Electronic Supplementary Material (ESI) for Dalton Transactions
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P–H Activation of Secondary Phosphanes on a Parent Amido Diiridium Complex

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Supporting Information

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Experimental Section

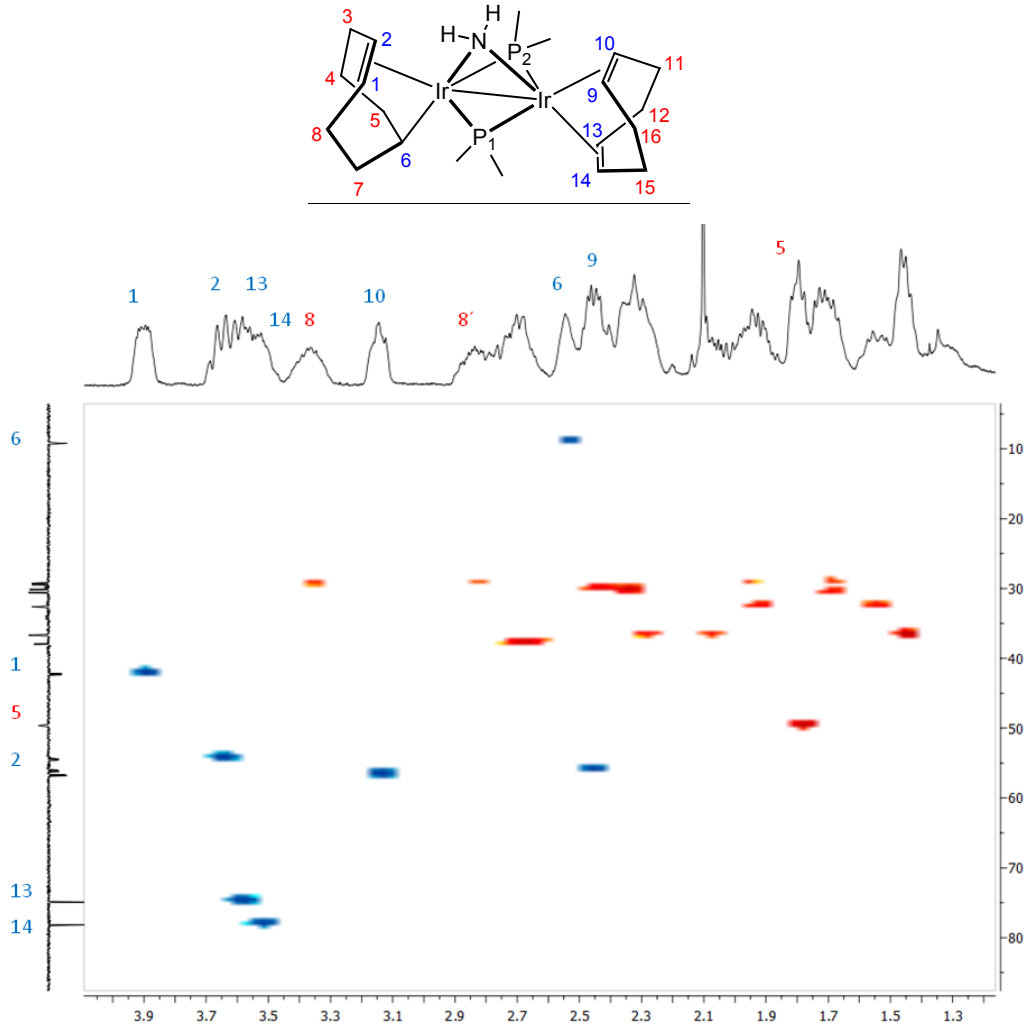
Formation of [{Rh(cod)}$_2$(μ-NH$_2$)(μ-PPh$_2$)]. An NMR tube was charged with [{Rh(μ-NH$_2$)(cod)}$_2$] (16.7 mg, 0.04 mmol), d$_8$-toluene (0.4 mL) and kept at –40 ^{o}C. To this solution, diphenylphosphane (6.4 μL, 0.04 mmol) was added *via* microsyringe and the reaction mixture was allowed to stand for 5 min at this temperature. At this point, multinuclear NMR spectra were recorded, showing the presence of the mixed-bridging complex, [{Rh(μ-NH$_2$)(cod)}$_2$] and [{Rh(μ-PPh$_2$)(cod)}$_2$] in a 1:0.5:0.4 ratio. NMR data of the mixed-bridging complex are as follows. ^{1}H NMR (300 MHz, d$_8$-toluene, 10 ^{o}C): δ 7.81 (m, 4H; H^o PPh$_2$), 7.05 (m, 6H; H^m + H^p PPh$_2$), 4.31 (m, 4H; =CH), 4.26 (m, 4H; =CH) (COD), 2.36 (m, 8H; CH$_2$), 1.91 (m, 8H; CH$_2$) (COD), –0.91 (br d, ^2J(H,Rh) = 6.1 Hz, 2H; NH$_2$); ^{31}P{^{1}H} RMN (121 MHz, d$_8$-toluene, 10 ^{o}C): δ 25.4 (t, ^1J(P,Rh) = 110 Hz); ^{13}C{^{1}H} RMN (75 MHz, C$_6$D$_6$, 10 ^{o}C): δ 139.8 (m, C^{ipso}), 135.6 (m, C^o), 127.7, 127.3 (m, C^m + C^p) (PPh$_2$), 89.0 (m, =CH), 71.1 (d, ^1J(C,Rh) = 11 Hz, =CH), 31.9, 30.6 (s, CH$_2$) (COD); ^{15}N-^{1}H HMQC (40 MHz, d$_8$-toluene, 10 ^{o}C): δ –16.1.

Preparation of [{Ir(μ-ND$_2$)(cod)}$_2$]. A suspension of [{Ir(μ-OMe)(cod)}$_2$] (0.100 g) in diethyl ether was stirred under an atmpsphere of ND$_3$ for 30 minutes, giving rise to the crystallization of a red solid quantitatively. This was islated by filtration *via* cannula and then vacuum-dried.

Catalytic isomerizations of olefins with 3.

An NMR tube was charged with complex **3** (3.3 mg) and dissolved in [D$_8$]toluene (0.4 mL). To this solution, a 100-fold excess of the correponding olefin was added via microsyringe and the mixture was stirred at the required temperature (RT to 60 ^{o}C). Measurements of the ^{1}H NMR spectra of the corresponding catalytic mixtures were carried out to determine the yield and the selectivity.

Figure S1. Selected view of the HSQC of complex **3** at RT in C_6D_6, together with the labelling scheme used.



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DFT calculations

Index

References for the computational study

Complete citation for reference 29:

Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng,

J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1. Comparison between X-ray data and DFT optimized key geometrical parameters of the Ir_2P_2N core for structures **2**, **3** and **7**. Distances in Å.

	2 X-ray	**C** DFT	**3** X-ray	**D** DFT	**7** X-ray	**E'** DFT
Ir1–Ir2	3.2928	3.390	2.6795	2.774	2.60679	2.657
Ir1–P1	2.3764	2.426	2.3321	2.368	2.2808	2.359
Ir1–P2	2.3669	2.439	2.3067	2.362	2.2783	2.359
Ir(2)–P(1)	2.419	2.494	2.3459	2.488	2.2989	2.335
Ir(2)−P(2)	2.3937	2.509	2.3459	2.457	2.2994	2.335
Ir(1)−N	2.175	2.236	2.180	2.277		
Ir(2)−N	2.131	2.167	2.125	2.123		
Ir(1)–H	1.608	1.600				
Ir(1)–C			2.098	2.138		

Figure S2. Computed DFT potential-energy profile (ΔE in kcalmol^{-1}) for the formation of complex **B** from **A** and one molecule of diphenylphosphane.

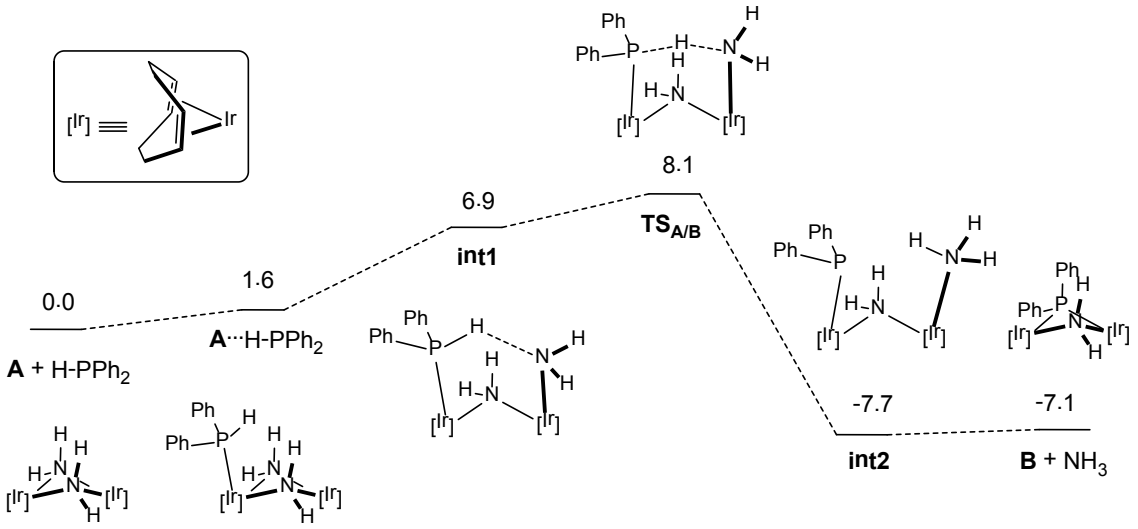

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Figure S3. Molecular structure of the B3LYP geometrically optimized transition structure $\mathbf{TS_{A/B}}$. Key geometrical parameters in Å. Hydrogen atoms are not included for clarity.

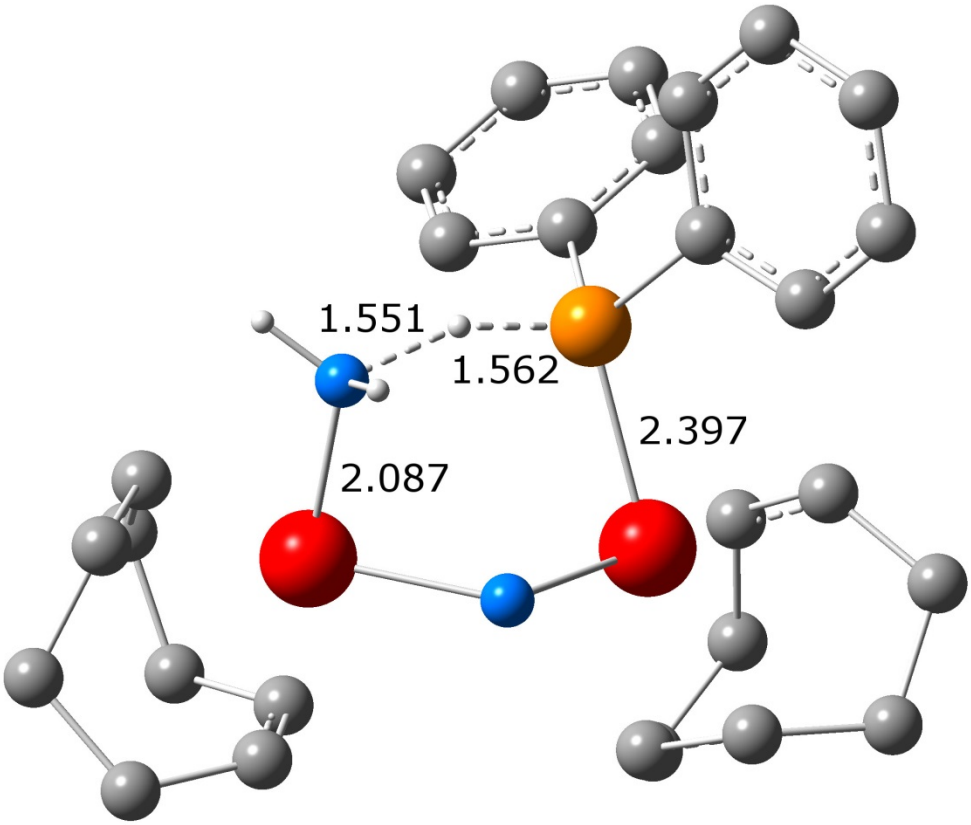

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Figure S4. Molecular structure of the B3LYP geometrically optimized transition structure $\mathbf{TS_{B/C}}$. Key geometrical parameters in Å. Hydrogen atoms and phenyl ligands of bridge phosphane are not included for clarity.

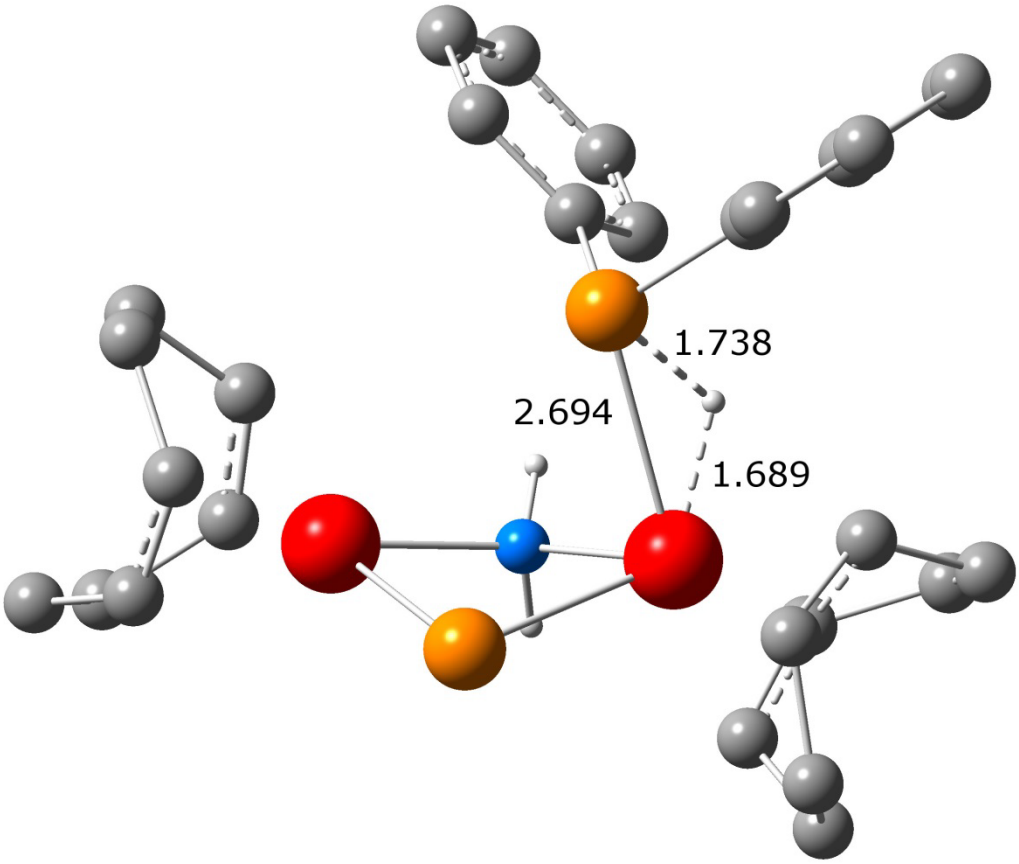

Figure S5. Molecular structure of the B3LYP geometrically optimized transition structure $\mathbf{TS_{C/D}}$. Key geometrical parameters in Å. Hydrogen atoms and phenyl ligands of bridge phosphane are not included for clarity.

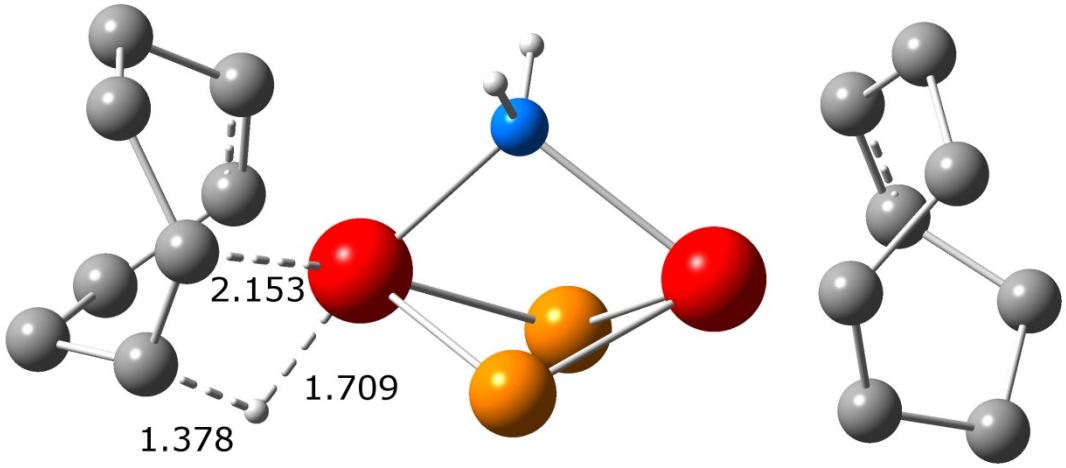

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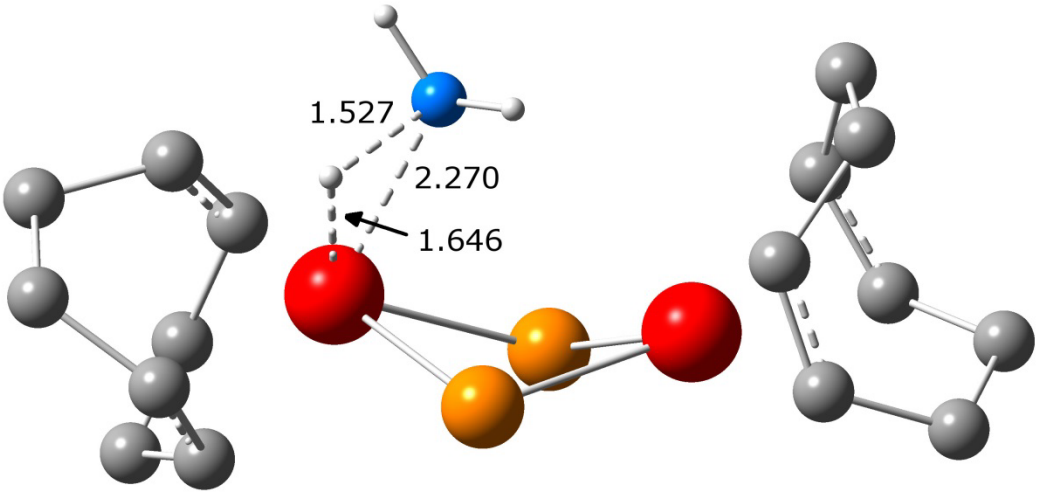
Figure S6. Molecular structure of the B3LYP geometrically optimized transition structure $\mathbf{TS_{C/E}}$. Key geometrical parameters in Å. Hydrogen atoms and phenyl ligands of bridge phosphanes are not included for clarity.



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List of Cartesian coordinates (in Å) and absolute energies (in a.u.) for all calculated structures.

A (E = -944.917520615 a.u.)

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77 -1.502338 -0.376994 0.011055
7 -0.011413 -1.113714 -1.307871
6 3.160252 -0.180813 -1.382542
6 2.325437 0.967266 -1.456732
6 2.626900 2.313295 -0.813455
1 3.369984 2.873890 -1.403293
1 1.701480 2.901251 -0.845627
6 3.090644 2.187974 0.658361
1 4.184395 2.140902 0.712918
1 2.804093 3.094893 1.203266
6 2.483100 0.968904 1.358821
6 3.105465 -0.308519 1.408035
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1 4.522334 -1.763772 0.792557
1 5.280362 -0.279368 1.355770
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6 0.485408 -2.665717 0.867834
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1 3.086720 -3.578580 -0.551546
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1 5.016605 -0.139887 -3.570129
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$TS_{A/B}$ (E = -1750.13700521 a.u.)

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1 2.460998 -3.298330 5.062372

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1 3.641759 -3.394105 2.100578
6 1.484706 -3.245698 2.446006
1 1.425465 -4.278092 2.083405
1 1.392622 -3.306904 3.536936
6 -4.002882 -0.482277 -1.638346
6 -4.091606 0.934814 -1.657335
6 -5.147470 1.734325 -0.890942
1 -6.063384 1.141781 -0.790524
1 -5.425566 2.619127 -1.474571
6 -4.634396 2.179348 0.497828
1 -4.118436 3.141688 0.396337
1 -5.476810 2.350529 1.186199
6 -3.640239 1.198557 1.098444
6 -3.795778 -0.212585 1.153040
6 -5.037159 -0.955218 0.650415
1 -5.210043 -1.833393 1.282532
1 -5.922360 -0.320690 0.770964
6 -4.892457 -1.408557 -0.822055
1 -4.434011 -2.404707 -0.844489
1 -5.883097 -1.515170 -1.291143
1 -3.246592 -0.732404 1.940192
1 -0.280478 -1.923954 2.648660
1 -1.355868 -2.378861 0.550220
1 3.655653 -1.179811 0.639783
1 -3.576521 -0.962815 -2.523171
1 -3.703228 1.439613 -2.544657
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1 -1.459518 0.466923 -2.999787
1 -0.693468 -0.727572 -2.141988
1 2.699033 -2.006474 -1.377919
15 1.861923 1.000633 -0.705773
1 -0.207722 0.803583 -1.937022
7 -0.732514 0.347266 0.878019
1 -0.413995 1.318417 0.921838
1 -1.041989 0.140460 1.830339
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6 2.049674 2.276724 1.869999
6 1.778754 3.742923 -0.023891
6 2.044793 3.381778 2.726367
1 2.155963 1.274433 2.276968
6 1.783350 4.849244 0.827920
1 1.668197 3.890174 -1.095334
6 1.912468 4.671287 2.207768
1 2.151415 3.233796 3.798572
1 1.679598 5.849856 0.415197
1 1.910283 5.531193 2.872793
6 3.624929 0.854312 -1.238285
6 4.717422 1.362691 -0.511833
6 3.897239 0.203546 -2.457352
6 6.024150 1.220964 -0.983406
1 4.544319 1.881637 0.426502
6 5.203455 0.048740 -2.922498
1 3.069162 -0.169444 -3.057213
6 6.275651 0.559945 -2.187511
1 6.849626 1.628305 -0.404028
1 5.382479 -0.458680 -3.867632
1 7.293571 0.450649 -2.552429

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77 1.596991 -0.552482 -0.279106
15 -0.026859 1.167001 0.146709
7 0.044615 -0.924653 -1.690932
6 -2.982176 -2.010413 -1.271474
6 -2.138660 -2.688184 -0.362541
6 -2.516102 -3.112046 1.046608
1 -3.113094 -4.038443 1.029498
1 -1.582541 -3.355016 1.568067
6 -3.256368 -2.007178 1.837081
1 -4.340299 -2.101951 1.704971
1 -3.074704 -2.155625 2.908083
6 -2.799335 -0.599357 1.443699
6 -3.418341 0.188138 0.434895

6 -4.601690 -0.236718 -0.420450
1 -4.676684 0.475397 -1.252137
1 -5.545033 -0.152538 0.142844
6 -4.443586 -1.662414 -0.998360
1 -4.883147 -2.401611 -0.319819
1 -5.011213 -1.739062 -1.933081
6 3.012900 -1.838510 -1.321920
6 2.397092 -2.601848 -0.303891
6 3.079132 -2.971713 1.012232
1 4.158017 -3.074626 0.850363
1 2.728306 -3.959763 1.332164
6 2.799297 -1.945063 2.136128
1 1.874875 -2.231209 2.653054
1 3.599619 -1.983210 2.893066
6 2.605644 -0.526436 1.622319
6 3.426970 0.118334 0.658626
6 4.692774 -0.503384 0.061370
1 5.431984 0.286186 -0.117777
1 5.153574 -1.182473 0.787745
6 4.409323 -1.242956 -1.265923
1 4.488891 -0.529538 -2.095083
1 5.173518 -2.015551 -1.448356
1 3.432720 1.208060 0.687423
1 -2.715412 -2.076806 -2.326809
1 -1.309505 -3.259796 -0.784585
1 -3.340311 1.269953 0.556635
1 2.636949 -1.979984 -2.336925
1 1.585245 -3.264877 -0.604940
1 2.084177 0.119532 2.326617
1 0.064318 -1.821062 -2.179444
1 0.051123 -0.197202 -2.408609
1 -2.302272 -0.049678 2.239786
6 -0.099816 2.147584 1.701322
6 -0.123575 3.552098 1.725031
6 -0.143091 1.459856 2.929894
6 -0.186556 4.244519 2.936710
1 -0.092572 4.109182 0.793995
6 -0.205874 2.153463 4.138295
1 -0.128170 0.373335 2.934682
6 -0.227588 3.550577 4.146833
1 -0.203983 5.331535 2.931173
1 -0.237905 1.601387 5.074222
1 -0.276596 4.091775 5.087865
6 0.029111 2.431119 -1.201859
6 1.250988 2.999046 -1.606508
6 -1.146191 2.834124 -1.859999
6 1.295060 3.942102 -2.635064
1 2.169944 2.691381 -1.116159
6 -1.101069 3.774066 -2.893005
1 -2.096031 2.399908 -1.562366
6 0.119086 4.329429 -3.282373
1 2.248761 4.368750 -2.935364
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1 0.154609 5.059018 -4.087260

B$^{\bullet+\bullet}$ H-PPh_2 (E = -2498.85306928 a.u.)

77 0.917574 -0.965346 -0.835853
77 -1.750108 1.255103 -0.223208
15 -1.200120 -0.986739 0.488750
7 -0.285597 0.631678 -1.656733
6 0.584560 -2.072199 -2.640844
6 1.766553 -1.237551 -2.789654
6 3.184603 -1.793063 -2.805591
1 3.397678 -2.331755 -3.744424
1 3.878858 -0.942428 -2.781627
6 3.463046 -2.701989 -1.589497
1 3.328894 -3.755957 -1.859851
1 4.512569 -2.604002 -1.287434
6 2.578609 -2.375576 -0.380423
6 1.349037 -3.016034 -0.116132
6 0.700737 -4.042572 -1.034598
1 -0.325789 -4.191314 -0.688295
1 1.210880 -5.014186 -0.923896
6 0.662893 -3.598466 -2.511149
1 1.534921 -3.980599 -3.056999
1 -0.210811 -4.048839 -2.995836
6 -2.525787 2.838238 -1.510650
6 -1.583098 3.426814 -0.644526
6 -1.953826 4.273182 0.570510
1 -2.896726 4.798891 0.383529
1 -1.197049 5.054830 0.705315
6 -2.053743 3.434691 1.867407
1 -1.057371 3.367629 2.322056
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1 -5.544025 2.230935 0.027042
1 -4.598119 3.566062 0.642974
6 -4.035602 2.921582 -1.368686
1 -4.467990 2.175721 -2.046741
1 -4.406638 3.901041 -1.710800
1 -4.096321 0.680735 1.019951
1 -0.308295 -1.729649 -3.169881
1 1.646007 -0.356881 -3.427917
1 1.062957 -3.112056 0.928777
1 -2.189110 2.615291 -2.525434
1 -0.582062 3.599301 -1.038503
1 -2.273181 1.327260 2.439668
1 0.286802 1.410117 -1.986421
1 -0.745011 0.259088 -2.489507
1 3.124950 -2.018397 0.487897
15 1.980355 0.711653 0.510637
6 -1.206228 -1.290149 2.316717
6 0.000106 -1.415675 3.023661
6 -2.407060 -1.349307 3.050113
6 0.012892 -1.586321 4.411384
1 0.938129 -1.388073 2.477421
6 -2.397584 -1.523783 4.434208
1 -3.357891 -1.265829 2.530774
6 -1.186253 -1.640748 5.122050
1 0.961891 -1.688257 4.932565
1 -3.338533 -1.566730 4.977263
1 -1.179880 -1.778235 6.200133
6 -2.464082 -2.206613 -0.099238
6 -2.611558 -3.477537 0.486607
6 -3.266464 -1.901346 -1.214482
6 -3.520763 -4.405651 -0.024910
1 -2.018151 -3.742885 1.357019
6 -4.166607 -2.833708 -1.734003
1 -3.193519 -0.912615 -1.661102
6 -4.298946 -4.091430 -1.141433
1 -3.618053 -5.378703 0.450709
1 -4.775533 -2.570245 -2.595653
1 -5.005719 -4.814868 -1.539254
6 3.547381 0.378684 1.436526

6 3.532426 0.235963 2.832418
6 4.765228 0.221741 0.755671
6 4.705720 -0.062663 3.529827
1 2.602943 0.366013 3.380985
6 5.937708 -0.067510 1.453617
1 4.798416 0.335484 -0.324764
6 5.910807 -0.214618 2.843036
1 4.676909 -0.166703 4.611404
1 6.873401 -0.178610 0.911901
1 6.824242 -0.442209 3.385721
6 2.381518 2.303678 -0.346040
6 2.296056 3.535265 0.322549
6 2.790266 2.288536 -1.687723
6 2.617721 4.723503 -0.334744
1 1.979431 3.564588 1.362108
6 3.118990 3.478019 -2.344377
1 2.839464 1.339144 -2.214411
6 3.031721 4.696782 -1.669783
1 2.546766 5.670048 0.194779
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1 3.281978 5.622676 -2.180673
1 1.269299 1.275628 1.599819

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77 0.932870 -1.027387 -0.789043
77 -1.685422 1.276537 -0.240458
15 -1.247961 -0.967350 0.521537
7 -0.218907 0.573993 -1.641687
6 0.352711 -2.342200 -2.386258
6 1.516048 -1.586396 -2.786283
6 2.918973 -2.165826 -2.887513
1 3.020564 -2.803879 -3.780752
1 3.613823 -1.328940 -3.027683
6 3.320037 -2.945336 -1.618854
1 3.110945 -4.013779 -1.743112
1 4.402389 -2.866677 -1.465636
6 2.614968 -2.434055 -0.359844
6 1.427045 -2.989575 0.148389
6 0.654700 -4.101386 -0.544869
1 -0.310450 -4.199930 -0.043365
1 1.179014 -5.059851 -0.400646
6 0.402177 -3.837085 -2.047481
1 1.164663 -4.330977 -2.662458
1 -0.552049 -4.295239 -2.328279
6 -2.398656 2.857469 -1.567813
6 -1.445594 3.431937 -0.703442
6 -1.797047 4.312215 0.492708
1 -2.717070 4.870431 0.285938
1 -1.010597 5.064710 0.620433
6 -1.940319 3.502496 1.804409
1 -0.953828 3.412758 2.274826
1 -2.575314 4.048604 2.520906
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1 -5.448570 2.378256 -0.047347
1 -4.463050 3.692007 0.552455
6 -3.906328 2.992892 -1.441753
1 -4.358161 2.250392 -2.110863
1 -4.240743 3.978271 -1.804066
1 -4.060983 0.799584 0.987640
1 -0.597925 -2.025375 -2.817623
1 1.337628 -0.766122 -3.485443
1 1.267602 -2.928511 1.222178
1 -2.061121 2.607720 -2.576375
1 -0.434959 3.561182 -1.088703
1 -2.225131 1.411248 2.407873
1 0.384176 1.335908 -1.954437
1 -0.677794 0.225228 -2.485476
1 3.264153 -1.940692 0.356967
15 2.017721 0.856098 0.802463
1 2.244149 0.034694 -0.713016
6 3.755107 0.392818 1.297306
6 3.917043 -0.213505 2.555428
6 4.905434 0.623638 0.522584
6 5.178909 -0.595347 3.017283
1 3.045142 -0.376170 3.184746
6 6.168316 0.253056 0.986650
1 4.815651 1.106139 -0.446510
6 6.309694 -0.362921 2.233201
1 5.277810 -1.063398 3.993490
1 7.044836 0.445386 0.372555
1 7.293961 -0.652041 2.592004
6 2.335520 2.410882 -0.181915
6 2.208989 3.626262 0.513982
6 2.673834 2.466090 -1.545398
6 2.427529 4.849661 -0.122180
1 1.933083 3.608323 1.565524
6 2.879471 3.690219 -2.189497
1 2.785230 1.543024 -2.110204
6 2.758980 4.885765 -1.478986
1 2.332148 5.775246 0.439961
1 3.140782 3.706812 -3.244888
1 2.920835 5.837518 -1.977947
6 -1.354416 -1.260198 2.344166
6 -0.193815 -1.239143 3.134442
6 -2.592173 -1.428257 2.993918
6 -0.262764 -1.386040 4.522006
1 0.768086 -1.088290 2.656915
6 -2.661629 -1.580518 4.379221
1 -3.507831 -1.449702 2.410274
6 -1.496511 -1.560918 5.150040
1 0.650834 -1.366104 5.111329
1 -3.629364 -1.711763 4.857074
1 -1.551260 -1.679653 6.228956
6 -2.518377 -2.138461 -0.147693
6 -2.741079 -3.411894 0.408719
6 -3.256999 -1.786973 -1.293292
6 -3.654944 -4.299412 -0.162399
1 -2.208743 -3.708310 1.307870
6 -4.161125 -2.679589 -1.873321
1 -3.136062 -0.790182 -1.711156
6 -4.364259 -3.941617 -1.311446
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1 -4.719351 -2.379874 -2.757106
1 -5.075161 -4.633350 -1.755484

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77 0.992634 -0.752950 -0.878917
77 -1.910393 1.142509 0.003206
15 -0.982732 -1.037021 0.485328
7 -0.326481 0.976536 -1.434663
6 0.793918 -2.690663 -2.113925
6 0.011675 -1.712227 -2.729255

6 0.402639 -0.947099 -3.980581
1 0.254746 -1.585790 -4.865723
1 -0.299694 -0.114725 -4.109368
6 1.845901 -0.396721 -3.957432
1 2.528651 -1.113990 -4.426987
1 1.893556 0.505484 -4.577745
6 2.363067 -0.055280 -2.560176
6 3.072456 -0.957621 -1.760477
6 3.359455 -2.404073 -2.121949
1 3.726893 -2.903955 -1.219483
1 4.182590 -2.447487 -2.852557
6 2.133689 -3.177690 -2.661127
1 2.108662 -3.132212 -3.755893
1 2.245980 -4.238362 -2.409763
6 -3.050767 2.525831 -1.228456
6 -2.289347 3.301313 -0.328801
6 -2.854106 3.983597 0.914236
1 -3.894590 4.278502 0.737634
1 -2.305517 4.916083 1.090770
6 -2.750476 3.090689 2.174681
1 -1.770857 3.248353 2.641327
1 -3.500825 3.396977 2.921274
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6 -3.832715 1.010907 1.024667
6 -4.945789 1.786246 0.317130
1 -5.838436 1.153447 0.250479
1 -5.239666 2.653847 0.918025
6 -4.535558 2.231459 -1.106001
1 -4.769976 1.427213 -1.814187
1 -5.130290 3.103362 -1.422424
1 -4.064966 -0.037881 1.203172
1 0.275758 -3.383681 -1.459169
1 -1.055268 -1.737379 -2.524857
1 3.750446 -0.542277 -1.021484
1 -2.669013 2.444769 -2.248729
1 -1.372234 3.739355 -0.721716
1 -2.433797 0.974052 2.650922
1 0.201231 1.848770 -1.489009
1 -0.722574 0.843815 -2.363762
1 2.521030 0.999786 -2.361589
15 1.812101 0.779357 0.895962
1 1.691049 -1.902700 -0.010391
6 3.389479 0.171031 1.685082
6 4.069523 1.082147 2.522846
6 3.882767 -1.144375 1.640587
6 5.190197 0.702689 3.257155
1 3.710489 2.105178 2.599697
6 4.999058 -1.533273 2.390064
1 3.390156 -1.880066 1.013376
6 5.663029 -0.612351 3.197354
1 5.691310 1.433881 3.887084
1 5.351300 -2.560691 2.329954
1 6.534021 -0.911245 3.774698
6 2.483884 2.281051 0.016735
6 1.622158 3.385817 -0.125483
6 3.789491 2.409396 -0.496945
6 2.027970 4.549948 -0.784242
1 0.628313 3.332291 0.310602
6 4.201934 3.574972 -1.144967
1 4.498341 1.595766 -0.374396
6 3.320434 4.648317 -1.301229
1 1.339256 5.386944 -0.874800
1 5.217066 3.645029 -1.529081
1 3.643834 5.555202 -1.805467
6 -0.793589 -1.549705 2.254906
6 -1.951362 -1.684548 3.044467
6 0.447980 -1.798479 2.852459
6 -1.864747 -2.048002 4.387947
1 -2.929809 -1.516766 2.603056
6 0.536813 -2.158329 4.200351
1 1.354114 -1.714576 2.266784
6 -0.617277 -2.282660 4.972850
1 -2.772508 -2.147739 4.977773
1 1.514215 -2.339312 4.639942
1 -0.548731 -2.562487 6.020854
6 -2.071215 -2.416194 -0.121568
6 -3.153260 -2.148056 -0.976821
6 -1.824157 -3.752806 0.239675
6 -3.958251 -3.182283 -1.462707
1 -3.363905 -1.115468 -1.246452
6 -2.631159 -4.785190 -0.240651
1 -1.004878 -3.984997 0.914995
6 -3.700366 -4.503877 -1.095752
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1 -2.426526 -5.810731 0.056626
1 -4.330080 -5.308351 -1.466506

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77 -0.188623 -1.641517 -0.318963
77 0.199707 1.709658 -0.655806
15 -1.527913 0.252268 0.435196
15 1.521279 -0.097257 0.442745
7 -0.008577 -0.059555 -1.889527
6 -0.348994 2.980093 -2.271641
6 1.104659 2.865895 -2.202010
6 2.000823 4.015844 -1.718649
1 1.549109 4.983534 -1.972226
1 2.956767 3.989026 -2.255929
6 2.272833 3.924186 -0.201118
1 3.174977 3.321002 -0.042178
1 2.488710 4.918582 0.224654
6 1.141346 3.254545 0.568969
6 -0.229283 3.578359 0.428650
6 -0.740421 4.715714 -0.462099
1 -1.610834 5.177699 0.019457
1 0.021152 5.502674 -0.517039
6 -1.121172 4.232612 -1.876716
1 -2.190063 3.984106 -1.890184
1 -0.986501 5.043946 -2.612233
1 -0.858729 3.349114 1.283575
1 -0.813718 2.447653 -3.108972
1 1.556144 2.265517 -2.996542
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1 0.790182 -0.182839 -2.509363
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1 -0.295773 -2.275211 1.146467
6 1.109549 -3.507759 -0.339626
6 1.102313 -2.992812 -1.639509
6 0.316446 -3.615399 -2.792274
1 0.250010 -4.698694 -2.642733
1 0.885292 -3.479432 -3.719132
6 -1.093358 -3.013461 -2.976128
1 -1.023346 -2.137887 -3.631769
1 -1.747294 -3.727469 -3.501730
6 -1.751713 -2.568984 -1.682491

6 -1.769504 -3.291626 -0.485854
6 -1.177398 -4.690382 -0.318861
1 -1.775425 -5.235798 0.419942
1 -1.293573 -5.240445 -1.259369
6 0.303382 -4.706046 0.130469
1 0.342519 -4.719308 1.225054
1 0.787660 -5.635679 -0.207533
1 -2.544061 -3.024673 0.227251
1 1.972213 -3.275624 0.278272
1 1.953115 -2.379386 -1.923992
1 -2.524270 -1.815486 -1.806517
6 1.983128 -0.105844 2.232996
6 2.957645 0.816970 2.663454
6 1.407187 -0.950382 3.191912
6 3.334310 0.892489 4.003483
1 3.436565 1.470602 1.939204
6 1.779714 -0.871166 4.537000
1 0.663238 -1.674850 2.883138
6 2.742349 0.049815 4.948467
1 4.089637 1.611653 4.310255
1 1.315235 -1.535514 5.261514
1 3.032315 0.110541 5.994134
6 3.167902 -0.516162 -0.311342
6 4.038776 -1.458669 0.266410
6 3.563534 0.102320 -1.509101
6 5.252294 -1.782145 -0.342286
1 3.776433 -1.926910 1.211278
6 4.775455 -0.226555 -2.123179
1 2.925429 0.868924 -1.938218
6 5.622878 -1.172221 -1.543865
1 5.911513 -2.509366 0.125510
1 5.063131 0.270325 -3.046617
1 6.569129 -1.423368 -2.015785
6 -2.058771 0.250020 2.211514
6 -2.533957 1.458126 2.754150
6 -2.074299 -0.890073 3.028940
6 -2.994837 1.525847 4.068841
1 -2.557081 2.350364 2.135358
6 -2.536605 -0.825091 4.346292
1 -1.723314 -1.836577 2.630169
6 -2.994970 0.383107 4.871915
1 -3.354581 2.471905 4.465412
1 -2.540641 -1.723021 4.959758
1 -3.352430 0.434348 5.897012
6 -3.205082 0.231026 -0.371213
6 -3.407655 0.971525 -1.547523
6 -4.281947 -0.520737 0.132728
6 -4.636741 0.945947 -2.212569
1 -2.594588 1.587925 -1.919190
6 -5.511954 -0.541255 -0.526904
1 -4.165254 -1.078717 1.057705
6 -5.692968 0.187153 -1.705941
1 -4.771189 1.532006 -3.118618
1 -6.332503 -1.124772 -0.116374
1 -6.652023 0.171396 -2.217020

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77 0.734843 1.545416 -0.453167
77 -0.635989 -1.617577 -0.602096
15 1.315828 -0.643908 0.400814
15 -1.438745 0.565460 0.254889
7 0.235459 0.107694 -1.971555
6 -0.669720 -3.444036 0.454230
6 0.047738 -3.648152 -0.800479
6 -0.558002 -4.416153 -1.984574
1 -1.209165 -5.226258 -1.630007
1 0.243151 -4.913247 -2.545863
6 -1.328024 -3.478553 -2.940465
1 -0.627704 -3.089957 -3.690712
1 -2.102733 -4.028868 -3.501194
6 -1.939140 -2.275183 -2.233391
6 -2.711176 -2.338874 -1.054860
6 -3.072399 -3.645722 -0.351746
1 -4.073476 -3.547737 0.085261
1 -3.145851 -4.450703 -1.092071
6 -2.052734 -4.014450 0.745701
1 -2.391920 -3.594173 1.701642
1 -2.016761 -5.107557 0.890045
1 -3.390351 -1.510386 -0.870553
1 -0.044315 -3.424898 1.350288
1 1.125578 -3.783320 -0.705572
1 -2.112769 -1.416141 -2.884094
1 -0.449605 0.454703 -2.638941
1 1.058254 -0.138393 -2.520853
1 1.175770 2.388790 0.966818
6 -0.165400 3.630433 -0.833596
6 0.422185 3.194666 -2.021102
6 1.732987 3.742050 -2.579037
1 1.836806 4.794075 -2.288703
1 1.674637 3.743082 -3.673547
6 2.960777 2.926894 -2.125032
1 3.156880 2.142071 -2.865125
1 3.861877 3.563079 -2.114823
6 2.751602 2.217729 -0.793597
6 2.334590 2.915613 0.438102
6 1.962257 4.411101 0.426707
1 2.186163 4.844197 1.408099
1 2.608331 4.929191 -0.288648
6 0.466769 4.647150 0.108278
1 -0.097201 4.622053 1.047858
1 0.328063 5.658839 -0.302236
1 2.903257 2.613525 1.321345
1 -1.240647 3.519907 -0.729137
1 -0.236609 2.733180 -2.752211
1 3.503734 1.450054 -0.620548
6 2.936630 -1.196299 -0.316620
6 4.158212 -0.927088 0.326880
6 2.973090 -1.840839 -1.564841
6 5.373025 -1.286708 -0.259312
1 4.161772 -0.445514 1.300565
6 4.189816 -2.192365 -2.155206
1 2.038128 -2.092518 -2.055568
6 5.394102 -1.917318 -1.505638
1 6.303918 -1.073685 0.260334
1 4.192752 -2.696651 -3.118432
1 6.339902 -2.199113 -1.960779
6 1.641416 -0.825006 2.209565
6 2.104428 -2.060905 2.700331
6 1.403002 0.207303 3.127889
6 2.325992 -2.250910 4.063967
1 2.304928 -2.875683 2.010287
6 1.622862 0.016164 4.494663
1 1.019672 1.159122 2.777256
6 2.086822 -1.211348 4.966882
1 2.685297 -3.212709 4.420966

1 1.422929 0.829084 5.187670
1 2.259305 -1.359893 6.029629
6 -1.827965 0.738832 2.057041
6 -2.072220 -0.399579 2.837888
6 -1.882541 1.999080 2.678491
6 -2.361181 -0.285285 4.201361
1 -2.017487 -1.376592 2.366914
6 -2.173223 2.116720 4.037625
1 -1.697564 2.894261 2.089631
6 -2.412741 0.971482 4.804311
1 -2.542663 -1.180622 4.790711
1 -2.213430 3.100247 4.500184
1 -2.637448 1.061717 5.864088
6 -2.980292 1.270039 -0.502234
6 -4.196623 1.332077 0.205713
6 -3.001338 1.676158 -1.851117
6 -5.368564 1.785280 -0.403732
1 -4.229484 1.023081 1.245201
6 -4.171264 2.127884 -2.462464
1 -2.089596 1.643987 -2.438456
6 -5.364844 2.187575 -1.740226
1 -6.289575 1.820917 0.173217
1 -4.147196 2.436822 -3.504814
1 -6.277235 2.541163 -2.212670

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77 0.000424 1.335822 -0.255432
77 0.071975 -1.434958 -0.357710
15 1.968265 0.069364 0.063337
15 -1.931517 -0.007644 0.014297
7 0.053645 -0.107980 -2.015121
6 0.782820 3.173473 -1.049304
6 -0.644251 3.126229 -1.252428
6 -1.681652 4.070064 -0.661254
1 -1.702435 4.982088 -1.282508
1 -2.664437 3.603101 -0.802246
6 -1.542305 4.490852 0.811040
1 -0.757162 5.247885 0.913489
1 -2.472660 4.994963 1.109212
6 -1.262471 3.337200 1.782537
1 -2.124550 2.659014 1.793567
1 -1.203896 3.771222 2.796468
6 0.027992 2.538563 1.512194
6 1.266883 3.461347 1.424400
1 2.153616 2.862083 1.661596
1 1.224496 4.264887 2.178975
6 1.454231 4.052586 0.004995
1 1.066468 5.078059 -0.056865
1 2.524613 4.132680 -0.224657
6 0.814175 -3.136094 -1.447770
6 -0.621170 -3.226816 -1.354490
6 -1.348319 -4.235243 -0.458023
1 -0.775094 -5.169656 -0.408201
1 -2.304527 -4.501490 -0.923260
6 -1.620663 -3.687954 0.962008
1 -2.610892 -3.221204 0.984245
1 -1.653911 -4.509388 1.695948
6 -0.613241 -2.642155 1.414872
6 0.776492 -2.790618 1.325073
6 1.458078 -4.066069 0.830559
1 2.385364 -4.206647 1.397346
1 0.824836 -4.927672 1.070708
6 1.771601 -4.033602 -0.678404
1 2.790006 -3.654177 -0.821329
1 1.765947 -5.054357 -1.094577
1 1.376441 -2.180912 1.991588
1 1.393485 2.965899 -1.929180
1 -0.940481 2.812848 -2.256950
1 0.175181 1.889086 2.385422
1 1.193430 -2.831535 -2.425138
1 -1.147720 -2.991176 -2.277966
1 -0.986353 -1.952281 2.166296
1 -0.756775 -0.189298 -2.625958
1 0.889573 -0.142932 -2.595160
6 -2.960327 -0.205922 1.527551
6 -4.270440 -0.718326 1.493563
6 -2.401370 0.104889 2.781206
6 -4.996056 -0.903322 2.671535
1 -4.728689 -0.969539 0.542487
6 -3.128548 -0.079391 3.957524
1 -1.394936 0.507331 2.828291
6 -4.429946 -0.583862 3.907522
1 -6.007653 -1.298161 2.621008
1 -2.678975 0.178022 4.913129
1 -4.998276 -0.725053 4.822920
6 -3.216082 0.057527 -1.315431
6 -4.115231 1.140880 -1.337431
6 -3.320132 -0.908553 -2.326984
6 -5.077604 1.253653 -2.339429
1 -4.063617 1.896844 -0.559446
6 -4.277879 -0.790249 -3.339842
1 -2.654415 -1.762414 -2.313848
6 -5.158476 0.290424 -3.349879
1 -5.762796 2.097458 -2.334418
1 -4.337463 -1.550970 -4.114310
1 -5.904766 0.382146 -4.134470
6 2.977473 -0.025047 1.598840
6 4.378855 -0.148585 1.594520
6 2.319114 0.010643 2.844161
6 5.093664 -0.223613 2.791241
1 4.916416 -0.183343 0.652945
6 3.035425 -0.063389 4.038337
1 1.238534 0.105479 2.875540
6 4.427353 -0.179669 4.017234
1 6.176401 -0.316334 2.762478
1 2.504656 -0.027306 4.986222
1 4.986439 -0.235596 4.947334
6 3.251739 0.205349 -1.261442
6 3.604834 -0.873648 -2.086315
6 3.896972 1.438857 -1.465713
6 4.565537 -0.724079 -3.091318
1 3.129523 -1.835671 -1.938423
6 4.862740 1.586374 -2.461397
1 3.641596 2.284579 -0.835228
6 5.196461 0.505306 -3.281811
1 4.822601 -1.572784 -3.720241
1 5.350304 2.547869 -2.600430
1 5.943432 0.621865 -4.062531

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77 -1.607193 -0.922374 -0.140019
15 -0.788545 1.350914 -0.000978
6 2.498960 2.612303 0.899113

6 2.472761 1.359600 1.527832
6 3.687659 0.460392 1.690172
1 4.332171 0.854914 2.492524
1 3.337618 -0.514864 2.037268
6 4.514672 0.271840 0.396457
1 5.343831 0.988480 0.364955
1 4.982835 -0.719110 0.418029
6 3.699959 0.395633 -0.889408
6 3.522034 1.602045 -1.576913
6 4.056544 2.950412 -1.129555
1 3.581122 3.716993 -1.750818
1 5.137554 3.011408 -1.332143
6 3.774846 3.260923 0.357305
1 4.623380 2.949718 0.977248
1 3.694942 4.346568 0.484590
6 -2.260193 -2.741676 0.867117
6 -2.248545 -3.025715 -0.515227
6 -3.499449 -3.097793 -1.388123
1 -4.347832 -3.468446 -0.801335
1 -3.340622 -3.838636 -2.180642
6 -3.847418 -1.737545 -2.038420
1 -3.279816 -1.635210 -2.971192
1 -4.912173 -1.709275 -2.321808
6 -3.499226 -0.540231 -1.171720
6 -3.762215 -0.412478 0.204625
6 -4.477928 -1.463042 1.047268
1 -5.052132 -0.959792 1.833884
1 -5.212831 -1.995437 0.433768
6 -3.498172 -2.466662 1.701828
1 -3.161577 -2.064079 2.664778
1 -4.019131 -3.410413 1.931210
1 -3.791921 0.599106 0.605356
1 1.718848 3.308885 1.181168
1 1.693807 1.210300 2.268939
1 3.294177 1.535698 -2.638668
1 -1.418042 -3.110160 1.451579
1 -1.393274 -3.583412 -0.889640
1 -3.359395 0.382606 -1.733123
1 3.590339 -0.517223 -1.468533
1 1.367955 2.578977 -1.221937
1 0.943420 1.196762 -3.064663
1 1.474188 -0.289708 -2.723995
7 0.828124 0.432184 -2.396304
15 0.790561 -1.269098 0.051574
6 -1.736646 2.543746 -1.070251
6 -2.592625 3.533620 -0.558482
6 -1.681266 2.379037 -2.468675
6 -3.333857 4.356227 -1.413027
1 -2.690901 3.673738 0.511897
6 -2.418583 3.203735 -3.317955
1 -1.071276 1.579389 -2.875083
6 -3.244520 4.202960 -2.795605
1 -3.983899 5.117333 -0.988228
1 -2.353836 3.057366 -4.393556
1 -3.819287 4.844522 -3.458469
6 -1.037256 2.051357 1.701158
6 -0.686744 3.377439 2.018560
6 -1.550354 1.243265 2.729102
6 -0.837967 3.872930 3.314560
1 -0.314690 4.037403 1.239754
6 -1.694472 1.735163 4.030211
1 -1.834920 0.220667 2.494482
6 -1.338168 3.050608 4.327841
1 -0.565479 4.902623 3.532307
1 -2.092769 1.088304 4.808114
1 -1.453510 3.435728 5.337584
6 1.486550 -2.437042 -1.206604
6 2.790931 -2.956899 -1.094714
6 0.755349 -2.742229 -2.367819
6 3.331166 -3.772782 -2.089922
1 3.387862 -2.732447 -0.214863
6 1.301167 -3.548167 -3.371324
1 -0.238492 -2.324387 -2.484025
6 2.586830 -4.072376 -3.234096
1 4.336597 -4.169722 -1.973128
1 0.715590 -3.765893 -4.261106
1 3.008132 -4.704784 -4.011093
6 1.133021 -2.133542 1.665502
6 1.484917 -3.492763 1.760144
6 0.910017 -1.439142 2.870293
6 1.636089 -4.117416 3.001740
1 1.637360 -4.079035 0.861208
6 1.062686 -2.060831 4.109279
1 0.592495 -0.403455 2.843075
6 1.433548 -3.405657 4.183658
1 1.909983 -5.169061 3.037831
1 0.887612 -1.490370 5.018188
1 1.554212 -3.891757 5.148023

$TS_{C/E}$ (E = -2498.79743092 a.u.)

77 0.938077 -1.514392 -0.755569
77 -1.073837 1.516249 -0.218694
15 1.247023 0.884271 0.195186
6 1.549078 -2.820169 0.832758
6 0.757469 -3.559477 -0.122366
6 1.312737 -4.572770 -1.113690
1 1.554258 -5.522002 -0.606723
1 0.514993 -4.803338 -1.830291
6 2.539058 -4.042469 -1.882757
1 3.466730 -4.332770 -1.378055
1 2.581125 -4.506148 -2.875426
6 2.505645 -2.525665 -2.051795
6 3.150887 -1.620756 -1.197336
6 3.879221 -2.027988 0.072824
1 4.085177 -1.112535 0.636493
1 4.861548 -2.458977 -0.179666
6 3.071020 -3.004823 0.959637
1 3.338148 -4.042966 0.727931
1 3.364234 -2.860237 2.006571
6 -3.159230 2.061050 0.176601
6 -3.064359 1.736060 -1.191774
6 -3.053877 2.764503 -2.319809
1 -3.646214 3.640471 -2.033530
1 -3.556931 2.336912 -3.194971
6 -1.623021 3.190134 -2.719453
1 -1.230950 2.480800 -3.458424
1 -1.642090 4.172323 -3.219313
6 -0.649917 3.211640 -1.556050
6 -0.907392 3.741123 -0.277666
6 -2.201048 4.437613 0.134503
1 -1.967040 5.219201 0.866661
1 -2.637671 4.957098 -0.725830
6 -3.231720 3.462825 0.753929
1 -3.043057 3.382046 1.831522
1 -4.249850 3.871800 0.651390
1 -0.031600 4.012114 0.309787

1 1.051569 -2.586607 1.771231
1 -0.256699 -3.804291 0.188366
1 3.434426 -0.655826 -1.609301
1 -3.578656 1.299007 0.833573
1 -3.396733 0.742016 -1.480826
1 0.393432 3.140579 -1.855233
1 2.311003 -2.175606 -3.063223
1 0.068474 -1.798482 -2.123523
1 0.532881 -0.880632 -3.578970
1 -0.509319 0.000028 -2.647407
7 0.420695 -0.418416 -2.675477
15 -1.205937 -0.860804 0.190249
6 -2.694528 -1.725451 -0.521074
6 -3.946085 -1.579648 0.108154
6 -2.640514 -2.482167 -1.701486
6 -5.095452 -2.160597 -0.427514
1 -4.020512 -1.021190 1.036513
6 -3.791657 -3.063269 -2.241568
1 -1.686604 -2.636853 -2.195025
6 -5.024099 -2.903555 -1.608591
1 -6.047720 -2.034239 0.081396
1 -3.718435 -3.649201 -3.154454
1 -5.918890 -3.358036 -2.025487
6 -1.432462 -1.286456 1.983478
6 -1.681321 -2.606799 2.401915
6 -1.375275 -0.282068 2.962510
6 -1.846745 -2.912095 3.753090
1 -1.768543 -3.401556 1.667449
6 -1.536499 -0.587460 4.316592
1 -1.203998 0.745202 2.657844
6 -1.769706 -1.903140 4.716885
1 -2.039302 -3.939419 4.052113
1 -1.480908 0.208302 5.054684
1 -1.898898 -2.141678 5.769408
6 2.575214 1.899680 -0.600200
6 3.528055 2.641322 0.119816
6 2.656880 1.900972 -2.009289
6 4.518667 3.370950 -0.544045
1 3.501862 2.653236 1.204312
6 3.649735 2.629390 -2.665598
1 1.940558 1.306975 -2.573488
6 4.583571 3.372354 -1.937743
1 5.241840 3.939340 0.036094
1 3.693394 2.615755 -3.752337
1 5.353267 3.942763 -2.451222
6 1.606737 1.129168 2.002166
6 1.187305 2.297716 2.664697
6 2.309116 0.170259 2.745753
6 1.465571 2.499652 4.017347
1 0.632669 3.050699 2.114914
6 2.585358 0.365726 4.101646
1 2.632005 -0.741530 2.260733
6 2.165178 1.531357 4.742262
1 1.132784 3.412497 4.505718
1 3.127667 -0.396411 4.655839
1 2.379347 1.685245 5.796749

E$^{+\cdot+\cdot}NH_3$ (E = -2498.86064397 a.u.)

77 -1.890764 -0.215633 -0.344458
77 1.891708 0.257117 -0.163941
15 0.224984 -1.509910 0.010896
6 -3.067631 0.311378 1.327414
6 -3.505654 1.088134 0.167319
6 -4.810459 0.840354 -0.579149
1 -5.683393 1.202769 -0.009569
1 -4.788418 1.437111 -1.501690
6 -4.991103 -0.646535 -0.948130
1 -5.594354 -1.158577 -0.190026
1 -5.554682 -0.735615 -1.885205
6 -3.655495 -1.374919 -1.105444
6 -3.048304 -2.122894 -0.082757
6 -3.583726 -2.202197 1.337098
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1 -4.464648 -2.864691 1.368513
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