
H -4.586995 -1.359885 -2.117741
H -4.593918 -1.289094 -0.360976
C -2.526686 0.160350 -2.712203
H -1.913301 1.054699 -2.823679
H -3.289627 0.182126 -3.495166
H -1.913484 -0.724044 -2.878984
C -0.245621 -2.306933 -0.739972
C 0.417849 -0.068118 -2.195471
N 1.373401 -0.426348 2.182089
N 1.336226 -1.491740 2.662835
O 0.759591 -2.544072 2.290848

60
ts-3-4-oh2 (SMD-BS2) el energy= -1774.63328964
Ru 0.185356 -0.427683 -0.516319
P -2.014185 0.286244 0.107176
O -0.650888 -3.192772 -1.457829
O 0.283903 0.593315 -3.338310
N 2.336220 -0.401096 -0.695757
N 0.683016 1.502203 0.101776
C 3.097597 -1.435496 -1.071322
H 2.574786 -2.328624 -1.381398
C 4.479844 -1.377437 -1.055037
H 5.057409 -2.238323 -1.361324
C 5.089216 -0.201716 -0.633319
H 6.167842 -0.121278 -0.599726
C 4.301048 0.871217 -0.250164
H 4.759055 1.789211 0.086286
C 2.912272 0.758690 -0.292800
C 1.993033 1.844239 0.102025
C 2.413242 3.115811 0.425552
H 3.457523 3.385483 0.419812
C 1.423466 4.070837 0.754136
H 1.724362 5.076867 1.020707
C 0.100891 3.740502 0.734528
H -0.658056 4.471473 0.980566
C -0.322481 2.411865 0.383707
C -1.646517 2.015837 0.324629
H -2.419492 2.718682 0.602433
C -2.611139 -0.401731 1.799940
C -4.052337 -0.003641 2.137408
H -4.193961 1.077628 2.103973
H -4.261242 -0.327197 3.161787
H -4.792409 -0.473396 1.492974
C -1.707938 0.210337 2.880608
H -0.658404 0.010013 2.687664
H -1.970188 -0.242004 3.842145
H -1.858958 1.286748 2.961096
C -2.467083 -1.928554 1.816628
H -3.075480 -2.414290 1.054979
H -2.797315 -2.305543 2.789767
H -1.428771 -2.220658 1.677399
C -3.433480 0.153063 -1.167687
C -4.511138 1.214315 -0.899034
H -5.004095 1.094937 0.061079
H -5.276848 1.133460 -1.675966
H -4.095002 2.220936 -0.951607
C -4.047340 -1.250921 -1.177671
H -3.291002 -2.021148 -1.333545
H -4.758343 -1.317060 -2.006307

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H    -4.589295 -1.482637 -0.263574
C    -2.861119  0.429598 -2.560258
H    -2.305410  1.366989 -2.593729
H    -3.690135  0.508638 -3.268744
H    -2.221709 -0.383364 -2.899870
C    -0.317005 -2.166988 -1.068434
C     0.113057  0.210836 -2.269471
N     2.125237 -2.876357  1.999789
H     2.555709 -1.922515  2.468225
N     1.157290 -2.687054  1.364073
O     0.648085 -1.088934  1.402504
H     1.587582 -0.582050  2.049117
O     2.530611 -0.519556  2.743548
H     3.236409 -0.020844  2.313918

60
ts-3-4-oh2-b (SMD-BS2)    el energy= -
1774.62989077
Ru    0.195952 -0.398831 -0.535134
H     2.457431 -2.368963  2.256201
P    -2.013973  0.268282  0.106079
O    -0.578882 -3.157052 -1.536147
O     0.266443  0.786608 -3.291218
N     2.344200 -0.337805 -0.703865
N     0.666091  1.515454  0.151364
C     3.119354 -1.354466 -1.100739
H     2.608730 -2.233634 -1.467002
C     4.499711 -1.292088 -1.048006
H     5.089562 -2.137729 -1.373062
C     5.093096 -0.129016 -0.569369
H     6.170195 -0.046982 -0.504906
C     4.291529  0.926268 -0.170057
H     4.735782  1.832066  0.214407
C     2.904895  0.808701 -0.246853
C     1.971101  1.874857  0.162737
C     2.372259  3.146309  0.507695
H     3.413138  3.428910  0.510951
C     1.368407  4.082447  0.847201
H     1.654701  5.087396  1.133289
C     0.050130  3.735651  0.812370
H    -0.720172  4.452597  1.064305
C    -0.352743  2.408967  0.432586
C    -1.672362  1.999810  0.344894
H    -2.456834  2.687627  0.628079
C    -2.592077 -0.444014  1.794794
C    -4.028539 -0.042865  2.148514
H    -4.168534  1.038716  2.116791
H    -4.227350 -0.366536  3.174865
H    -4.775717 -0.511280  1.511170
C    -1.674776  0.156269  2.870095
H    -0.627647 -0.027541  2.654471
H    -1.914498 -0.316676  3.827527
H    -1.835635  1.229159  2.973751
C    -2.454714 -1.971546  1.798634
H    -3.070365 -2.449942  1.038666
H    -2.779147 -2.353381  2.771853
H    -1.418088 -2.267118  1.651916
C    -3.433835  0.118778 -1.165372
C    -4.522606  1.167906 -0.894530
H    -5.010449  1.043659  0.067761
H    -5.290184  1.077540 -1.668579
H    -4.117867  2.179038 -0.949210
C    -4.032495 -1.291807 -1.170871
H    -3.267845 -2.055465 -1.319121
H    -4.739108 -1.369202 -2.002224
H    -4.576354 -1.523629 -0.257954
C    -2.869695  0.398506 -2.560468
H    -2.350262  1.355699 -2.604346
H    -3.700564  0.439048 -3.270119
H    -2.199953 -0.394514 -2.890298
C    -0.278424 -2.120201 -1.148512
C     0.110807  0.333907 -2.248423
N     2.621029 -1.315740  2.629174
N     1.828051 -0.540265  2.238633
O     0.627477 -1.262148  1.331660
O     1.695149 -3.383637  1.506952
H     2.137529 -3.696022  0.708494
H     1.055987 -2.404476  1.281988

59
complex-1-no-hydride (C1)   el energy=
-1850.34521289
Ru    0.086042  0.073782 -0.038017
P     2.247737  1.051571  0.098962
O     0.985156 -2.810986 -0.649959
O    -0.129060 -0.536148  2.881574
N    -2.034762 -0.014526 -0.509566
N    -0.494263  2.043327  0.130513
C    -2.738326 -1.120296 -0.824955
H    -2.169660 -2.039458 -0.918707
```

C	-4.110234	-1.100892	-1.019583
H	-4.643451	-2.011928	-1.269962
C	-4.779014	0.118944	-0.873735
C	-6.272142	0.195229	-1.124550
C	-4.063566	1.259528	-0.537036
H	-4.582115	2.201653	-0.408015
C	-2.677421	1.177538	-0.359477
C	-1.830924	2.329456	-0.010628
C	-2.316979	3.603489	0.151403
H	-3.367381	3.835440	0.028569
C	-1.399457	4.641014	0.492174
C	-1.951095	6.033196	0.687807
C	-0.070341	4.377781	0.631593
H	0.629105	5.165888	0.888474
C	0.435272	3.041279	0.431814
C	1.775083	2.720099	0.517737
H	2.503861	3.470066	0.805405
C	2.742799	1.058708	-1.749614
C	3.645383	2.258107	-2.080809
H	3.168928	3.204534	-1.805051
H	3.833271	2.274025	-3.162766
H	4.615987	2.200433	-1.580738
C	1.408521	1.224716	-2.513514
H	0.736994	0.352599	-2.382033
H	1.601706	1.279199	-3.593330
H	0.875730	2.135791	-2.224260
C	3.417961	-0.254834	-2.170234
H	4.398417	-0.383822	-1.702497
H	3.577016	-0.239689	-3.256468
H	2.809444	-1.136000	-1.941066
C	3.603619	0.462903	1.272155
C	4.959907	1.094495	0.906168
H	5.344990	0.732368	-0.051575
H	5.692563	0.823954	1.677208
H	4.910480	2.189204	0.871548
C	3.692560	-1.073322	1.232308
H	2.761294	-1.538378	1.574342
H	4.491256	-1.401021	1.909486
H	3.926474	-1.460753	0.236559
C	3.202760	0.914213	2.690751
H	3.165595	2.003987	2.781101
H	3.952184	0.539641	3.399612
H	2.232709	0.513153	2.999713
C	0.651547	-1.741775	-0.417683
C	-0.010524	-0.316940	1.762520
F	-0.993451	6.920253	0.988994
F	-2.574989	6.450182	-0.429912
F	-2.860311	6.041834	1.679578
F	-6.808609	1.280696	-0.548238
F	-6.515523	0.259808	-2.443098
F	-6.889503	-0.893169	-0.643278

60

complex-1 (C1) el energy= -1851.14432611

Ru	0.027487	0.008737	0.016886
H	0.045975	0.142455	-1.619941
P	2.179625	1.011815	-0.067809
O	0.995797	-2.837837	-0.472554
O	-0.466019	-0.214043	3.101803
N	-2.123163	-0.083389	-0.244512
N	-0.573971	2.033789	0.094879
C	-2.837403	-1.201046	-0.454343
H	-2.272557	-2.127146	-0.461435
C	-4.210300	-1.189028	-0.657483
H	-4.749116	-2.114039	-0.832975
C	-4.865258	0.045066	-0.640243
C	-6.364040	0.105858	-0.805007
C	-4.132592	1.204908	-0.429278
H	-4.628739	2.167438	-0.431910
C	-2.748533	1.123396	-0.229470
C	-1.893674	2.307162	-0.007525
C	-2.395769	3.593593	0.093628
H	-3.453133	3.813075	0.024711
C	-1.458539	4.636232	0.313948
C	-1.983223	6.041379	0.424763
C	-0.119287	4.374458	0.412662
H	0.590847	5.177681	0.576384
C	0.374455	3.025331	0.291857
C	1.718424	2.687910	0.353162
H	2.458697	3.476918	0.446628
C	2.923903	1.071199	-1.845251
C	4.327566	1.699875	-1.883148
H	4.345000	2.686136	-1.404031
H	4.624760	1.841268	-2.931713
H	5.089051	1.069327	-1.414742
C	1.993596	1.967170	-2.686022
H	0.959254	1.611703	-2.665222
H	2.339476	1.955703	-3.729033
H	2.006140	3.001839	-2.328664

C	2.958381	-0.334226	-2.469235
H	3.585120	-1.033103	-1.907157
H	3.368137	-0.268461	-3.487100
H	1.951868	-0.756622	-2.539350
C	3.529193	0.472126	1.177849
C	4.544782	1.601889	1.438605
H	5.110817	1.888957	0.550782
H	5.266373	1.262894	2.194971
H	4.045406	2.493179	1.833993
C	4.243405	-0.804839	0.705189
H	3.529977	-1.602591	0.466103
H	4.894363	-1.173999	1.510053
H	4.874356	-0.634564	-0.172029
C	2.831460	0.168645	2.514164
H	2.193578	0.999750	2.834303
H	3.593981	0.009353	3.288902
H	2.224810	-0.739016	2.453437
C	0.614761	-1.768168	-0.262699
C	-0.194105	-0.120023	1.991714
F	-1.015532	6.943515	0.668038
F	-2.611335	6.418823	-0.711001
F	-2.893215	6.145475	1.418696
F	-6.772189	1.316559	-1.224012
F	-6.794553	-0.808501	-1.693967
F	-6.986516	-0.148728	0.362502

63

ts-1-2 (C1) el energy= -2035.78105752

Ru	-0.784237	-0.969920	-0.425666
H	-0.562120	-1.073923	1.348378
P	-2.845339	0.171466	-0.042899
O	-2.069515	-3.739485	-0.678930
O	-0.495321	-0.566264	-3.452633
N	1.357881	-1.296709	-0.358135
N	-0.009837	0.961822	-0.135796
C	1.970659	-2.489370	-0.441911
H	1.323219	-3.344569	-0.591155
C	3.345211	-2.631033	-0.311640
H	3.803307	-3.612406	-0.370927
C	4.106547	-1.482579	-0.082926
C	5.609620	-1.582093	0.019537
C	3.477228	-0.248328	0.006969
H	4.057952	0.644086	0.204248
C	2.087265	-0.170779	-0.138055
C	1.335768	1.098087	-0.058955
C	1.946317	2.332441	0.063267
H	3.021363	2.446095	0.111316
C	1.101251	3.473101	0.099605
C	1.749085	4.823760	0.241086
C	-0.258179	3.349473	0.016719
H	-0.896392	4.225872	0.043849
C	-0.869852	2.049729	-0.102975
C	-2.240549	1.848195	-0.175957
H	-2.906069	2.701753	-0.089246
C	-3.506599	-0.055933	1.754701
C	-4.882715	0.594733	1.980717
H	-4.881715	1.655539	1.703755
H	-5.123713	0.538598	3.051401
H	-5.690467	0.091657	1.441913
C	-2.512150	0.660034	2.689953
H	-1.483238	0.322446	2.559464
H	-2.798725	0.453505	3.730264
H	-2.535950	1.743360	2.534971
C	-3.570942	-1.551098	2.111524
H	-4.261251	-2.106224	1.468502
H	-3.921879	-1.661887	3.146828
H	-2.589008	-2.025866	2.040826
C	-4.281325	-0.024501	-1.290376
C	-5.215612	1.201640	-1.265439
H	-5.720624	1.342482	-0.308663
H	-5.991724	1.069910	-2.031933
H	-4.666026	2.118342	-1.506355
C	-5.068688	-1.319943	-1.030668
H	-4.410569	-2.196116	-1.005951
H	-5.789821	-1.471873	-1.845726
H	-5.635189	-1.290951	-0.095811
C	-3.673504	-0.104149	-2.700651
H	-2.985744	0.726499	-2.892828
H	-4.482304	-0.050152	-3.441903
H	-3.145684	-1.048501	-2.859524
C	-1.541794	-2.727142	-0.538508
C	-0.709334	-0.713783	-2.334473
N	0.117014	-1.462860	2.466488
N	0.237574	-2.640993	2.407192
O	-0.032183	-3.567306	1.650091
F	0.862544	5.834235	0.200194
F	2.421330	4.921308	1.408441
F	2.651724	5.034990	-0.742015
F	5.982129	-2.707692	0.654086

F 6.170881 -1.607899 -1.205181
F 6.134895 -0.536837 0.682135

63
ts-3-4 (C1) el energy= -2035.76946893
Ru -0.804584 -1.012569 -0.435850
H 0.665354 -1.136192 2.447335
P -2.870045 0.127898 -0.027914
O -2.056081 -3.800687 -0.647127
O -0.572717 -0.525568 -3.441796
N 1.367112 -1.322399 -0.494250
N -0.028129 0.920156 -0.169257
C 1.986810 -2.504560 -0.608713
H 1.350242 -3.355012 -0.828713
C 3.357423 -2.650511 -0.436815
H 3.823682 -3.626055 -0.521660
C 4.101320 -1.510747 -0.126318
C 5.600252 -1.606049 0.031706
C 3.461997 -0.283419 -0.004086
H 4.029524 0.600016 0.261259
C 2.078142 -0.205128 -0.200659
C 1.316692 1.058227 -0.095174
C 1.924949 2.292285 0.036244
H 3.000224 2.408763 0.071245
C 1.076616 3.431362 0.084511
C 1.721657 4.781884 0.239287
C -0.282059 3.305612 0.003195
H -0.922341 4.180132 0.040532
C -0.891764 2.004525 -0.124045
C -2.261875 1.802151 -0.190079
H -2.925926 2.655552 -0.090175
C -3.517892 -0.083445 1.770806
C -4.891393 0.568389 2.004501
H -4.894707 1.629108 1.725924
H -5.119092 0.514333 3.078221
H -5.706354 0.063913 1.477422
C -2.505937 0.630220 2.689461
H -1.500367 0.229606 2.551198
H -2.804173 0.457045 3.733305
H -2.495057 1.710393 2.510311
C -3.562067 -1.579167 2.132358
H -4.222746 -2.154853 1.475764
H -3.942102 -1.689219 3.158088
H -2.554420 -2.000383 2.092547
C -4.313087 -0.083588 -1.265961
C -5.245127 1.144857 -1.240743
H -5.735959 1.297129 -0.278564
H -6.032007 1.006065 -1.994933
H -4.696984 2.057516 -1.499523
C -5.100698 -1.374141 -0.983993
H -4.445863 -2.253114 -0.967865
H -5.837872 -1.527038 -1.784428
H -5.647219 -1.339138 -0.037971
C -3.728515 -0.177105 -2.684632
H -3.052607 0.656915 -2.900644
H -4.551077 -0.140431 -3.411788
H -3.194872 -1.118596 -2.841853
C -1.568985 -2.762569 -0.571985
C -0.776264 -0.703596 -2.324540
N 1.123732 -2.220025 2.825071
N 0.338026 -2.793016 2.166469
O -0.437255 -1.342523 1.568012
F 2.637190 4.997097 -0.730923
F 0.835308 5.792018 0.190798
F 2.378371 4.875181 1.415938
F 6.083441 -0.614404 0.799876
F 5.960391 -2.776783 0.585567
F 6.211563 -1.523567 -1.166400

63
complex-3(C1) el energy= -2035.82365549
Ru -0.747502 -1.020738 -0.400060
H 0.608173 -1.805181 3.541467
P -2.829816 0.094294 0.034541
O -1.939607 -3.841247 -0.593255
O -0.635828 -0.575166 -3.404033
N 1.409412 -1.298291 -0.496108
N -0.010653 0.929487 -0.193295
C 2.038135 -2.479521 -0.565071
H 1.406989 -3.346459

-0.722035			
C	3.414760	-2.599916	
-0.420687			
H	3.890272	-3.573287	
-0.470461			
C	4.151570	-1.439149	
-0.182154			
C	5.655546	-1.507696	
-0.062168			
C	3.499823	-0.214874	
-0.093144			
H	4.061338	0.685313	
0.124458			
C	2.111709	-0.161908	
-0.257474			
C	1.334152	1.092428	
-0.171168			
C	1.922627	2.340359	
-0.104509			
H	2.996248	2.476003	
-0.109472			
C	1.055620	3.465682	
-0.066387			
C	1.680475	4.831719	
0.024205			
C	-0.302430	3.314545	
-0.102228			
H	-0.956971	4.178826	
-0.076596			
C	-0.891584	2.000015	
-0.169788			
C	-2.259567	1.771824	
-0.202722			
H	-2.937209	2.615931	
-0.117543			
C	-3.404981	-0.065971	
1.862322			
C	-4.769161	0.595259	
2.123591			
H	-4.782948	1.644357	
1.804494			
H	-4.956953	0.582587	
3.206250			
H	-5.602436	0.071331	
1.646301			
C	-2.359889	0.678477	
2.719010			
H	-1.353203	0.286019	
2.565326			
H	-2.621362	0.539388	
3.777751			
H	-2.364167	1.752272	
2.505209			
C	-3.443980	-1.548411	
2.273841			
H	-4.155372	-2.132910	
1.682091			
H	-3.754945	-1.621276	
3.325473			
H	-2.454023	-1.999338	
2.183573			
C	-4.309732	-0.188498	
-1.143019			
C	-5.258602	1.027155	
-1.135914			
H	-5.717926	1.212242	
-0.163776			
H	-6.068955	0.846072	
-1.855415			
H	-4.733878	1.935795	
-1.451003			
C	-5.069056	-1.476351	
-0.782361			
H	-4.400858	-2.344561	
-0.742754			
H	-5.823338	-1.676264	
-1.555910			
H	-5.593278	-1.404654	
0.174230			
C	-3.770123	-0.333092	
-2.575159			
H	-3.123605	0.506267	
-2.851533			
H	-4.616813	-0.348813	
-3.274729			
H	-3.218976	-1.268500	
-2.708650			
C	-1.471910	-2.796286	
-0.515129			
C	-0.792776	-0.733088	

-2.277197
N 0.655468 -2.708732
3.021805
N 0.165228 -2.542281
1.893736
O -0.290858 -1.296467
1.642092
F 2.567102 5.027228
-0.976328
F 0.775125 5.824156
-0.037071
F 2.364334 4.977675
1.179510
F 6.142712 -0.488133
0.666622
F 6.050241 -2.656978
0.511739
F 6.233123 -1.446195
-1.278273

56
complex-1-no-hydride (C2) el energy= -
1513.31951889
Ru -0.855823 1.029494 0.106337
P -1.853053 -1.123119 -0.044331
O -3.441985 2.690087 -0.129545
O -0.947392 1.172862 3.091105
N 0.668186 2.543689 -0.206483
N 0.873050 -0.087528 0.016930
C 0.462989 3.871188 -0.313526
H -0.572485 4.195745 -0.309811
C 1.506160 4.779730 -0.422691
H 1.293415 5.840284 -0.512112
C 2.816269 4.291882 -0.411307
H 3.660585 4.971205 -0.490443
C 3.031921 2.923052 -0.295058
H 4.042410 2.530762 -0.281002
C 1.940103 2.053152 -0.194560
C 2.065303 0.590000 -0.076839
C 3.269343 -0.069951 -0.073623
H 4.210917 0.457328 -0.159218
C 3.264066 -1.490894 0.048026
C 4.596480 -2.200376 0.070980
C 2.092352 -2.179691 0.136990
H 2.086739 -3.260432 0.227272
C 0.830935 -1.480639 0.105540
C -0.390271 -2.123996 0.150694
H -0.440833 -3.200539 0.272576
C -2.317030 -1.166317 -1.900834
C -2.237208 -2.594730 -2.463205
H -1.247980 -3.033797 -2.297501
H -2.418382 -2.562139 -3.545971
H -2.988008 -3.258034 -2.025288
C -1.234871 -0.306941 -2.594948
H -1.286860 0.758379 -2.293691
H -1.397867 -0.308091 -3.681119
H -0.224396 -0.684124 -2.409378
C -3.703368 -0.560989 -2.164782
H -4.508082 -1.173359 -1.747333
H -3.866577 -0.507561 -3.249244
H -3.803903 0.454955 -1.768391
C -3.207034 -1.746113 1.113894
C -3.839225 -3.042617 0.574118
H -4.412097 -2.877877 -0.343090
H -4.533421 -3.435517 1.327972
H -3.089621 -3.819550 0.382965
C -4.277957 -0.655288 1.295022
H -3.859711 0.244509 1.759752
H -5.063123 -1.034372 1.961221
H -4.755943 -0.367061 0.354369
C -2.541310 -2.037582 2.473449
H -1.795839 -2.835385 2.403805
H -3.317837 -2.357592 3.179917
H -2.056283 -1.154363 2.899897
C -2.482287 2.074138 -0.036143
C -0.949107 1.104846 1.946371
F 4.463084 -3.529515 0.175206
F 5.288697 -1.934574 -1.053306
F 5.340071 -1.770167 1.107233

57
complex-1 (C2) el energy= -
1514.11317050
Ru 1.952051 5.670530 11.245788
H 0.897909 6.901852 11.514121
P 0.323800 4.854368 9.720045
O 0.708046 4.420623 13.729200
O 4.299548 3.637515 10.851703
N 3.422911 7.069110 12.010406
N 2.599578 6.708830 9.521267

C	3.763121	7.215718	13.300458
H	3.266408	6.547008	13.995879
C	4.687128	8.160575	13.730926
H	4.927825	8.240488	14.786678
C	5.281292	8.989276	12.776851
H	6.006922	9.743674	13.070081
C	4.930277	8.839314	11.440276
H	5.373735	9.476426	10.683513
C	3.993361	7.866462	11.068606
C	3.562302	7.645815	9.671341
C	4.098860	8.333838	8.595836
H	4.877975	9.075838	8.710708
C	3.595573	8.015081	7.308332
C	4.168842	8.749522	6.128350
C	2.616162	7.073772	7.143608
H	2.233305	6.839289	6.156365
C	2.069454	6.381332	8.283161
C	1.058840	5.434018	8.196939
H	0.607114	5.229413	7.230740
C	-1.384516	5.733424	9.883724
C	-2.437733	5.178981	8.909175
H	-2.076791	5.185964	7.873662
H	-3.330293	5.819142	8.948196
H	-2.757668	4.163646	9.161582
C	-1.155642	7.214344	9.523674
H	-0.376401	7.666752	10.143987
H	-2.090902	7.767461	9.688648
H	-0.865580	7.329179	8.474327
C	-1.905192	5.647840	11.328435
H	-2.072646	4.618306	11.659222
H	-2.865682	6.177831	11.399679
H	-1.207163	6.122134	12.024297
C	0.059250	2.968001	9.529474
C	-0.472881	2.606674	8.128792
H	-1.457232	3.028000	7.917523
H	-0.558115	1.513623	8.052037
H	0.220818	2.939965	7.349132
C	-0.873253	2.423533	10.624050
H	-0.536210	2.717805	11.625245
H	-0.874927	1.325123	10.585118
H	-1.908110	2.755645	10.499247
C	1.431752	2.291723	9.684080
H	2.178766	2.739631	9.019605
H	1.339627	1.228439	9.422991
H	1.795241	2.351296	10.713589
C	1.205352	4.881536	12.793908
C	3.383019	4.320020	10.953181
F	3.630701	8.362824	4.957418
F	3.975040	10.083194	6.240220
F	5.505373	8.564444	6.038894

60

ts-1-2 (C2) el energy= -1698.75033898

Ru	0.807272	0.809046	-0.432425
H	0.698771	1.052909	1.336141
P	1.710123	-1.362823	-0.023897
O	3.536501	2.169614	-0.722752
O	0.317649	0.643724	-3.455488
N	-0.662843	2.399423	-0.382908
N	-1.001801	-0.216474	-0.126730
C	-0.397462	3.711995	-0.484114
H	0.642586	3.971822	-0.640412
C	-1.385457	4.682068	-0.364653
H	-1.122772	5.732125	-0.447427
C	-2.697669	4.269171	-0.126690
H	-3.497785	4.996990	-0.018611
C	-2.972352	2.910049	-0.023583
H	-3.982443	2.568432	0.171829
C	-1.936262	1.978660	-0.157856
C	-2.138998	0.517119	-0.063098
C	-3.385108	-0.068843	0.063255
H	-4.297397	0.511753	0.101153
C	-3.433773	-1.486443	0.119629
C	-4.781967	-2.137903	0.262310
C	-2.292970	-2.237936	0.051581
H	-2.338858	-3.320570	0.094511
C	-1.005894	-1.602490	-0.074949
C	0.193013	-2.299427	-0.137801
H	0.181685	-3.380343	-0.034463
C	2.380655	-1.574198	1.772300
C	3.049506	-2.938889	2.013501
H	2.384287	-3.769755	1.750320
H	3.278218	-3.032103	3.084388
H	3.991771	-3.058338	1.471424
C	1.162763	-1.498342	2.714089
H	0.572260	-0.591650	2.576349
H	1.521487	-1.505633	3.752601
H	0.501141	-2.358768	2.572027
C	3.367108	-0.442166	2.107694
H	4.250716	-0.451314	1.461580

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H     3.713947 -0.558190  3.143929
H     2.897723  0.541240  2.022056
C     2.949323 -2.121845 -1.267383
C     2.914934 -3.662453 -1.224206
H     3.226182 -4.076299 -0.263838
H     3.599849 -4.053121 -1.989516
H     1.912175 -4.038435 -1.455546
C     4.374296 -1.597623 -1.022102
H     4.406282 -0.502025 -1.009854
H     5.028173 -1.937854 -1.837165
H     4.804365 -1.963032 -0.085469
C     2.516474 -1.696874 -2.680329
H     1.459585 -1.918934 -2.863655
H     3.110977 -2.251700 -3.418883
H     2.691514 -0.631186 -2.851132
C     2.493394  1.709882 -0.565851
C     0.581030  0.636443 -2.337767
N     0.421946  1.799733  2.450399
N     1.080270  2.782863  2.380338
O     1.881015  3.317633  1.620995
F    -4.716617 -3.481447  0.261128
F    -5.386142 -1.763464  1.411532
F    -5.608855 -1.771778 -0.742555

60
ts-3-4 (C2)       el energy= -
1698.73890469
Ru    0.801306  0.886327 -0.430965
H    -0.349787  1.871250  2.418190
P     1.840631 -1.228564  0.003153
O     3.423554  2.454832 -0.646786
O     0.349417  0.597180 -3.436231
N    -0.797739  2.381148 -0.517801
N    -0.943418 -0.252173 -0.166031
C    -0.627169  3.702981 -0.652270
H     0.384539  4.029325 -0.870243
C    -1.670946  4.609829 -0.504660
H    -1.485251  5.673637 -0.615448
C    -2.938123  4.113203 -0.195895
H    -3.779453  4.787382 -0.057522
C    -3.115147  2.740204 -0.059104
H    -4.088709  2.336093  0.194462
C    -2.025265  1.878523 -0.231285
C    -2.125411  0.406293 -0.111826
C    -3.330870 -0.258338  0.014727
H    -4.279873  0.261135  0.033548
C    -3.286868 -1.676655  0.080985
C    -4.589672 -2.413195  0.231664
C    -2.100054 -2.352509  0.019525
H    -2.075185 -3.435485  0.070664
C    -0.855622 -1.634973 -0.105928
C     0.384968 -2.253938 -0.157281
H     0.439501 -3.332651 -0.043903
C     2.486237 -1.411619  1.806025
C     3.237170 -2.730486  2.055306
H     2.633353 -3.604100  1.781498
H     3.449892 -2.807297  3.130794
H     4.196560 -2.788791  1.533034
C     1.243994 -1.407870  2.719393
H     0.651408 -0.503692  2.570148
H     1.582827 -1.428684  3.765134
H     0.615945 -2.287592  2.544206
C     3.378073 -0.208301  2.161045
H     4.251583 -0.120806  1.506576
H     3.748979 -0.326861  3.189259
H     2.794109  0.714035  2.111078
C     3.149960 -1.895215 -1.222474
C     3.210534 -3.435609 -1.182555
H     3.524123 -3.832376 -0.216044
H     3.936143 -3.779927 -1.932472
H     2.238703 -3.871985 -1.438474
C     4.534330 -1.285864 -0.943499
H     4.500567 -0.190138 -0.937458
H     5.227853 -1.589824 -1.739966
H     4.961030 -1.618815  0.006377
C     2.728198 -1.497834 -2.646319
H     1.696287 -1.795105 -2.860618
H     3.382223 -2.007217 -3.367196
H     2.831375 -0.422134 -2.813891
C     2.429190  1.883396 -0.568649
C     0.611254  0.635174 -2.317266
N    -0.087083  3.024021  2.791156
N     0.897755  3.008933  2.149944
O     0.678297  1.380512  1.570090
F    -5.452684 -2.083950 -0.755395
F    -4.441053 -3.749742  0.208454
F    -5.198388 -2.094464  1.395298

60
complex-3(C2)        el energy= -
```

1698.79305630

Ru	0.767868	0.909650	-0.401521
H	0.103482	2.343635	3.529648
P	1.804872	-1.213379	0.038023
O	3.384611	2.499078	-0.598083
O	0.418210	0.617149	-3.405215
N	-0.814656	2.395736	-0.507617
N	-0.971211	-0.240154	-0.194496
C	-0.632021	3.720479	-0.590480
H	0.388340	4.049081	-0.752584
C	-1.679274	4.625539	-0.455215
H	-1.485681	5.691312	-0.525102
C	-2.958457	4.125420	-0.210072
H	-3.802473	4.798949	-0.085148
C	-3.144435	2.749696	-0.114606
H	-4.126630	2.342168	0.096806
C	-2.051745	1.889910	-0.269670
C	-2.156249	0.416609	-0.178656
C	-3.363374	-0.252326	-0.112102
H	-4.313370	0.265665	-0.122482
C	-3.318812	-1.671379	-0.065576
C	-4.624919	-2.412483	0.024179
C	-2.129309	-2.344773	-0.093894
H	-2.104206	-3.428415	-0.061133
C	-0.883136	-1.623447	-0.163599
C	0.360397	-2.239560	-0.192341
H	0.414601	-3.320217	-0.100451
C	2.374029	-1.416017	1.863676
C	3.095145	-2.748955	2.126955
H	2.491732	-3.609143	1.812874
H	3.259267	-2.845075	3.209365
H	4.075591	-2.812910	1.645942
C	1.094508	-1.405773	2.725480
H	0.506664	-0.499555	2.569286
H	1.391593	-1.441481	3.783460
H	0.469361	-2.280169	2.516932
C	3.274019	-0.234886	2.267812
H	4.188880	-0.176705	1.669671
H	3.575957	-0.355250	3.317797
H	2.733487	0.709292	2.179244
C	3.165550	-1.857441	-1.141607
C	3.221871	-3.398399	-1.129320
H	3.489181	-3.814293	-0.156762
H	3.981543	-3.729569	-1.850814
H	2.262596	-3.827595	-1.438821
C	4.537711	-1.257937	

-0.790696
H 4.505396 -0.162632
-0.756326
H 5.262317 -1.541915
-1.566461
H 4.925293 -1.618497
0.165880
C 2.806297 -1.429730
-2.573757
H 1.787940 -1.729447
-2.842207
H 3.496253 -1.917958
-3.275405
H 2.909459 -0.349597
-2.712114
C 2.393281 1.926096
-0.517315
C 0.636732 0.651656
-2.277746
N 0.622463 3.094483
3.023682
N 0.935740 2.668251
1.900359
O 0.554110 1.400586
1.639262
F -5.450920 -2.067773
-0.988704
F -4.472163 -3.748160
-0.016212
F -5.276699 -2.114556
1.169535

56
complex-1-no-hydride (C3) el energy=
-1513.31631799
Ru -0.499286 -0.622638 -0.140553
P -2.699192 0.252805 0.069757
O -1.206348 -3.593804 0.274502
O -0.609095 -0.931309 -3.113186
N 1.659717 -0.647912 0.090733
N -0.023167 1.380971 -0.159980
C 2.437989 -1.742796 0.210256
H 1.919474 -2.693725 0.273062
C 3.820723 -1.674531 0.250453
H 4.414182 -2.577663 0.345617
C 4.420409 -0.413487 0.154667
C 5.927964 -0.288664 0.240745
C 3.627790 0.716549 0.019018
H 4.091490 1.691029 -0.071390
C 2.233240 0.584873 -0.008138
C 1.309060 1.719730 -0.138971
C 1.719974 3.030611 -0.221693
H 2.770533 3.293261 -0.191515
C 0.735652 4.051396 -0.348734
H 1.049569 5.088594 -0.428054
C -0.590791 3.728862 -0.365983
H -1.354398 4.495322 -0.459843
C -1.018611 2.356285 -0.252109
C -2.347123 1.973681 -0.224205
H -3.134373 2.707922 -0.356535
C -2.980614 0.049071 1.953278
C -3.889357 1.160822 2.502581
H -3.487562 2.153196 2.273445
H -3.952131 1.061852 3.594638
H -4.907754 1.100528 2.109339
C -1.577931 0.210076 2.583348
H -0.892331 -0.610790 2.295463
H -1.653432 0.156445 3.677808
H -1.117242 1.169291 2.327532
C -3.548699 -1.332878 2.307682
H -4.570295 -1.466925 1.940035
H -3.582610 -1.432507 3.400647
H -2.934792 -2.154266 1.923483
C -4.159160 -0.288963 -0.997555
C -5.488536 0.232225 -0.420294
H -5.745414 -0.241970 0.531437
H -6.294007 0.001403 -1.129207
H -5.479232 1.319248 -0.277732
C -4.182037 -1.824238 -1.107001
H -3.280202 -2.205204 -1.598810
H -5.041796 -2.124686 -1.719048
H -4.280510 -2.318981 -0.136518
C -3.945957 0.318538 -2.398360
H -3.963082 1.412331 -2.379143
H -4.757464 -0.023480 -3.053385
H -3.003181 0.000696 -2.853650
C -0.943578 -2.491525 0.114325
C -0.604171 -0.829886 -1.970655
F 6.351895 0.880130 -0.263505
F 6.326017 -0.357621 1.521369

F 6.525829 -1.283782 -0.430482

57
complex-1 (C5) el energy= -1514.10829980
Ru -0.445476 -0.687782 -0.110098
H -0.354212 -0.564188 1.525783
P -2.637039 0.198973 0.135407
O -1.221632 -3.586319 0.414467
O -0.164602 -0.850913 -3.223726
N 1.719587 -0.662281 -0.002154
N 0.036768 1.369574 -0.210266
C 2.507430 -1.741794 0.139063
H 1.994831 -2.697293 0.172369
C 3.887603 -1.657020 0.240432
H 4.487684 -2.553920 0.355083
C 4.471682 -0.386598 0.192607
C 5.970309 -0.258774 0.301566
C 3.665458 0.731486 0.047792
H 4.108869 1.718389 0.016515
C 2.274393 0.577547 -0.050089
C 1.345068 1.713344 -0.198652
C 1.766228 3.029340 -0.322409
H 2.815874 3.296718 -0.321506
C 0.767346 4.023267 -0.466237
H 1.060797 5.065847 -0.569192
C -0.560373 3.682180 -0.472477
H -1.330632 4.441651 -0.577005
C -0.973532 2.308804 -0.332609
C -2.300926 1.894351 -0.307680
H -3.088281 2.642041 -0.335210
C -3.253632 0.202622 1.963650
C -4.682705 0.753405 2.108584
H -4.787289 1.738678 1.638443
H -4.910673 0.875416 3.176902
H -5.441244 0.084169 1.691697
C -2.315550 1.145007 2.742630
H -1.267826 0.846090 2.644942
H -2.584764 1.112182 3.807756
H -2.408813 2.177940 2.392278
C -3.165484 -1.205114 2.576353
H -3.794092 -1.934418 2.056580
H -3.499997 -1.167315 3.622942
H -2.135152 -1.572203 2.566112
C -4.042594 -0.415587 -1.011120
C -5.136214 0.655779 -1.189229
H -5.654905 0.902936 -0.261260
H -5.888180 0.282322 -1.898534
H -4.715241 1.577016 -1.606626
C -4.648359 -1.732504 -0.498993
H -3.875881 -2.489279 -0.317405
H -5.333920 -2.135311 -1.257900
H -5.223171 -1.601464 0.422482
C -3.427753 -0.673519 -2.396731
H -2.861674 0.194052 -2.752970
H -4.233824 -0.872047 -3.116587
H -2.768138 -1.545577 -2.387168
C -0.914279 -2.495378 0.190428
C -0.360136 -0.785345 -2.095132
F 6.377410 1.021360 0.245890
F 6.415868 -0.781134 1.460909
F 6.584267 -0.928094 -0.693995

60
ts-1-2 (C3) el energy= -1698.74580798
Ru 0.501670 -0.419603 0.473391
H 0.273549 -0.768502 -1.266229
P 2.715710 0.321589 -0.023715
O 1.342002 -3.277003 1.190273
O 0.267537 0.508776 3.386781
N -1.664153 -0.422933 0.395414
N 0.038737 1.537950 -0.137577
C -2.454613 -1.479549 0.648597
H -1.947271 -2.388301 0.948002
C -3.833722 -1.430209 0.504329
H -4.438242 -2.308348 0.703882
C -4.406928 -0.229644 0.076665
C -5.906189 -0.114671 -0.050991
C -3.594308 0.863579 -0.188129
H -4.029742 1.790758 -0.538802
C -2.208141 0.752551 -0.019509
C -1.270407 1.862101 -0.276015
C -1.679440 3.141740 -0.613044
H -2.727014 3.397819 -0.713838
C -0.674277 4.122359 -0.805405
H -0.961825 5.137647 -1.069612
C 0.650127 3.801912 -0.661075
H 1.424425 4.550053 -0.807529
C 1.055255 2.463045 -0.316291

C 2.380348 2.066933 -0.166319
H 3.171431 2.781761 -0.372861
C 3.340947 -0.294590 -1.742345
C 4.802658 0.092038 -2.029198
H 4.966467 1.170881 -1.922015
H 5.036183 -0.170551 -3.070556
H 5.519977 -0.436575 -1.395138
C 2.474543 0.406918 -2.806883
H 1.405300 0.252889 -2.656344
H 2.732636 -0.000844 -3.794071
H 2.662679 1.485185 -2.818407
C 3.172545 -1.819350 -1.858942
H 3.766380 -2.364663 -1.118488
H 3.504193 -2.146366 -2.854315
H 2.128446 -2.120435 -1.741001
C 4.099487 0.100509 1.278320
C 5.214863 1.148086 1.090199
H 5.741596 1.054234 0.139256
H 5.956182 1.023890 1.891785
H 4.812930 2.164537 1.165693
C 4.674743 -1.325386 1.246089
H 3.887015 -2.081992 1.337974
H 5.359396 -1.456854 2.095640
H 5.243060 -1.532275 0.335025
C 3.482368 0.339719 2.666339
H 2.932537 1.286249 2.705755
H 4.287014 0.385134 3.412876
H 2.812215 -0.474586 2.955456
C 0.977989 -2.230112 0.880934
C 0.460242 0.149656 2.313124
N -0.458669 -1.222803 -2.333816
N -0.764336 -2.342843 -2.095078
O -0.648973 -3.171265 -1.198023
F -6.263285 0.886844 -0.875080
F -6.446091 -1.252874 -0.522419
F -6.472192 0.129253 1.147902

60
ts-3-4(C3) el energy= -
1698.73418730
Ru -0.513825 -0.462883 -0.489508
H 0.918668 -0.846422 2.381595
P -2.730589 0.289727 0.017331
O -1.338802 -3.325687 -1.202839
O -0.319525 0.552463 -3.361307
N 1.679372 -0.444664 -0.514359
N -0.036521 1.490587 0.117323
C 2.468065 -1.490303 -0.796727
H 1.966171 -2.374019 -1.176346
C 3.842284 -1.466665 -0.599122
H 4.447974 -2.337791 -0.823827
C 4.405410 -0.299789 -0.077536
C 5.898917 -0.206160 0.120611
C 3.591251 0.785239 0.218849
H 4.019129 1.683085 0.647108
C 2.212472 0.698972 -0.014565
C 1.273416 1.804018 0.266444
C 1.688700 3.075494 0.624121
H 2.737782 3.325892 0.724047
C 0.687801 4.060207 0.824826
H 0.980331 5.070122 1.103845
C -0.637149 3.750599 0.668209
H -1.407671 4.501204 0.821651
C -1.049236 2.418090 0.303612
C -2.375901 2.033673 0.144295
H -3.160713 2.752156 0.362434
C -3.364797 -0.314251 1.731347
C -4.823066 0.083633 2.016539
H -4.980651 1.163952 1.911669
H -5.054252 -0.178522 3.058547
H -5.547088 -0.439823 1.385335
C -2.483601 0.376505 2.791245
H -1.427756 0.154407 2.628262
H -2.767005 -0.007508 3.781774
H -2.630713 1.461535 2.787414
C -3.190094 -1.839359 1.844260
H -3.746515 -2.387737 1.077008
H -3.564727 -2.173113 2.822679
H -2.130242 -2.097050 1.776456
C -4.110951 0.072393 -1.290548
C -5.215735 1.131854 -1.103084
H -5.738614 1.048622 -0.149318
H -5.961514 1.009867 -1.900873
H -4.804088 2.143725 -1.186550
C -4.701434 -1.346965 -1.250311
H -3.923486 -2.112227 -1.354299
H -5.399254 -1.470115 -2.090383
H -5.257100 -1.549165 -0.330917
C -3.501003 0.299951 -2.683100
H -2.953697 1.246937 -2.734738

H -4.310074 0.336889 -3.425425
H -2.830884 -0.515316 -2.969959
C -1.009985 -2.256137 -0.938974
C -0.507737 0.160223 -2.296901
N 1.532457 -1.904086 2.595266
N 0.840652 -2.460745 1.824684
O -0.127447 -1.065189 1.449310
F 6.417763 -1.385559 0.504759
F 6.512308 0.146133 -1.027155
F 6.223030 0.713005 1.047440

60
complex-3(C3) el energy= -1698.78854657
Ru -0.470247 -0.494176 -0.441062
H 0.982945 -1.437602 3.431855
P -2.694003 0.260977 0.062506
O -1.237609 -3.426253 -0.917144
O -0.429722 0.252712 -3.385158
N 1.703936 -0.441666 -0.529550
N -0.030733 1.516523 -0.045077
C 2.500308 -1.506266 -0.697928
H 2.003656 -2.437766 -0.943514
C 3.879065 -1.437413 -0.544849
H 4.492818 -2.321682 -0.676697
C 4.435914 -0.207755 -0.188526
C 5.932729 -0.066962 -0.052389
C 3.611121 0.893348 0.003194
H 4.033843 1.841377 0.311727
C 2.229154 0.759207 -0.175818
C 1.276576 1.871548 0.013701
C 1.671974 3.183656 0.205944
H 2.717572 3.465016 0.235431
C 0.654863 4.164162 0.332371
H 0.932359 5.204920 0.484512
C -0.666904 3.812639 0.259726
H -1.449664 4.560390 0.353094
C -1.058254 2.440001 0.060404
C -2.380141 2.014284 -0.022073
H -3.175786 2.736402 0.135956
C -3.238911 -0.153723 1.860370
C -4.685338 0.273700 2.163252
H -4.853689 1.333832 1.938300
H -4.868803 0.136310 3.238129
H -5.432802 -0.321550 1.630566
C -2.314695 0.655205 2.793935
H -1.261554 0.427600 2.620315
H -2.554646 0.387319 3.833018
H -2.473919 1.731604 2.672606
C -3.058929 -1.656711 2.137508
H -3.678368 -2.283629 1.488524
H -3.352586 -1.869197 3.175270

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H          -2.013784       -1.947864
2.017286
C          -4.116832       -0.138240
-1.152307
C          -5.236024        0.917831
-1.051350
H          -5.719881        0.943448
-0.073712
H          -6.009077        0.685975
-1.797052
H          -4.850035        1.918572
-1.274366
C          -4.676201       -1.550955
-0.915602
H          -3.886385       -2.310671
-0.944489
H          -5.393783       -1.791202
-1.712452
H          -5.203679       -1.642765
0.037499
C          -3.563226       -0.074061
-2.584938
H          -3.049976        0.873654
-2.777646
H          -4.398360       -0.154683
-3.294075
H          -2.877623       -0.900889
-2.792351
C          -0.926681       -2.336567
-0.733120
C          -0.559072       -0.036426
-2.280672
N           1.164198       -2.272781
2.833000
N           0.656140       -2.074996
1.717274
O           0.022787       -0.892631
1.574533
F           6.489778       -1.187854
0.437604
F           6.501099        0.172008
-1.251468
F           6.266057        0.952766
0.759417
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```
56
complex-1-no-hydride (C5)   el energy=
-1215.61566699
Ru  -0.100898 -0.875955  0.100476
P    1.869306  0.449472 -0.030767
O    1.239457 -3.630432 -0.236945
O   -0.065002 -1.134822  3.078774
N   -2.189336 -1.363201 -0.221151
N   -0.988785  0.977621  0.052957
C   -2.707410 -2.600418 -0.355286
H   -1.992316 -3.416372 -0.377178
C   -4.071135 -2.829988 -0.460376
H   -4.443103 -3.843405 -0.572681
C   -4.934848 -1.730694 -0.415162
H   -6.010060 -1.868763 -0.489886
C   -4.404876 -0.454071 -0.270958
H   -5.062583  0.406650 -0.230319
C   -3.018239 -0.280918 -0.176312
C   -2.360193  1.027682 -0.030545
C   -3.038268  2.221673  0.007134
H   -4.119274  2.251158 -0.071781
C   -2.315665  3.448881  0.152738
C   -3.072849  4.747928  0.210019
C   -0.950452  3.394577  0.230948
H   -0.367734  4.305498  0.338128
C   -0.234793  2.146510  0.168652
C    1.145799  2.056860  0.210173
H    1.750976  2.944563  0.358976
C    2.288608  0.290909 -1.893105
C    2.971239  1.564483 -2.418233
H    2.358438  2.451386 -2.226727
H    3.109695  1.472810 -3.503992
H    3.957788  1.723259 -1.974527
C    0.919639  0.147842 -2.597144
H    0.408404 -0.797211 -2.331086
H    1.063933  0.107700 -3.685298
H    0.253613  0.988630 -2.379280
C    3.152042 -0.943262 -2.191940
H    4.158265 -0.856041 -1.771356
H    3.263681 -1.043698 -3.279727
H    2.704618 -1.871857 -1.822119
C    3.355954  0.240378  1.115092
C    4.573637  1.025067  0.592465
H    4.974002  0.606022 -0.335305
H    5.371912  0.978271  1.344374
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H     4.341782   2.083623   0.425854
C     3.696593  -1.253960   1.257695
H     2.870023  -1.812241   1.710957
H     4.566702  -1.360194   1.917899
H     3.948009  -1.725924   0.303551
C     2.948828   0.803375   2.491239
H     2.733943   1.875292   2.448784
H     3.780212   0.648938   3.191040
H     2.072823   0.297364   2.907870
C     0.740573  -2.608393  -0.104641
C    -0.037606  -1.044168   1.935071
H    -2.399404   5.603039   0.321897
H    -3.665388   4.894915  -0.702771
H    -3.775720   4.752105   1.053664
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57
complex-1 (C5)      el energy= -
1216.40013388
Ru    1.954120   5.663806  11.249275
H     0.900405   6.895657  11.521613
P     0.330133   4.850503   9.716478
O     0.711453   4.403826  13.728267
O     4.300539   3.637325  10.828232
N     3.424416   7.065113  12.011411
N     2.596690   6.704636   9.524619
C     3.766292   7.211107  13.301185
H     3.272085   6.539850  13.996074
C     4.687875   8.157447  13.732476
H     4.929835   8.236578  14.788031
C     5.277921   8.989212  12.777833
H     6.001721   9.745588  13.071077
C     4.925279   8.840128  11.442142
H     5.365192   9.479890  10.685560
C     3.990278   7.864978  11.067917
C     3.557953   7.644569   9.671842
C     4.088668   8.332562   8.593163
H     4.867068   9.076468   8.720549
C     3.599550   8.033141   7.291449
C     4.162613   8.767038   6.100580
C     2.619500   7.081147   7.152300
H     2.226968   6.839830   6.167139
C     2.075324   6.379833   8.285381
C     1.070156   5.420264   8.197419
H     0.613890   5.220717   7.231999
C    -1.378668   5.732760   9.881849
C    -2.430729   5.181861   8.904104
H    -2.064335   5.185706   7.870353
H    -3.321302   5.825432   8.937805
H    -2.755794   4.167954   9.155992
C    -1.144428   7.212549   9.520949
H    -0.367163   7.662923  10.145181
H    -2.079253   7.768822   9.679243
H    -0.846258   7.323804   8.473505
C    -1.903526   5.650709  11.324891
H    -2.075043   4.622120  11.656200
H    -2.862372   6.184369  11.394411
H    -1.204538   6.122507  12.021554
C     0.054189   2.963524   9.537296
C    -0.472103   2.599202   8.135337
H    -1.455119   3.021601   7.919274
H    -0.558117   1.505960   8.059545
H     0.225704   2.932120   7.359214
C    -0.886413   2.427126  10.628700
H    -0.553818   2.724367  11.630462
H    -0.892463   1.328387  10.594466
H    -1.919352   2.762772  10.496965
C     1.422193   2.280611   9.701406
H     2.172862   2.720656   9.035969
H     1.325521   1.215649   9.448104
H     1.782850   2.346868  10.731591
C     1.209468   4.869146  12.794604
C     3.383404   4.317975  10.942641
H     3.697823   8.434408   5.166255
H     4.003282   9.850204   6.193515
H     5.246692   8.608875   6.016947
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ts-1-2 (C5)     el energy= -
1401.03819514
Ru    0.114947  -0.661783  -0.453814
H     0.326742  -0.891386   1.304917
P    -1.955379   0.440983  -0.007927
O    -1.145658  -3.414917  -0.916769
O     0.427387  -0.032866  -3.438527
N     2.258602  -0.972501  -0.393351
N     0.868287   1.252167  -0.024190
C     2.881235  -2.150877  -0.559313
H     2.239065  -2.995834  -0.777002
C     4.257503  -2.290563  -0.429921
H     4.716390  -3.264829  -0.566783
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C	5.012398	-1.159756	-0.110977
H	6.090867	-1.228081	0.007950
C	4.367963	0.059923	0.058860
H	4.934064	0.947536	0.317321
C	2.977624	0.141755	-0.089449
C	2.212765	1.396166	0.070075
C	2.804832	2.627997	0.280995
H	3.881755	2.735637	0.344453
C	1.969133	3.774612	0.396691
C	2.594766	5.126251	0.629821
C	0.609023	3.618962	0.293392
H	-0.048829	4.480637	0.378501
C	0.006109	2.330485	0.075887
C	-1.366938	2.122832	-0.028829
H	-2.040289	2.961820	0.120812
C	-2.628698	0.078262	1.764117
C	-4.009073	0.705088	2.027711
H	-4.011267	1.782278	1.822733
H	-4.256495	0.575334	3.090788
H	-4.811371	0.236532	1.450667
C	-1.643363	0.731544	2.753260
H	-0.613205	0.404055	2.607306
H	-1.937771	0.456959	3.775833
H	-1.666557	1.822569	2.667601
C	-2.687074	-1.438059	2.016570
H	-3.374340	-1.949950	1.335486
H	-3.038197	-1.623259	3.041465
H	-1.702960	-1.902264	1.912810
C	-3.385687	0.312070	-1.272141
C	-4.330571	1.526082	-1.173292
H	-4.847053	1.595648	-0.214573
H	-5.097376	1.443525	-1.956228
H	-3.784174	2.460669	-1.341811
C	-4.164601	-1.003553	-1.106291
H	-3.498779	-1.873829	-1.133182
H	-4.877767	-1.107497	-1.936123
H	-4.739373	-1.041138	-0.176591
C	-2.768165	0.331323	-2.680309
H	-2.086119	1.178633	-2.809361
H	-3.571893	0.427183	-3.423228
H	-2.229420	-0.595471	-2.896111
C	-0.626605	-2.410589	-0.699232
C	0.205460	-0.265920	-2.335623
N	1.005827	-1.360702	2.409360
N	1.124500	-2.531345	2.271634
O	0.858547	-3.410974	1.459556
H	1.838125	5.916136	0.684382
H	3.167802	5.137780	1.567125
H	3.295481	5.380024	-0.177407

60

ts-3-4 (C5) el energy= -1401.02681692

Ru	0.092083	-0.725996	-0.435891
H	1.538269	-0.988651	2.425238
P	-1.976026	0.405574	-0.002501
O	-1.158491	-3.498797	-0.800630
O	0.360843	-0.093642	-3.407915
N	2.260392	-1.033023	-0.487505
N	0.863621	1.191682	-0.072143
C	2.879926	-2.208204	-0.660646
H	2.241183	-3.043461	-0.929014
C	4.250860	-2.362993	-0.490451
H	4.709656	-3.336285	-0.634195
C	4.998372	-1.245359	-0.114784
H	6.070889	-1.323979	0.044347
C	4.355137	-0.025364	0.062400
H	4.916230	0.850364	0.368382
C	2.971581	0.068907	-0.136301
C	2.208663	1.326925	0.020358
C	2.809184	2.556776	0.215066
H	3.887277	2.658841	0.267591
C	1.980687	3.711318	0.314140
C	2.616089	5.061333	0.529060
C	0.620254	3.564182	0.210145
H	-0.031669	4.431399	0.283358
C	0.007771	2.276310	0.010783
C	-1.366312	2.078761	-0.091053
H	-2.030316	2.926912	0.049449
C	-2.649374	0.109967	1.776682
C	-4.023913	0.754882	2.022800
H	-4.020708	1.826324	1.788218
H	-4.265370	0.656746	3.090631
H	-4.833818	0.275802	1.464858
C	-1.647809	0.779602	2.738818
H	-0.642920	0.377563	2.599194
H	-1.963390	0.568215	3.770803
H	-1.626277	1.865562	2.600127
C	-2.701419	-1.399527	2.072742
H	-3.355430	-1.944281	1.383925

H -3.093060 -1.554332 3.088599
H -1.694534 -1.821683 2.025260
C -3.408394 0.242699 -1.262262
C -4.340502 1.469508 -1.197697
H -4.849353 1.576700 -0.238627
H -5.113214 1.368577 -1.972637
H -3.785247 2.391820 -1.401321
C -4.200118 -1.057692 -1.045787
H -3.545113 -1.936630 -1.057201
H -4.926896 -1.177115 -1.861640
H -4.759186 -1.062152 -0.106340
C -2.807124 0.209017 -2.676616
H -2.128863 1.051622 -2.846742
H -3.620374 0.275757 -3.412422
H -2.269790 -0.724487 -2.865869
C -0.670126 -2.466304 -0.665637
C 0.144701 -0.326912 -2.302451
N 1.981985 -2.104345 2.760729
N 1.169325 -2.619011 2.082662
O 0.432713 -1.144417 1.561545
H 1.865438 5.857638 0.571093
H 3.187859 5.081825 1.467004
H 3.320029 5.298045 -0.280561

60
complex-3(C5) el energy= -1401.08118955
Ru 0.134930 -0.731457 -0.414470
H 1.477799 -1.634857 3.503538
P -1.941361 0.389197 0.043542
O -1.071817 -3.536212 -0.713341
O 0.264526 -0.181353 -3.397852
N 2.288076 -1.015895 -0.512943
N 0.879063 1.206956 -0.141981
C 2.910286 -2.196976 -0.629080
H 2.271505 -3.051496 -0.822088
C 4.287170 -2.329900 -0.489451
H 4.749700 -3.307024 -0.587210
C 5.035143 -1.187112 -0.202358
H 6.112678 -1.248704 -0.071794
C 4.386239 0.036252 -0.071976
H 4.946800 0.931462 0.172548
C 2.997563 0.108153 -0.234356
C 2.225378 1.363584 -0.111068
C 2.813572 2.609167 -0.003105
H 3.891314 2.727358 0.001826
C 1.972340 3.756393 0.071453
C 2.595457 5.123217 0.196806
C 0.611207 3.587281 0.024420
H -0.050232 4.448731 0.076776
C 0.011466 2.283857 -0.091762
C -1.362563 2.063776 -0.148330
H -2.035155 2.908519 -0.031030
C -2.529573 0.171417 1.862756
C -3.889668 0.834998 2.138535
H -3.893686 1.892516 1.847763
H -4.082856 0.794007 3.219803
H -4.724925 0.331225 1.643020
C -1.483354 0.882068

2.746249
H -0.479809 0.483574
2.587154
H -1.752954 0.718254
3.799724
H -1.474564 1.960690
2.558375
C -2.581153 -1.321665
2.231067
H -3.293811 -1.883488
1.619177
H -2.896939 -1.424159
3.279096
H -1.594090 -1.776827
2.130809
C -3.421241 0.143444
-1.144283
C -4.364343 1.362893
-1.107530
H -4.832880 1.518014
-0.134377
H -5.168188 1.211112
-1.841344
H -3.829834 2.277933
-1.385529
C -4.189143 -1.150140
-0.825458
H -3.524839 -2.022079
-0.807000
H -4.940639 -1.324529
-1.608214
H -4.717997 -1.103557
0.130308
C -2.876532 0.037701
-2.577927
H -2.224741 0.882025
-2.824964
H -3.719860 0.045482
-3.282058
H -2.327572 -0.895311
-2.735199
C -0.597482 -2.497074
-0.594021
C 0.102580 -0.379056
-2.277166
N 1.503054 -2.531220
2.969307
N 1.009623 -2.331984
1.846624
O 0.578754 -1.074923
1.622783
H 1.835608 5.911324
0.225574
H 3.198687 5.197353
1.112032
H 3.267907 5.327625
-0.647598

56
complex-1-no-hydride (C6) el energy=
-1215.61666240
Ru 0.108017 -0.645648 -0.114476
P -2.070002 0.296252 0.040303
O -0.690877 -3.592897 0.300282
O 0.059623 -0.967023 -3.085948
N 2.251669 -0.734774 0.168550
N 0.644302 1.343407 -0.134383
C 2.997987 -1.848578 0.319005
H 2.451233 -2.784203 0.378399
C 4.378732 -1.816884 0.395526
H 4.930149 -2.744244 0.522854
C 5.048755 -0.584013 0.304595
C 6.548869 -0.511020 0.377612
C 4.266737 0.559630 0.142861
H 4.750107 1.527448 0.064921
C 2.871788 0.475323 0.077844
C 1.986182 1.640630 -0.083224
C 2.436121 2.938263 -0.164685
H 3.492918 3.169968 -0.111894
C 1.485174 3.986143 -0.321004
H 1.831351 5.013256 -0.399653
C 0.150202 3.704315 -0.366850
H -0.587790 4.492534 -0.482623
C -0.320034 2.346129 -0.255122
C -1.660612 2.002497 -0.255222
H -2.422236 2.759894 -0.405960
C -2.407661 0.111459 1.916690
C -3.299220 1.250995 2.436252
H -2.865783 2.230231 2.208086
H -3.389860 1.163618 3.527412

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H    -4.309478   1.214379   2.019709
C    -1.017868   0.238820   2.581962
H    -0.350078  -0.604963   2.321104
H    -1.123470   0.201290   3.674654
H    -0.522436   1.180828   2.326758
C    -3.020944  -1.252436   2.265196
H    -4.036593  -1.361633   1.873428
H    -3.083830  -1.345146   3.357571
H    -2.419715  -2.091705   1.899734
C    -3.519775  -0.211006  -1.058508
C    -4.847469   0.352012  -0.518227
H    -5.140797  -0.107531   0.430163
H    -5.642060   0.139301  -1.244987
H    -4.810001   1.439306  -0.382372
C    -3.584902  -1.745664  -1.159152
H    -2.681756  -2.155762  -1.624406
H    -4.436889  -2.025684  -1.791582
H    -3.722462  -2.230694  -0.188455
C    -3.255306   0.379763  -2.457588
H    -3.237848   1.473610  -2.444755
H    -4.061431   0.058745  -3.129804
H    -2.312214   0.029774  -2.887896
C    -0.393539  -2.499005   0.139748
C     0.039695  -0.859040  -1.943635
H     6.910214   0.518034   0.290315
H     6.910642  -0.923519   1.328170
H     7.004770  -1.105048  -0.424765

57
complex-1 (C6)        el energy= -
1216.40082975
Ru    0.142058  -0.704584  -0.081104
H     0.171810  -0.595018   1.558663
P    -2.030848   0.244113   0.074526
O    -0.731222  -3.584063   0.389546
O     0.564205  -0.860607  -3.177061
N     2.300000  -0.743218   0.115327
N     0.688729   1.339346  -0.143782
C     3.055563  -1.841376   0.279342
H     2.518460  -2.784432   0.282651
C     4.431860  -1.790958   0.438800
H     4.992268  -2.713136   0.569028
C     5.078428  -0.545675   0.432713
C     6.571449  -0.443421   0.606323
C     4.284041   0.585722   0.262228
H     4.745476   1.567480   0.259203
C     2.896097   0.477177   0.102994
C     2.005598   1.643172  -0.076614
C     2.466876   2.947846  -0.175692
H     3.522934   3.184588  -0.132077
C     1.503830   3.970649  -0.352985
H     1.831154   5.005061  -0.437345
C     0.167798   3.669235  -0.415407
H    -0.575675   4.451019  -0.546404
C    -0.288171   2.307823  -0.302812
C    -1.627898   1.930931  -0.338730
H    -2.391154   2.702115  -0.391527
C    -2.731323   0.250354   1.873063
C    -4.149084   0.840666   1.959929
H    -4.204556   1.832405   1.494902
H    -4.421701   0.960209   3.018183
H    -4.906642   0.196984   1.502834
C    -1.802453   1.158636   2.701988
H    -0.760843   0.828690   2.648594
H    -2.120787   1.126775   3.753692
H    -1.848557   2.196158   2.355767
C    -2.710354  -1.164034   2.476043
H    -3.337156  -1.870273   1.923207
H    -3.087697  -1.125315   3.508121
H    -1.691450  -1.560778   2.504918
C    -3.401978  -0.320828  -1.138300
C    -4.456613   0.781873  -1.355206
H    -5.011693   1.033635  -0.449716
H    -5.184281   0.437388  -2.103643
H    -3.990921   1.695425  -1.740853
C    -4.066020  -1.624823  -0.666958
H    -3.322803  -2.403318  -0.456886
H    -4.726517  -2.003142  -1.460110
H    -4.678986  -1.485738   0.228494
C    -2.733117  -0.584357  -2.497644
H    -2.127921   0.270151  -2.819499
H    -3.511218  -0.754736  -3.254754
H    -2.098008  -1.473875  -2.466556
C    -0.386472  -2.499587   0.186124
C     0.316978  -0.793421  -2.058123
H     6.909139   0.597867   0.581409
H     6.885684  -0.881177   1.562766
H     7.096504  -0.991208  -0.187115

60
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ts-1-2 (C6) el energy= -1401.03896557

Ru	-0.066168	-0.395224	0.501220
H	-0.306834	-0.802422	-1.221170
P	2.144993	0.328518	-0.032639
O	0.773901	-3.225586	1.316323
O	-0.292187	0.630302	3.381748
N	-2.229043	-0.399347	0.437123
N	-0.532612	1.542214	-0.172101
C	-3.024184	-1.442663	0.729310
H	-2.519044	-2.340244	1.065464
C	-4.401549	-1.393839	0.582470
H	-4.997331	-2.269209	0.826832
C	-5.002604	-0.218991	0.106529
C	-6.494106	-0.132244	-0.084573
C	-4.165883	0.855718	-0.187885
H	-4.592133	1.778240	-0.567280
C	-2.780033	0.756630	-0.016884
C	-1.843228	1.861141	-0.311435
C	-2.251636	3.131112	-0.684500
H	-3.299729	3.385183	-0.784661
C	-1.247203	4.103675	-0.914391
H	-1.535753	5.110893	-1.207841
C	0.078464	3.787307	-0.770486
H	0.852496	4.529500	-0.946030
C	0.483378	2.460092	-0.385930
C	1.810210	2.067392	-0.230197
H	2.599830	2.774392	-0.467747
C	2.764114	-0.345773	-1.732003
C	4.223372	0.032932	-2.040318
H	4.385740	1.115077	-1.969765
H	4.452278	-0.263877	-3.073617
H	4.944993	-0.472890	-1.392548
C	1.890281	0.317212	-2.814962
H	0.822531	0.162997	-2.653882
H	2.145992	-0.120732	-3.789927
H	2.072936	1.395509	-2.861329
C	2.596921	-1.873726	-1.796252
H	3.198093	-2.393205	-1.043217
H	2.919993	-2.233966	-2.783106
H	1.554280	-2.171473	-1.658174
C	3.536533	0.150190	1.268471
C	4.651472	1.190298	1.041265
H	5.175467	1.063231	0.092563
H	5.395275	1.094650	1.844641
H	4.249121	2.208608	1.081799
C	4.111417	-1.276090	1.281648
H	3.323451	-2.028696	1.400680
H	4.798983	-1.380129	2.132814
H	4.676577	-1.513066	0.375866
C	2.925355	0.435550	2.650405
H	2.375951	1.383095	2.659864
H	3.732839	0.504933	3.392208
H	2.255107	-0.367927	2.968133
C	0.409343	-2.190042	0.969583
C	-0.103125	0.235487	2.319489
N	-1.046374	-1.298522	-2.273436
N	-1.338222	-2.413124	-1.997769
O	-1.207174	-3.216700	-1.080732
H	-7.022540	-0.344099	0.853893
H	-6.799061	0.860219	-0.432173
H	-6.835485	-0.871172	-0.821232

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ts-3-4 (C6) el energy= -1401.02765700

Ru	0.050979	-0.466867	-0.498297
H	1.528387	-0.835698	2.330824
P	-2.157499	0.298624	0.031974
O	-0.788200	-3.329783	-1.192645
O	0.217233	0.532190	-3.375550
N	2.236931	-0.457437	-0.555193
N	0.543030	1.487611	0.094739
C	3.023811	-1.502723	-0.847110
H	2.518062	-2.381493	-1.234142
C	4.396811	-1.483224	-0.652526
H	4.988243	-2.361046	-0.898452
C	4.995753	-0.333949	-0.117126
C	6.476887	-0.283443	0.151219
C	4.165652	0.748217	0.172960
H	4.591113	1.650772	0.598825
C	2.786510	0.677569	-0.056352
C	1.856950	1.793652	0.226105
C	2.280511	3.066558	0.569118
H	3.332013	3.312781	0.652403
C	1.286663	4.056607	0.775030
H	1.587068	5.067433	1.043172
C	-0.042110	3.753023	0.637561
H	-0.807368	4.508103	0.795558
C	-0.463255	2.420733	0.286037
C	-1.794424	2.040753	0.142377

H -2.572982 2.764073 0.367579
C -2.777228 -0.292460 1.756466
C -4.229685 0.115358 2.056327
H -4.382076 1.195887 1.945482
H -4.450787 -0.138233 3.102760
H -4.963949 -0.407999 1.436833
C -1.879898 0.399157 2.802228
H -0.827593 0.167165 2.629805
H -2.156286 0.025192 3.798731
H -2.018138 1.485330 2.790900
C -2.609436 -1.817677 1.876919
H -3.179184 -2.367742 1.120696
H -2.972218 -2.143640 2.862560
H -1.552020 -2.081621 1.795957
C -3.555210 0.078921 -1.257799
C -4.653689 1.143841 -1.065386
H -5.168203 1.066919 -0.106490
H -5.407370 1.022370 -1.855965
H -4.237733 2.153334 -1.156302
C -4.150888 -1.337703 -1.202728
H -3.376687 -2.106396 -1.309901
H -4.858189 -1.463693 -2.034570
H -4.697412 -1.532016 -0.276108
C -2.959681 0.295187 -2.658386
H -2.409093 1.239570 -2.721297
H -3.776389 0.330406 -3.392564
H -2.295225 -0.524228 -2.946551
C -0.453527 -2.259991 -0.935175
C 0.040332 0.146716 -2.306344
N 2.141936 -1.901204 2.540600
N 1.412996 -2.452124 1.798488
O 0.454707 -1.059445 1.443521
H 7.048965 -0.581176 -0.736423
H 6.799029 0.720117 0.447726
H 6.745832 -0.977793 0.958323

60
complex-3(C6) el energy= -1401.08194921
Ru 0.088783 -0.504821 -0.439911
H 1.571742 -1.410618 3.424861
P -2.125778 0.276322 0.070803
O -0.702909 -3.432596 -0.898687
O 0.127370 0.221892 -3.387888
N 2.256704 -0.474177 -0.546994
N 0.550362 1.503803 -0.055705
C 3.047847 -1.542420 -0.723551
H 2.544232 -2.468073 -0.978919
C 4.424849 -1.483378 -0.569325
H 5.020999 -2.379420 -0.718975
C 5.021913 -0.270785 -0.196958
C 6.510453 -0.170310 0.009893
C 4.184620 0.829009 -0.011444
H 4.607511 1.779549 0.296205
C 2.801778 0.715995 -0.191653
C 1.862413 1.843181 -0.004956
C 2.270614 3.153032 0.177451
H 3.319274 3.423466 0.198145
C 1.264552 4.144069 0.303845
H 1.553525 5.183028 0.448562
C -0.061795 3.806924 0.240850
H -0.836298 4.563209 0.334765
C -0.467079 2.438000 0.049984
C -1.794753 2.024747 -0.025258
H -2.581486 2.756148

0.135716
C -2.671074 -0.124368
1.872375
C -4.111630 0.319453
2.179107
H -4.269542 1.380062
1.948603
H -4.292775 0.190013
3.255488
H -4.867451 -0.270652
1.652341
C -1.734884 0.679132
2.798678
H -0.685039 0.438353
2.622346
H -1.974480 0.420192
3.840249
H -1.881762 1.756580
2.670917
C -2.504915 -1.627533
2.156524
H -3.134477 -2.251357
1.514249
H -2.794264 -1.832202
3.197197
H -1.463490 -1.929735
2.031051
C -3.558596 -0.114308
-1.135797
C -4.667009 0.953042
-1.036569
H -5.148542 0.986693
-0.057972
H -5.444054 0.727209
-1.780148
H -4.270651 1.948992
-1.262974
C -4.130999 -1.520325
-0.890890
H -3.348171 -2.287378
-0.917952
H -4.853195 -1.757991
-1.684510
H -4.656516 -1.602446
0.064250
C -3.009350 -0.062612
-2.570639
H -2.486256 0.878589
-2.768726
H -3.847513 -0.137642
-3.277003
H -2.332749 -0.897323
-2.775908
C -0.382671 -2.344136
-0.720448
C -0.000637 -0.058005
-2.280417
N 1.725290 -2.264426
2.844340
N 1.199012 -2.082331
1.733634
O 0.585220 -0.893106
1.576925
H 7.053766 -0.481571
-0.891539
H 6.815279 0.851725
0.257520
H 6.833428 -0.829684
0.826018

59
complex-1-no-hydride (C7) el energy=
-1254.94217238
Ru 0.026240 -0.819016 0.130035
P 2.113795 0.306238 -0.053018
O 1.080709 -3.695640 -0.199478
O 0.094291 -1.050322 3.109415
N -2.100460 -1.101108 -0.153943
N -0.677049 1.112532 0.075751
C -2.748075 -2.279207 -0.267312
H -2.122988 -3.166085 -0.291281
C -4.125916 -2.368407 -0.349892
H -4.595439 -3.343388 -0.446000
C -4.899114 -1.194762 -0.305743
C -6.399497 -1.252714 -0.387706
C -4.218582 0.016400 -0.181980
H -4.782874 0.941786 -0.141101
C -2.822053 0.054076 -0.108622
C -2.038540 1.295248 0.013988
C -2.595634 2.550093 0.050856

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H    -3.669829   2.684112 -0.010282
C    -1.753983   3.701696  0.171996
C    -2.379553   5.069055  0.229788
C    -0.399345   3.515318  0.226833
H     0.271248   4.365895  0.314414
C     0.189689   2.202796  0.164915
C     1.555730   1.978887  0.182226
H     2.247321   2.804788  0.308880
C     2.484988   0.088113 -1.919218
C     3.279955   1.283108 -2.470262
H     2.759613   2.227569 -2.280286
H     3.391143   1.166854 -3.556821
H     4.284323   1.349633 -2.043450
C     1.097444   0.071603 -2.600623
H     0.503311  -0.818225 -2.318077
H     1.219466   0.010672 -3.690545
H     0.518424   0.973713 -2.379191
C     3.218513  -1.228015 -2.214978
H     4.234800  -1.235301 -1.809906
H     3.302615  -1.351868 -3.302836
H     2.687626  -2.103292 -1.825995
C     3.592737  -0.036495  1.070986
C     4.873736   0.615774  0.518438
H     5.214135   0.147601 -0.409827
H     5.676196   0.498118  1.258084
H     4.746252   1.690191  0.341135
C     3.785992  -1.555482  1.229983
H     2.918078  -2.022665  1.708438
H     4.655095  -1.738904  1.874465
H     3.969163  -2.063356  0.278714
C     3.268157   0.581060  2.445745
H     3.163149   1.668759  2.392389
H     4.090819   0.350297  3.134817
H     2.351835   0.172417  2.882074
C     0.687971  -2.627809 -0.069860
C     0.109083  -0.973785  1.964206
H    -1.623943   5.855124  0.321849
H    -2.971331   5.266187 -0.674024
H    -3.063284   5.148653  1.085359
H    -6.847829  -0.255935 -0.336262
H    -6.718001  -1.725317 -1.325698
H    -6.809075  -1.856931  0.431845

60
complex-1 (C7)      el energy= -
1255.72445120
Ru    0.032107   0.005709   0.021355
H     0.040945   0.134213  -1.617289
P     2.181463   1.016430  -0.066578
O     0.993919  -2.844122  -0.458200
O    -0.466069  -0.194597   3.103323
N    -2.119645  -0.082844  -0.231309
N    -0.567836   2.032822   0.091148
C    -2.843428  -1.197163  -0.426781
H    -2.283251  -2.126715  -0.426440
C    -4.216032  -1.178662  -0.621215
H    -4.749938  -2.112734  -0.775863
C    -4.893157   0.050264  -0.618380
C    -6.383283   0.118040  -0.829842
C    -4.131605   1.198698  -0.415100
H    -4.616703   2.168999  -0.413346
C    -2.746042   1.122449  -0.221059
C    -1.888707   2.307708  -0.006010
C    -2.382801   3.597779   0.094633
H    -3.444587   3.806179   0.026497
C    -1.462734   4.661516   0.306747
C    -1.976439   6.074534   0.422709
C    -0.122951   4.373582   0.397424
H     0.599099   5.171719   0.553977
C     0.373648   3.027360   0.284587
C     1.722395   2.687577   0.352150
H     2.462815   3.478477   0.431943
C     2.929155   1.058782  -1.845760
C     4.332619   1.686898  -1.889769
H     4.349738   2.675095  -1.414357
H     4.629659   1.823832  -2.939329
H     5.094620   1.058766  -1.418572
C     1.998571   1.950515  -2.690473
H     0.965099   1.592728  -2.667215
H     2.344879   1.937544  -3.733737
H     2.008098   2.985307  -2.333260
C     2.962165  -0.349625  -2.462272
H     3.593743  -1.044257  -1.900055
H     3.364654  -0.290440  -3.483857
H     1.955598  -0.773555  -2.521288
C     3.535695   0.477299   1.176255
C     4.553846   1.605795   1.431147
H     5.123413   1.883523   0.542433
H     5.272424   1.272484   2.193333
H     4.053743   2.501499   1.815505
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C 4.246958 -0.803613 0.710866
H 3.530765 -1.599932 0.475209
H 4.897515 -1.171326 1.517144
H 4.877945 -0.639243 -0.167606
C 2.838805 0.182874 2.515083
H 2.200675 1.016966 2.826762
H 3.600920 0.028341 3.291624
H 2.230571 -0.724064 2.459734
C 0.614731 -1.771662 -0.251725
C -0.191428 -0.109445 1.991911
H -1.160870 6.787132 0.586229
H -2.513726 6.374822 -0.487489
H -2.683946 6.169109 1.258038
H -6.747433 1.150257 -0.799784
H -6.661499 -0.313629 -1.800126
H -6.915006 -0.453755 -0.058092

63
ts-1-2 (C7) el energy= -
1440.36274682
Ru -0.034842 -0.605016 -0.499628
H 0.197030 -0.874355 1.250041
P -2.173017 0.341260 -0.018705
O -1.108038 -3.420209 -1.050338
O 0.226608 0.139260 -3.462526
N 2.123413 -0.770491 -0.447822
N 0.589007 1.341536 -0.010225
C 2.832504 -1.894818 -0.645945
H 2.255937 -2.777683 -0.895089
C 4.211292 -1.939848 -0.511328
H 4.735025 -2.877591 -0.676592
C 4.906629 -0.776411 -0.149522
C 6.402770 -0.788123 0.024160
C 4.158514 0.382358 0.048741
H 4.658538 1.300123 0.339257
C 2.767256 0.375991 -0.105210
C 1.920927 1.572179 0.091397
C 2.428419 2.833843 0.342531
H 3.495715 3.011331 0.411235
C 1.517411 3.917079 0.493486
C 2.050584 5.299554 0.771652
C 0.170718 3.673856 0.382868
H -0.543612 4.486088 0.494858
C -0.343888 2.355398 0.123099
C -1.700255 2.058927 0.010126
H -2.428277 2.845454 0.186592
C -2.814770 -0.118587 1.743003
C -4.233175 0.405492 2.028079
H -4.309270 1.485404 1.853663
H -4.466494 0.229490 3.087724
H -5.004646 -0.099973 1.440158
C -1.871670 0.570175 2.749125
H -0.822285 0.318748 2.589829
H -2.141437 0.244857 3.763606
H -1.969891 1.659150 2.697258
C -2.769634 -1.642135 1.950752
H -3.425302 -2.178995 1.257847
H -3.101036 -1.880562 2.971247
H -1.757270 -2.035721 1.828848
C -3.595530 0.150921 -1.284288
C -4.620960 1.293881 -1.148624
H -5.137068 1.300053 -0.187220
H -5.383421 1.182064 -1.932215
H -4.140126 2.268138 -1.290481
C -4.281229 -1.219327 -1.154146
H -3.557348 -2.040676 -1.207826
H -4.989858 -1.348628 -1.984344
H -4.847073 -1.322381 -0.223994
C -2.986483 0.252911 -2.692614
H -2.365831 1.149140 -2.799011
H -3.798026 0.313301 -3.430805
H -2.385005 -0.627279 -2.936010
C -0.657149 -2.390588 -0.800649
C 0.024324 -0.144133 -2.367542
N 0.910331 -1.332719 2.340624
N 1.104436 -2.488098 2.166425
O 0.893559 -3.359059 1.329349
H 1.242466 6.034570 0.850087
H 2.621454 5.319244 1.710178
H 2.732710 5.626080 -0.025306
H 6.696802 -1.485224 0.819624
H 6.901620 -1.119193 -0.895875
H 6.786367 0.204268 0.282738

63
ts-3-4(C7) el energy= -
1440.35150001
Ru -0.050046 -0.722559 -0.394287
H 1.503366 -0.733663 2.414973
P -2.181510 0.275280 0.060858

O -1.102420 -3.592452 -0.593634
O 0.076189 -0.209959 -3.398086
N 2.129878 -0.872356 -0.508285
N 0.588324 1.260620 -0.139809
C 2.837602 -2.002282 -0.647850
H 2.262723 -2.895342 -0.870948
C 4.215834 -2.045341 -0.499526
H 4.740959 -2.989579 -0.615812
C 4.906383 -0.868190 -0.177568
C 6.397551 -0.875807 0.034102
C 4.157759 0.300530 -0.043846
H 4.655207 1.229064 0.215707
C 2.768912 0.288190 -0.217942
C 1.922056 1.495925 -0.094935
C 2.435808 2.773584 0.025882
H 3.504678 2.954710 0.039186
C 1.527954 3.868694 0.099411
C 2.068357 5.269640 0.233465
C 0.179406 3.619623 0.045634
H -0.531941 4.440208 0.101190
C -0.342218 2.283209 -0.076715
C -1.700745 1.982102 -0.124282
H -2.420803 2.785727 0.001289
C -2.775476 0.016276 1.873700
C -4.185998 0.569098 2.139625
H -4.271299 1.625635 1.857611
H -4.384963 0.503725 3.218700
H -4.975050 0.005832 1.632702
C -1.796550 0.802535 2.768496
H -0.769180 0.470513 2.609870
H -2.060617 0.616438 3.819659
H -1.862116 1.879444 2.581453
C -2.705019 -1.477226 2.239475
H -3.338664 -2.100524 1.599877
H -3.050932 -1.611524 3.274715
H -1.671473 -1.826436 2.175139
C -3.636770 -0.051994 -1.139314
C -4.655468 1.104839 -1.097029
H -5.138287 1.221209 -0.125684
H -5.444082 0.910176 -1.837337
H -4.177765 2.054255 -1.363195
C -4.321078 -1.395311 -0.836183
H -3.602422 -2.223155 -0.832148
H -5.063402 -1.606476 -1.618815
H -4.846744 -1.396281 0.122378
C -3.080506 -0.108793 -2.571272
H -2.471807 0.771490 -2.802631
H -3.919812 -0.135269 -3.279924
H -2.482417 -1.009096 -2.738091
C -0.687551 -2.522085 -0.521274
C -0.086464 -0.407056 -2.276474
N 2.052586 -1.793429 2.780560
N 1.258376 -2.401697 2.159669
O 0.383930 -1.020637 1.608114
H 1.262740 6.010886 0.264040
H 2.663848 5.375237 1.150726
H 2.729411 5.518400 -0.608093
H 6.913522 -1.348336 -0.811101
H 6.792775 0.138095 0.155199
H 6.656032 -1.449885 0.933807

63
complex-3(C7) el energy= -1440.40582712
Ru -0.015520 -0.700587 -0.415663
H 1.415062 -1.486637 3.495147
P -2.159353 0.281264 0.050687
O -1.033676 -3.580140 -0.700526
O 0.062295 -0.150720 -3.400557
N 2.148997 -0.839559 -0.526176
N 0.599364 1.283877 -0.149739
C 2.856485 -1.972962 -0.640759
H 2.282866 -2.871353 -0.839594
C 4.235038 -2.008978 -0.493455
H 4.761182 -2.954679 -0.591067
C 4.923984 -0.824983 -0.195046
C 6.417347 -0.824788 0.001473

C	4.172887	0.343730	2.246444
-0.072833			
H	4.667601	1.276321	1.640533
0.177314			
C	2.784383	0.325068	3.296697
-0.243069			
C	1.932589	1.528674	2.141636
-0.120862			
C	2.437167	2.810638	-1.128557
-0.015656			
H	3.504846	2.999249	-1.091445
-0.013504			
C	1.522077	3.899670	-0.115636
0.059080			
C	2.053572	5.304952	-1.818741
0.181920			
C	0.174845	3.641172	-1.377492
0.015430			
H	-0.541895	4.457163	-0.799436
0.068458			
C	-0.337494	2.300859	-0.780957
-0.097533			
C	-1.694427	1.989882	-1.576759
-0.148803			
H	-2.420907	2.788496	0.159421
-0.029352			
C	-2.723518	0.030494	-2.564743
1.873499			
C	-4.123664	0.601634	-2.818642
2.155586			
H	-4.200976	1.655677	-3.264257
1.862389			
H	-4.307728	0.550549	-2.721355
3.238047			
H	-4.925665	0.041208	-0.587041
1.665955			
C	-1.722440	0.812196	-2.278533
2.749167			
H	-0.695298	0.482030	2.965938
2.584152			
H	-1.973645	0.632878	1.846678
3.804697			
H	-1.787636	1.888539	1.620679
2.559299			
C	-2.672799	-1.461621	0.205982
H	-3.349788	-2.072040	1.640533
H	-2.974885	-1.581665	3.296697
H	-1.658023	-1.849951	2.141636
C	-3.625504	-0.067720	-1.128557
C	-4.647028	1.086686	-1.091445
H	-5.117937	1.215776	-0.115636
H	-5.444155	0.878356	-1.818741
H	-4.175899	2.033528	-1.377492
C	-4.303834	-1.407823	-0.799436
H	-3.582793	-2.233424	-0.780957
H	-5.046617	-1.635793	-1.576759
H	-4.828820	-1.391543	0.159421
C	-3.082597	-0.143763	-2.564743
H	-2.488967	0.740466	-2.818642
H	-3.928335	-0.194449	-3.264257
H	-2.474228	-1.039339	-2.721355
C	-0.628946	-2.511180	-0.587041
C	-0.080565	-0.355991	-2.278533
N	1.501813	-2.382238	2.965938
N	0.984849	-2.226701	1.846678
O	0.460537	-1.006522	1.620679
H	1.243447	6.041489	0.205982

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H           2.647598        5.421364
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H           2.713912        5.550739
-0.661006
H           6.929651       -1.222387
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H           6.798772        0.183404
0.193547
H           6.696619       -1.462561
0.850212

53
complex-1-no-hydride (C8)  el energy= -
1176.28774605
Ru    5.945095   5.008664   9.798333
P     6.923852   7.243889   9.605804
O     4.089489   5.017269   7.358073
O     3.644503   5.500948  11.628669
N     7.351575   4.908708  11.398667
N     7.016408   1.332441  11.617818
C     7.679705   7.337343  11.323654
H     8.545227   8.007425  11.359074
H     6.909782   7.786269  11.965219
C     8.034320   5.976250  11.870574
C     9.018980   5.801876  12.843260
H     9.564257   6.663264  13.217010
C     9.284309   4.517534  13.326764
H    10.048307   4.370264  14.085856
C     8.570651   3.429078  12.830135
H     8.742917   2.410515  13.160697
C     7.599411   3.654313  11.856482
C     6.789247   2.593640  11.229450
C     5.841554   2.980552  10.251429
C     5.075864   1.953160   9.685385
H     4.310454   2.171974   8.943910
C     5.302607   0.632663  10.080168
H     4.728276  -0.185575   9.653516
C     6.280077   0.374391  11.049197
H     6.474380  -0.642850  11.385055
C     8.392834   7.152662   8.402701
C     9.216300   8.447322   8.335265
H     8.653432   9.269246   7.882813
H    10.103823   8.277881   7.711486
H     9.568824   8.770149   9.322137
C     7.861544   6.780942   7.003644
H     7.305420   5.834777   7.020652
H     8.711243   6.650176   6.321723
H     7.210744   7.547429   6.576607
C     9.291949   5.996623   8.890265
H     9.749955   6.193284   9.865033
H    10.103102   5.849683   8.166393
H     8.748418   5.042742   8.959380
C     5.901191   8.835177   9.462111
C     4.612958   8.599617  10.275564
H     3.992263   7.816223   9.828930
H     4.024551   9.525654  10.285322
H     4.810012   8.331572  11.320718
C     6.645746  10.058581  10.028919
H     6.860399   9.954218  11.098330
H     6.006716  10.943503   9.913955
H     7.584309  10.261830   9.507163
C     5.516855   9.077774   7.992105
H     6.374045   9.382097   7.383607
H     4.780810   9.890379   7.947973
H     5.057018   8.193526   7.534188
C     4.780382   5.012841   8.269656
C     4.519911   5.328087  10.908157

54
complex-1 (C8)       el energy= -
1177.08669782
Ru    5.894152   4.996397   9.774754
H     7.070080   4.427649   8.759852
P     6.931677   7.164792   9.558092
O     4.186669   4.896373   7.265719
O     3.560323   5.536861  11.767188
N     7.359655   4.853336  11.348394
N     6.895258   1.303995  11.700073
C     7.694863   7.269482  11.277105
H     8.546822   7.956789  11.327220
H     6.908896   7.687586  11.920765
C     8.068878   5.905384  11.806395
C     9.076954   5.724049  12.752018
H     9.645525   6.580001  13.104608
C     9.333297   4.436306  13.236365
H    10.117185   4.278102  13.973650
C     8.579825   3.365642  12.772433
H     8.728366   2.346520  13.112418
C     7.586171   3.601695  11.815062
C     6.727323   2.558370  11.240632
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C 5.794457 2.959849 10.251449
C 4.990666 1.929976 9.739602
H 4.246376 2.146002 8.975153
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H 4.528024 -0.185033 9.817598
C 6.111306 0.359326 11.184149
H 6.256454 -0.651976 11.564794
C 8.444141 7.237204 8.388886
C 9.132002 8.609964 8.323402
H 8.506081 9.371343 7.848429
H 10.047352 8.521130 7.721879
H 9.429557 8.973556 9.314632
C 7.992843 6.806046 6.980514
H 7.536381 5.811901 7.005410
H 8.868359 6.766403 6.317758
H 7.274858 7.503797 6.538352
C 9.471516 6.208002 8.904987
H 9.919204 6.512194 9.857969
H 10.284700 6.126632 8.170955
H 9.024598 5.217010 9.027443
C 5.915252 8.782403 9.451698
C 4.615431 8.543748 10.243510
H 4.014154 7.748105 9.795607
H 4.021401 9.467983 10.240256
H 4.801698 8.276320 11.290283
C 6.623332 10.013320 10.047232
H 6.851330 9.877481 11.110920
H 5.955209 10.882431 9.969173
H 7.550834 10.265928 9.530015
C 5.532726 9.041012 7.983287
H 6.389528 9.347735 7.375337
H 4.791295 9.850581 7.939138
H 5.082400 8.153067 7.522822
C 4.813665 4.943357 8.234794
C 4.438458 5.401834 11.035922

57
ts-1-2 (C8) el energy= -
1361.72315969
Ru -0.324455 -0.571334 0.448048
H -0.535389 -0.559086 -1.333247
P 1.930466 0.261147 0.099056
O 0.276566 -3.556089 0.670739
O -0.633052 -0.347483 3.488876
C -2.411749 -0.604220 0.314389
N -0.756422 1.513731 0.170293
C -3.317454 -1.670781 0.389656
H -2.961858 -2.677841 0.592478
C -4.677016 -1.439827 0.179429
H -5.396652 -2.254476 0.228187
C -5.111668 -0.138258 -0.104888
H -6.167934 0.070269 -0.275469
N -4.284194 0.902401 -0.184512
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C -1.486923 4.109774 -0.414045
H -1.765932 5.133084 -0.654479
C -0.150166 3.794296 -0.144381
H 0.621128 4.559014 -0.161312
C 0.189071 2.476762 0.157618
C 1.596012 2.065788 0.524302
H 1.703216 2.136289 1.615493
C 2.546564 0.325272 -1.710500
C 3.970252 0.879592 -1.880265
H 4.080800 1.879628 -1.443268
H 4.187886 0.968765 -2.953599
H 4.733485 0.225290 -1.449344
C 1.587829 1.246392 -2.494177
H 0.541480 0.953959 -2.394019
H 1.843448 1.186034 -3.560514
H 1.690377 2.295068 -2.192678
C 2.465188 -1.098325 -2.294410
H 3.170846 -1.784061 -1.814607
H 2.709805 -1.064510 -3.364641
H 1.461011 -1.517575 -2.190524
C 3.352689 -0.210944 1.286257
C 4.434892 0.875212 1.428688
H 4.951737 1.091530 0.492226
H 5.189721 0.533342 2.150365
H 4.021124 1.813739 1.816116
C 3.974743 -1.538572 0.815899
H 3.208988 -2.307572 0.656939
H 4.661925 -1.909094 1.588713
H 4.549584 -1.428235 -0.108419
C 2.726475 -0.449643 2.673193
H 2.186345 0.426394 3.050672
H 3.527745 -0.675095 3.390001

H 2.034553 -1.295889 2.661074
C 0.006933 -2.447333 0.514551
C -0.456515 -0.435710 2.354344
N -1.126913 -0.784849 -2.536152
N -1.362249 -1.946546 -2.570273
O -1.243381 -2.940269 -1.869076

57
ts-3-4 (C8) el energy= -1361.71147172
Ru 0.340098 -0.670296 -0.330249
H 1.841422 -0.203126 2.419835
P -1.978499 0.160772 -0.060729
O -0.042647 -3.680356 -0.019637
O 0.481474 -0.828371 -3.374985
C 2.427081 -0.632105 -0.335401
N 0.703678 1.442814 -0.394072
C 3.368062 -1.667883 -0.337545
H 3.046520 -2.703375 -0.431360
C 4.725636 -1.372670 -0.200266
H 5.472772 -2.163484 -0.192395
C 5.119301 -0.036105 -0.061270
H 6.171130 0.224723 0.054988
N 4.255798 0.979284 -0.061608
H -2.416107 2.609786 -0.461055
C 2.953322 0.674825 -0.199887
C 1.998700 1.795191 -0.217593
C 2.357997 3.139791 -0.083535
H 3.405418 3.378321 0.065183
C 1.361434 4.107221 -0.143959
H 1.612340 5.159873 -0.034968
C 0.032834 3.723998 -0.354715
H -0.760593 4.462826 -0.420753
C -0.271146 2.369177 -0.486331
C -1.667899 1.876002 -0.779583
H -1.771301 1.764230 -1.867718
C -2.584970 0.507177 1.715804
C -4.014623 1.061946 1.807526
H -4.144296 1.980745 1.221889
H -4.221938 1.314689 2.856733
H -4.774083 0.339409 1.493946
C -1.622779 1.542845 2.335441
H -0.590112 1.188562 2.282898
H -1.890648 1.668292 3.394053
H -1.708664 2.526932 1.859517
C -2.463050 -0.807550 2.511207
H -3.115716 -1.595748 2.121511
H -2.755263 -0.622428 3.554475
H -1.426447 -1.154610 2.498150
C -3.403093 -0.502774 -1.150580
C -4.495389 0.539247 -1.455546
H -5.006063 0.898911 -0.560789
H -5.252951 0.081245 -2.106751
H -4.092312 1.406497 -1.991772
C -4.014433 -1.741905 -0.471143
H -3.242652 -2.472278 -0.198848
H -4.705819 -2.233059 -1.169485
H -4.580468 -1.489956 0.430244
C -2.789074 -0.955909 -2.488370
H -2.268754 -0.145902 -3.012044
H -3.594387 -1.307318 -3.147840
H -2.083334 -1.779571 -2.349673
C 0.104987 -2.545130 -0.128965
C 0.362336 -0.780841 -2.229342
N 2.211613 -1.187838 3.057311
N 1.290371 -1.794633 2.655479
O 0.614064 -0.468992 1.727948

57
complex-3(C8) el energy= -1361.76466888
Ru 0.379850 -0.685135 -0.345353
H 1.625798 -0.230144 3.684043
P -1.935662 0.147501 -0.023463
O 0.052446 -3.698091 0.032834
O 0.410914 -0.946999 -3.374377
C 2.461144 -0.643691 -0.433509
N 0.726762 1.424075 -0.486315
C 3.400214 -1.679260 -0.432611
H 3.077601 -2.716969 -0.481903
C 4.760801 -1.377002 -0.347255

H	5.509823	-2.165941	2.234863
-0.339619			
C	5.154843	-0.036444	3.373961
-0.260137			
H	6.209294	0.229362	1.809285
-0.186724			
N	4.289310	0.977624	2.598308
-0.259172			
H	-2.398326	2.579115	2.272298
-0.490595			
C	2.984536	0.667080	3.646885
-0.346676			
C	2.025943	1.783258	2.552984
-0.360383			
C	2.384182	3.132140	-1.039302
-0.274556			
H	3.434877	3.377053	-1.348536
-0.164370			
C	1.383197	4.094923	-0.452083
-0.332084			
H	1.634090	5.150786	-1.953804
-0.260585			
C	0.049580	3.703492	-1.933330
-0.492055			
H	-0.747491	4.438591	-0.292783
-0.555638			
C	-0.253527	2.345003	-0.011736
-0.575118			
C	-1.656994	1.838456	-0.951055
-0.809137			
H	-1.795187	1.690973	0.612117
-1.889106			
C	-2.482919	0.556662	-2.377536
1.759290			
C	-3.906707	1.122796	-2.948333
1.876240			
H	-4.051099	2.019317	-2.996933
1.260472			
H	-4.079770	1.416077	-2.230236
2.921041			
H	-4.678381	0.392770	-0.092429
1.614301			
C	-1.499680	1.611636	-2.228694
2.310544			
H	-0.463100	1.274808	3.485030

H	-1.728620	1.768614	3.373961
H	-1.610604	2.580321	1.809285
C	-2.349963	-0.729368	2.598308
H	-3.039837	-1.514334	2.272298
H	-2.583968	-0.499247	3.646885
H	-1.329268	-1.114759	2.552984
C	-3.391104	-0.562796	-1.039302
C	-4.495399	0.465299	-1.348536
H	-4.975855	0.860712	-0.452083
H	-5.273801	-0.019750	-1.953804
H	-4.113015	1.310171	-1.933330
C	-3.976980	-1.775222	-0.292783
H	-3.195015	-2.491298	-0.011736
H	-4.684826	-2.297072	-0.951055
H	-4.520084	-1.487830	0.612117
C	-2.818316	-1.065779	-2.377536
H	-2.317929	-0.275308	-2.948333
H	-3.643111	-1.443634	-2.996933
H	-2.106422	-1.882711	-2.230236
C	0.179540	-2.563897	-0.092429
C	0.333250	-0.853133	-2.228694
N	1.708277	-1.251680	3.485030

N 1.256422 -1.470130 2.350941
O 0.762629 -0.385439 1.712370

59
complex-1-no-hydride (C9) el energy= -1254.94084813
Ru -0.039224 0.055648 0.046178
P -2.304857 0.983294 0.078216
O 0.311094 -0.800365 2.879337
O -0.627719 -2.824014 -0.824716
N 0.421046 2.090933 0.471388
N 3.889845 1.594692 -0.337966
C -4.079970 2.306402 -1.770979
C -1.919307 2.566447 1.014626
C -0.497345 3.025423 0.800580
C -2.757107 1.530744 -1.685764
C 2.140876 3.751154 0.416734
C 4.708465 0.588611 -0.682722
C 1.722001 2.433798 0.279485
C 2.894478 -1.012586 -0.550911
C 4.237870 -0.730791 -0.799842
C 2.604849 1.314029 -0.102279
C 2.022546 0.027899 -0.206510
C -0.406922 -1.749954 -0.497703
C 0.154076 -0.486292 1.786980
C -4.791559 1.268296 1.466002
C -4.413295 -0.883881 0.198504
C -3.748216 0.217441 1.042262
C -3.136149 -0.428835 2.301066
C 1.215184 4.744785 0.760123
C -2.807000 0.284291 -2.592293
C -1.603136 2.429301 -2.179265
C -0.121162 4.359199 0.944818
H 2.536960 -2.037356 -0.628001
H -2.626804 3.368954 0.780541
H -2.057553 2.327086 2.077395
H 3.188589 3.973385 0.239788
H 4.926037 -1.526053 -1.074945
H -2.988523 0.601816 -3.626951
H -3.602219 -0.412456 -2.316942
H -4.979580 -0.475299 -0.644126
H -3.683001 -1.606011 -0.186421
H -4.943079 1.673958 -1.542357
H -1.856122 -0.263659 -2.578717
H -0.628513 1.921542 -2.136624
H -4.369397 2.024007 2.137738
H -1.518966 3.364147 -1.615663
H -2.480757 -1.267503 2.045143
H -5.246879 1.780016 0.614371
H -2.565927 0.281617 2.911913
H -4.212711 2.681450 -2.794388
H -0.872847 5.099204 1.205688
H -1.782357 2.689783 -3.229855
H -4.098810 3.174385 -1.101124
H -5.596483 0.763123 2.015252
H -3.946220 -0.818604 2.930245
H -5.120443 -1.436509 0.829921
C 1.646314 6.174118 0.939891
H 2.120413 6.303597 1.922634
H 2.385772 6.461876 0.184378
H 0.798600 6.864431 0.884798
C 6.149001 0.944427 -0.933513
H 6.229197 1.620263 -1.794462
H 6.565867 1.474583 -0.069020
H 6.758080 0.057009 -1.130937

60
complex-1 (C9) el energy= -1255.73479116
Ru -0.034915 0.008775 0.037551
P -2.253117 0.959648 0.006891
O 0.347583 -0.770595 3.029297
O -0.559064 -2.801309 -0.987625
N 0.450361 2.075767 0.396730
N 3.953849 1.553689 -0.220844
C -4.243391 2.239642 -1.683943
C -1.878629 2.552272 0.941398
C -0.463374 3.021480 0.698970
C -2.858821 1.573121 -1.701212
C 2.173259 3.734856 0.340800
C 4.779853 0.542368 -0.492119
C 1.752299 2.405453 0.227297
C 2.944476 -1.039996 -0.484007
C 4.303222 -0.775226 -0.629145
C 2.642155 1.278830 -0.078704
C 2.046754 0.001230 -0.198475
C -0.361786 -1.741882 -0.570772
C 0.144678 -0.461050 1.939466

C	-4.742015	1.250406	1.481054
C	-4.380116	-0.885658	0.177514
C	-3.702144	0.216289	1.011396
C	-3.084594	-0.446581	2.257449
C	1.248599	4.735169	0.627986
C	-2.860425	0.379929	-2.675481
C	-1.831863	2.608923	-2.204732
C	-0.093262	4.357533	0.811271
H	2.581091	-2.060081	-0.596535
H	0.051780	0.369377	-1.575015
H	-2.598914	3.351258	0.732706
H	-1.982260	2.298276	2.005172
H	3.227324	3.945456	0.190839
H	5.003547	-1.579585	-0.850062
H	-3.125979	0.735386	-3.680769
H	-3.586291	-0.389625	-2.394476
H	-4.954660	-0.481334	-0.661657
H	-3.646506	-1.598896	-0.217868
H	-5.047198	1.533063	-1.456340
H	-1.869978	-0.082553	-2.725648
H	-0.813370	2.210333	-2.184192
H	-4.294272	2.013894	2.127881
H	-1.858166	3.535542	-1.620189
H	-2.418738	-1.269561	1.984377
H	-5.245790	1.756698	0.655494
H	-2.512719	0.259237	2.871238
H	-4.450390	2.656587	-2.679479
H	-0.847874	5.104358	1.047087
H	-2.076245	2.868076	-3.243951
H	-4.296719	3.068864	-0.967799
H	-5.513270	0.738022	2.073159
H	-3.892153	-0.849626	2.884041
H	-5.078164	-1.445431	0.815129
C	1.660335	6.180771	0.742471
H	2.738438	6.301183	0.595781
H	1.143371	6.796508	-0.005583
H	1.401620	6.587295	1.729071
C	6.247411	0.863438	-0.643056
H	6.400631	1.941646	-0.539366
H	6.850078	0.350820	0.119524
H	6.629458	0.546519	-1.622999

63

ts-1-2 (C9) el energy= -1440.37173606

Ru	-0.297158	-0.558980	0.566766
H	-0.558815	-0.800787	-1.190609
P	1.934411	0.235901	0.032614
O	0.339538	-3.481906	1.176139
O	-0.516629	0.083351	3.554963
N	-0.757791	1.463316	0.018647
C	-3.288986	-1.661804	0.750424
H	-2.925018	-2.631829	1.079785
C	-4.651954	-1.464549	0.549216
H	-5.359782	-2.271414	0.732197
C	-5.122671	-0.216469	0.098216
C	-2.972567	0.590914	0.057868
C	-2.067488	1.714993	-0.216264
C	-2.479619	2.966634	-0.682664
H	-3.539347	3.114724	-0.863858
C	-1.538878	3.969189	-0.906073
C	-0.190871	3.682774	-0.626713
H	0.573777	4.442559	-0.769807
C	0.172683	2.425399	-0.157048
C	1.594855	2.079384	0.219731
H	2.310380	2.702835	-0.327555
C	2.492100	0.057437	-1.788475
C	3.902892	0.594440	-2.078853
H	4.016091	1.644687	-1.783299
H	4.084694	0.540497	-3.161220
H	4.687252	0.009275	-1.590191
C	1.497525	0.855670	-2.657750
H	0.458586	0.572058	-2.482547
H	1.718982	0.651531	-3.713917
H	1.597233	1.936410	-2.505559
C	2.410122	-1.432554	-2.172258
H	3.133821	-2.042876	-1.622612
H	2.628016	-1.542140	-3.243260
H	1.412669	-1.839629	-1.987255
C	3.399691	-0.062550	1.223929
C	4.475101	1.038832	1.182243
H	4.958708	1.129952	0.208219
H	5.256691	0.801860	1.917436
H	4.064548	2.018645	1.453471
C	4.019431	-1.438145	0.917003
H	3.256300	-2.225399	0.887587
H	4.733968	-1.697661	1.710050
H	4.563929	-1.450332	-0.031884
C	2.821670	-0.114210	2.650994
H	2.283491	0.801135	2.923330

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H     3.648528 -0.233503  3.364321
H     2.139750 -0.959080  2.778269
C     0.054055 -2.405705  0.880790
C    -0.373760 -0.160510  2.438355
N    -1.188104 -1.191754 -2.334057
N    -1.430272 -2.344171 -2.195902
O    -1.296591 -3.230967 -1.365851
N    -4.288323  0.796146 -0.143176
H     1.732887  2.296269  1.287886
C    -2.388282 -0.615589  0.503419
C    -6.594752  0.026070 -0.130737
H    -7.006334 -0.679759 -0.864747
H    -7.169849 -0.100026  0.796872
H    -6.747522  1.044226 -0.500184
C    -1.940678  5.320851 -1.437981
H    -1.501677  6.129535 -0.840135
H    -1.587094  5.452347 -2.469765
H    -3.028562  5.442451 -1.437535

63
ts-3-4 (C9)    el energy= -
1440.36017353
Ru    0.288021 -0.553036 -0.659772
H     2.020078 -1.044467  1.936156
P    -1.962248  0.174083  0.079057
O    -0.191255 -3.487475 -1.341422
O     0.183698  0.322815 -3.580570
N     0.732949  1.451638 -0.047582
C     3.269534 -1.518029 -1.267654
H     2.905248 -2.459719 -1.674136
C     4.640667 -1.298519 -1.159213
H     5.349984 -2.057931 -1.483894
C     5.115609 -0.090813 -0.615697
C     2.956570  0.640493 -0.323719
C     2.050240  1.712532  0.118421
C     2.472149  2.929836  0.657792
H     3.538895  3.089522  0.777616
C     1.529654  3.889765  1.023590
C     0.172505  3.597647  0.808423
H    -0.593626  4.326728  1.060638
C    -0.201149  2.372245  0.264185
C    -1.638465  2.027471 -0.047523
H    -1.837337  2.293495 -1.094779
C    -2.408708 -0.088703  1.916594
C    -3.799452  0.427056  2.316482
H    -3.932544  1.491103  2.083684
H    -3.911172  0.316917  3.404225
H    -4.613884 -0.135527  1.850238
C    -1.354075  0.662407  2.757189
H    -0.345850  0.329595  2.497393
H    -1.531942  0.429189  3.816564
H    -1.431852  1.750396  2.645725
C    -2.284386 -1.596009  2.214078
H    -3.002355 -2.196734  1.645882
H    -2.482390 -1.767156  3.281649
H    -1.269354 -1.935609  1.991204
C    -3.497526 -0.065553 -1.035854
C    -4.565498  1.032662 -0.877430
H    -4.988254  1.077117  0.127609
H    -5.390879  0.830470 -1.574338
H    -4.169707  2.024273 -1.126719
C    -4.105007 -1.452584 -0.756762
H    -3.346217 -2.242588 -0.815788
H    -4.871620 -1.670480 -1.512984
H    -4.584419 -1.511081  0.224639
C    -3.011666 -0.051945 -2.497222
H    -2.502226  0.880457 -2.765892
H    -3.880552 -0.153494 -3.161865
H    -2.330650 -0.882493 -2.702243
C    -0.006511 -2.383373 -1.077206
C     0.156996 -0.017456 -2.479233
N     2.414867 -2.189647  2.166624
N     1.440385 -2.619255  1.670736
O     0.731958 -1.061662  1.315957
C     2.368358 -0.535854 -0.837979
N     4.278396  0.865800 -0.207429
H    -2.324886  2.618631  0.568182
C     1.944259  5.199931  1.642340
H     3.012235  5.390642  1.495157
H     1.379250  6.038443  1.217201
H     1.751353  5.193294  2.724029
C     6.594521  0.169806 -0.465080
H     7.122527  0.050267 -1.420532
H     6.754385  1.188034 -0.098923
H     7.050371 -0.531568  0.247179

63
complex-3(C9)          el energy= -
1440.41339222
Ru          0.055843      -0.868926
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-0.344965			
H	1.317766	-0.581247	
3.694634			
P	-2.175859	0.167135	
-0.020122			
O	-0.537737	-3.846825	
-0.015179			
O	0.086182	-1.082977	
-3.376876			
N	0.588812	1.200746	
-0.450972			
C	2.984915	-2.116112	
-0.436047			
H	2.578278	-3.122949	
-0.503500			
C	4.362474	-1.931929	
-0.340359			
H	5.035980	-2.787210	
-0.342667			
C	4.889428	-0.632491	
-0.228188			
C	2.769711	0.249043	
-0.316737			
C	1.912992	1.445062	
-0.316492			
C	2.386158	2.754855	
-0.210277			
H	3.455611	2.900019	
-0.096387			
C	1.489683	3.821600	
-0.250751			
C	0.125625	3.532235	
-0.424144			
H	-0.604192	4.336025	
-0.482384			
C	-0.299848	2.211406	
-0.528280			
C	-1.743142	1.839437	
-0.775621			
H	-1.890190	1.724252	
-1.858286			
C	-2.694026	0.595141	
1.767130			
C	-4.061108	1.286338	
1.887141			
H	-4.119000	2.202744	
1.286587			
H	-4.213995	1.576211	
2.936091			
H	-4.894215	0.634370	
1.608133			
C	-1.622738	1.547841	
2.340569			
H	-0.620422	1.119530	
2.265619			
H	-1.844458	1.708943	
3.404980			
H	-1.641304	2.529744	
1.853405			
C	-2.682883	-0.711012	
2.585226			
H	-3.440855	-1.423984	
2.245000			
H	-2.898439	-0.477429	
3.637047			
H	-1.701421	-1.187254	
2.535221			
C	-3.684446	-0.393497	
-1.052218			
C	-4.690218	0.733958	
-1.350809			
H	-5.139198	1.157054	
-0.450648			
H	-5.505017	0.329974	
-1.967682			
H	-4.229866	1.549978	
-1.920140			
C	-4.381281	-1.559645	
-0.327653			
H	-3.668878	-2.348779	
-0.057386			
H	-5.131393	-2.003643	
-0.996250			
H	-4.899182	-1.239328	
0.580986			
C	-3.150770	-0.926074	
-2.395034			
H	-2.580075	-0.174365	
-2.952088			
H	-4.001818	-1.222241	

-3.023396
H -2.513248 -1.803447
-2.255188
C -0.310510 -2.726308
-0.122967
C 0.008417 -1.001590
-2.230013
N 1.321300 -1.602943
3.479691
N 0.855883 -1.766954
2.341502
O 0.449637 -0.637613
1.720763
C 2.133789 -1.005737
-0.425290
N 4.097320 0.442745
-0.218598
H -2.415841 2.638160
-0.445229
C 1.959013 5.246050
-0.103209
H 3.040870 5.327081
-0.249974
H 1.459694 5.907188
-0.821997
H 1.728244 5.625254
0.901904
C 6.375679 -0.400598
-0.104871
H 6.924986 -0.868250
-0.932836
H 6.583127 0.673362
-0.106156
H 6.767882 -0.829564
0.827417

59
complex-1-no-hydride (C10) el
energy= -1850.34186333
Ru -0.044058 0.063373 0.033021
P -2.309325 0.987468 0.073981
O 0.304234 -0.805214 2.863698
O -0.649889 -2.814207 -0.835693
N 0.424574 2.097389 0.473829
N 3.896313 1.586269 -0.293953
C -4.063973 2.322085 -1.783568
C -1.920486 2.568060 1.014859
C -0.498734 3.027040 0.807709
C -2.747969 1.535432 -1.692750
C 2.159075 3.746255 0.445254
C 4.693153 0.573039 -0.633795
C 1.727914 2.429839 0.295695
C 2.895878 -1.017428 -0.550146
C 4.248335 -0.744159 -0.776492
C 2.608396 1.309077 -0.080628
C 2.025887 0.023174 -0.205744
C -0.423573 -1.741976 -0.511093
C 0.150460 -0.486397 1.773716
C -4.792933 1.270014 1.457630
C -4.414360 -0.881794 0.188196
C -3.750469 0.217311 1.035995
C -3.138205 -0.430445 2.293819
C 1.217178 4.714965 0.778702
C -2.804089 0.287840 -2.597401
C -1.582620 2.422109 -2.180998
C -0.120933 4.359420 0.966536
H 2.534478 -2.038811 -0.645545
H -2.625317 3.372829 0.781031
H -2.061093 2.328052 2.077243
H 3.207501 3.976909 0.291191
H 4.944232 -1.530161 -1.050189
H -2.979310 0.605917 -3.632773
H -3.605684 -0.402114 -2.324470
H -4.982323 -0.470999 -0.652147
H -3.684483 -1.602946 -0.199406
H -4.932793 1.696521 -1.557921
H -1.857441 -0.267670 -2.581162
H -0.612420 1.904461 -2.133091
H -4.373475 2.021850 2.135384
H -1.492732 3.358551 -1.620895
H -2.485833 -1.271398 2.037013
H -5.241612 1.785817 0.604891
H -2.566521 0.278206 2.905540
H -4.189265 2.696698 -2.807921
H -0.857865 5.107127 1.240440
H -1.751368 2.681809 -3.233307
H -4.078945 3.191445 -1.115446
H -5.602385 0.764741 1.999745
H -3.948441 -0.818733 2.923439
H -5.120363 -1.436505 0.818812

C 1.625083 6.172678 0.883993
C 6.147957 0.948588 -0.859157
F 0.876669 6.813611 1.795915
F 2.912207 6.294148 1.225621
F 1.444753 6.782852 -0.299203
F 6.258817 1.839527 -1.855971
F 6.675475 1.496485 0.244684
F 6.880718 -0.132026 -1.181717

60
complex-1 (C10) el energy= -1851.15512172
Ru -0.029319 0.012124 0.035417
P -2.251134 0.960493 0.011088
O 0.329087 -0.816975 3.020137
O -0.574967 -2.782956 -1.019394
N 0.458657 2.074023 0.412878
N 3.950538 1.544407 -0.220870
C -4.235719 2.261389 -1.667093
C -1.872319 2.540547 0.966608
C -0.459119 3.012180 0.727238
C -2.850560 1.595438 -1.690681
C 2.192102 3.725533 0.364598
C 4.754439 0.523441 -0.505208
C 1.760845 2.399984 0.242812
C 2.938547 -1.048530 -0.505652
C 4.301589 -0.791753 -0.656381
C 2.646009 1.273083 -0.075842
C 2.046413 -0.008304 -0.206265
C -0.369424 -1.730945 -0.592144
C 0.135987 -0.487304 1.935923
C -4.737071 1.236103 1.484990
C -4.374883 -0.886667 0.157791
C -3.698327 0.204824 1.006774
C -3.084234 -0.471944 2.246878
C 1.251282 4.701813 0.660704
C -2.851379 0.413513 -2.678929
C -1.823897 2.638098 -2.180270
C -0.089436 4.348682 0.852360
H 2.571743 -2.065830 -0.625803
H 0.051224 0.385909 -1.572955
H -2.591117 3.343764 0.770971
H -1.971873 2.273196 2.027427
H 3.243102 3.947135 0.219117
H 5.002957 -1.587267 -0.887655
H -3.121196 0.780841 -3.678482
H -3.574377 -0.361281 -2.405380
H -4.947698 -0.471980 -0.677235
H -3.641757 -1.596503 -0.244633
H -5.039753 1.551855 -1.450531
H -1.860157 -0.045875 -2.739663
H -0.804538 2.241352 -2.166649
H -4.290785 1.988909 2.145239
H -1.853191 3.558745 -1.586297
H -2.420670 -1.294798 1.967947
H -5.235189 1.755138 0.664216
H -2.513658 0.226221 2.870607
H -4.439928 2.690079 -2.657880
H -0.830397 5.100154 1.104569
H -2.067649 2.909835 -3.216027
H -4.291637 3.082355 -0.941770
H -5.512383 0.717653 2.065898
H -3.894157 -0.879549 2.866947
H -5.074315 -1.452974 0.787645
C 1.649252 6.155853 0.730501
C 6.215465 0.879744 -0.655300
F 0.954198 6.808558 1.684712
F 2.956098 6.308652 0.994519
F 1.395109 6.779413 -0.438116
F 6.717445 1.410212 0.476777
F 6.409871 1.783797 -1.634499
F 6.962254 -0.205606 -0.955687

63
ts-1-2 (C10) el energy= -2035.79017006
Ru -0.298684 -0.554270 0.571160
H -0.570833 -0.786587 -1.192250
P 1.935203 0.234611 0.025188
O 0.351176 -3.477226 1.168803
O -0.480269 0.070518 3.566986
N -0.764039 1.466390 0.023026
C -3.281788 -1.669900 0.777313
H -2.913742 -2.638233 1.105263
C -4.651432 -1.480760 0.587944
H -5.360899 -2.280419 0.774991
C -5.098964 -0.232732 0.141159
C -2.975691 0.587601 0.077147
C -2.075067 1.713169 -0.204900
C -2.498721 2.961403 -0.672341

H	-3.556000	3.120355	-0.850524
C	-1.542135	3.942704	-0.892734
C	-0.193058	3.683180	-0.623367
H	0.558783	4.452146	-0.767037
C	0.170925	2.424480	-0.153918
C	1.592167	2.077866	0.218547
H	2.305011	2.704916	-0.327534
C	2.479377	0.059568	-1.799702
C	3.890378	0.594151	-2.095020
H	4.006703	1.644775	-1.802063
H	4.067335	0.538414	-3.177821
H	4.675562	0.008291	-1.608953
C	1.483855	0.862518	-2.663621
H	0.444080	0.580242	-2.490866
H	1.703044	0.661968	-3.720637
H	1.587291	1.942791	-2.510211
C	2.391930	-1.430113	-2.183788
H	3.117580	-2.042250	-1.638982
H	2.603384	-1.539107	-3.255864
H	1.394886	-1.836103	-1.994139
C	3.404134	-0.063977	1.210687
C	4.475134	1.041689	1.164630
H	4.952924	1.136358	0.188202
H	5.261350	0.805025	1.894596
H	4.063723	2.019659	1.441269
C	4.026438	-1.437000	0.896330
H	3.266920	-2.227862	0.870991
H	4.746662	-1.694495	1.684564
H	4.565494	-1.445743	-0.055579
C	2.833361	-0.120733	2.640129
H	2.296860	0.793577	2.919300
H	3.664117	-0.241454	3.348277
H	2.154197	-0.967706	2.768660
C	0.060364	-2.402982	0.876404
C	-0.350920	-0.165253	2.448271
N	-1.203276	-1.168225	-2.313086
N	-1.447161	-2.321882	-2.174503
O	-1.305926	-3.200841	-1.337820
N	-4.286370	0.789430	-0.113318
H	1.729622	2.292650	1.287210
C	-2.386268	-0.623349	0.522699
C	-6.568346	0.046694	-0.082877
C	-1.934836	5.283513	-1.465209
F	-1.195518	6.277293	-0.931305
F	-1.732487	5.312296	-2.797416
F	-3.227654	5.565664	-1.244364
F	-6.815040	0.423570	-1.350726
F	-7.010967	1.035541	0.718095
F	-7.323878	-1.043814	0.169633

63

ts-3-4 (C10) el energy= -2035.77801338

Ru	0.316852	-0.649993	-0.518743
H	1.863887	-0.883129	2.262558
P	-1.955379	0.201560	-0.020392
O	-0.226391	-3.630316	-0.873062
O	0.408802	-0.126836	-3.527525
N	0.783624	1.401042	-0.106584
C	3.295246	-1.759747	-0.802896
H	2.928828	-2.732126	-1.124911
C	4.667203	-1.569565	-0.622087
H	5.376090	-2.371119	-0.802884
C	5.114851	-0.317966	-0.189651
C	2.991200	0.504878	-0.131072
C	2.093471	1.642946	0.123914
C	2.523964	2.900697	0.555505
H	3.580957	3.059379	0.735661
C	1.571737	3.896022	0.735443
C	0.224561	3.639687	0.460670
H	-0.522364	4.418413	0.572867
C	-0.146285	2.367623	0.029492
C	-1.566384	2.019459	-0.342490
H	-1.681468	2.160955	-1.425863
C	-2.518665	0.166392	1.802431
C	-3.916966	0.752751	2.049950
H	-4.006752	1.785835	1.691403
H	-4.097978	0.769880	3.133564
H	-4.716008	0.156906	1.599001
C	-1.497276	0.990516	2.614861
H	-0.483592	0.613726	2.456431
H	-1.740627	0.882347	3.680962
H	-1.545315	2.060442	2.379244
C	-2.453717	-1.298398	2.278458
H	-3.149461	-1.947322	1.736318
H	-2.725007	-1.339694	3.342564
H	-1.435758	-1.680657	2.165438
C	-3.422474	-0.133176	-1.199342
C	-4.462119	1.002497	-1.236907
H	-4.939341	1.179206	-0.271743

H -5.252522 0.737169 -1.952554
H -4.022246 1.946443 -1.579866
C -4.088371 -1.462530 -0.798434
H -3.353315 -2.272755 -0.717258
H -4.814593 -1.749230 -1.571069
H -4.627480 -1.392815 0.150645
C -2.849147 -0.303042 -2.618530
H -2.295064 0.578453 -2.960809
H -3.679767 -0.458694 -3.320206
H -2.186066 -1.170044 -2.685066
C -0.017826 -2.508878 -0.734966
C 0.306472 -0.331140 -2.398536
N 2.201201 -1.992831 2.645758
N 1.271662 -2.475938 2.120395
O 0.624322 -0.939094 1.520864
C 2.401027 -0.713517 -0.553667
N 4.301784 0.708071 0.052993
H -2.274519 2.696825 0.146193
C 1.973226 5.250328 1.270222
C 6.584320 -0.036286 0.031852
F 3.260641 5.528935 1.014013
F 1.220869 6.231323 0.732196
F 1.802049 5.306059 2.605573
F 7.027193 0.942003 -0.781515
F 6.829262 0.356432 1.294796
F 7.338938 -1.130362 -0.206606

63
complex-3(C10) el energy= -
2035.83106182
Ru -0.719524 -1.191731
-0.350790
H 0.585494 -1.037726
3.683563
P -2.834384 0.064086
-0.019148
O -1.634640 -4.084144
0.004484
O -0.743681 -1.431930
-3.384404
N 0.026154 0.811677
-0.461191
C 2.058064 -2.745999
-0.437261
H 1.548708 -3.704506
-0.502089
C 3.451341 -2.712976
-0.338347
H 4.037426 -3.626249
-0.335214
C 4.082619 -1.470730
-0.231365
C 2.093098 -0.366114
-0.321706
C 1.366915 0.913306
-0.321675
C 1.980526 2.164263
-0.209242
H 3.057103 2.210492
-0.092247
C 1.178198 3.297148
-0.252280
C -0.203900 3.176128
-0.432047
H -0.834625 4.056625
-0.493937
C -0.760430 1.903751
-0.539958
C -2.232005 1.678733
-0.786620
H -2.386965 1.569934
-1.868785
C -3.291461 0.548264
1.769472
C -4.581318 1.373915
1.895659
H -4.550526 2.291240
1.294756
H -4.696982 1.678581
2.944924
H -5.477535 0.808879
1.623281
C -2.125793 1.390441
2.331361
H -1.171050 0.865859
2.248394
H -2.319495 1.572641
3.397476
H -2.054151 2.370712
1.845464

C -3.407104 -0.750543 -0.431545
2.591472
N 3.426577 -0.311862
H -4.233558 -1.385326 -0.221629
2.256167
H -2.818809 2.545281
H -3.595018 -0.492954 -0.464496
3.642721
C 1.780774 4.669358
H -2.478579 -1.322929 -0.062909
2.541465
C 5.586818 -1.354590
C -4.396234 -0.341619 -0.122042
-1.042991
F 3.081721 4.695495
C -5.279149 0.885357 -0.389498
-1.338185
F 1.144708 5.589999
H -5.671850 1.358241 -0.815175
-0.436658
F 1.674036 5.063656
H -6.138025 0.566753 1.221022
-1.944746
F 6.104836 -0.670825
H -4.741112 1.644978 -1.161107
-1.917414
F 5.954732 -0.710290
C -5.205829 -1.426066 0.999707
-0.308391
F 6.176935 -2.568781
H -4.578810 -2.285010 -0.105267
-0.039338

H -6.002281 -1.791155 3
-0.970750
N20 (wB97XD-SMD-BS2) el
H -5.681803 -1.050160 energy= -184.660675320
0.601789
N 0.000000 0.000000
C -3.930488 -0.930332 -1.189063
-2.387650
N 0.000000 0.000000
H -3.286110 -0.245343 -0.074027
-2.950442
O 0.000000 0.000000
H -4.812435 -1.132904 1.103770
-3.010101

H -3.392354 -1.872591 54
-2.251675
complex-1(C4,wB97XD-SMD-BS2)
C -1.285988 -2.997609 el energy= -1512.90072253
-0.113315
Ru -0.351525 -0.711032
C -0.801859 -1.332280 0.018296
-2.239013
H -0.333047 -0.594276
N 0.475583 -2.052069 -1.612997
3.463606
P 1.794896 0.276303
N -0.004246 -2.163586 -0.058936
2.326974
O 0.532943 -3.556320
O -0.283157 -0.991988 -0.408849
1.704926
O -0.886610 -0.997185
C 1.328996 -1.554158 3.040949

N	-2.484978	-0.809791	-1.846437
-0.213152			
N	-0.945204	1.302321	
0.086408			
C	-3.192439	-1.930938	
-0.381117			
H	-2.632020	-2.855308	
-0.373542			
C	-4.560568	-1.925598	
-0.557794			
H	-5.088342	-2.859913	
-0.691244			
C	-5.221728	-0.707661	
-0.561657			
H	-6.294062	-0.661144	
-0.702678			
C	-4.493474	0.452864	
-0.385185			
H	-4.991483	1.411374	
-0.387196			
C	-3.116905	0.382007	
-0.206022			
C	-2.261111	1.575267	
-0.002850			
C	-2.754113	2.853786	
0.098698			
H	-3.810137	3.066185	
0.031505			
C	-1.823392	3.894738	
0.301410			
H	-2.178408	4.915525	
0.384901			
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