

Supporting Information

A “phosphorus derivative” of aziridines: on the importance of ring strain energy and three heteropolar bonds in azaphosphiridines

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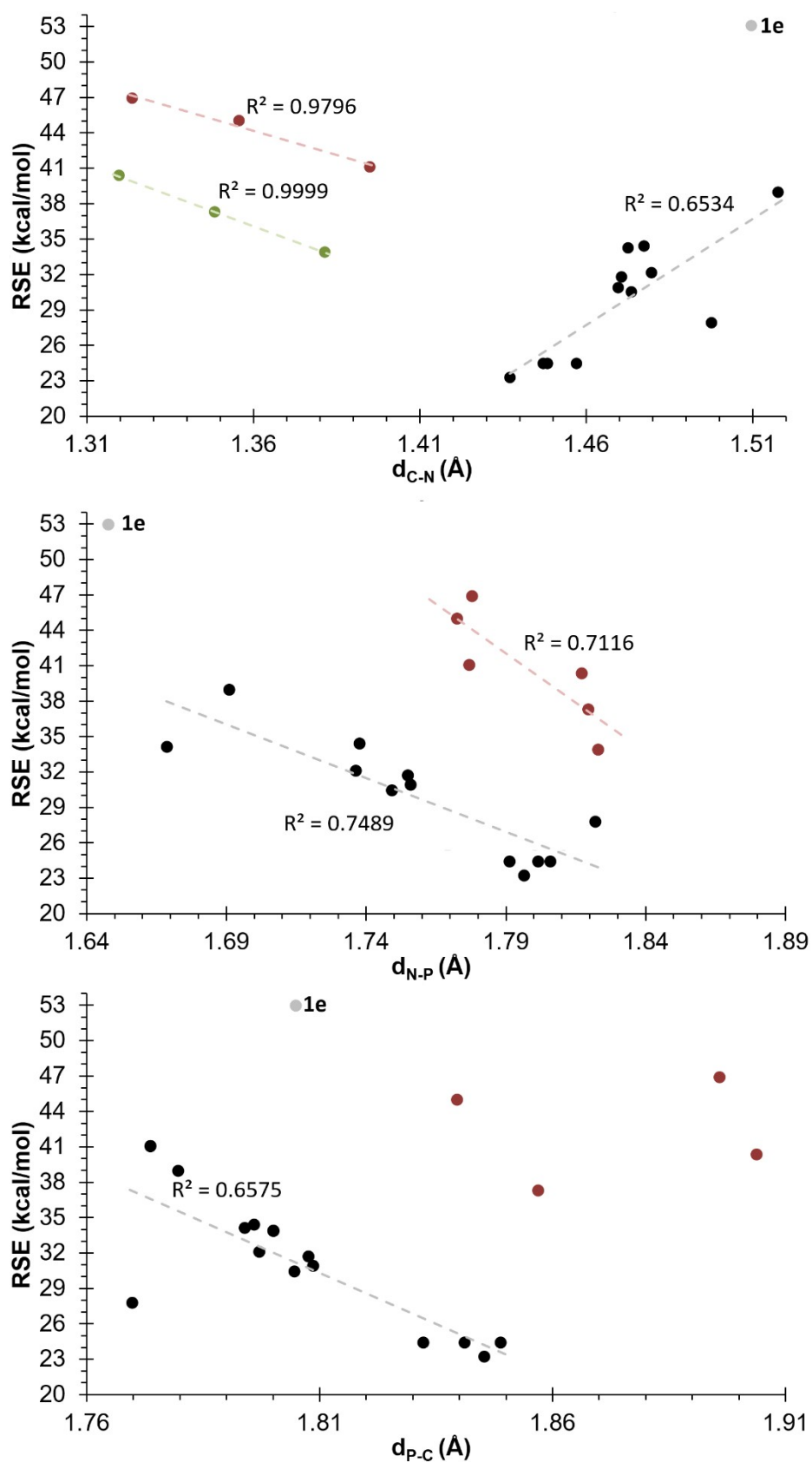


Figure S1. Plot of RSEs (kcal/mol) versus endocyclic C-N (a), N-P (b) and P-C (c) bond distances for the azaphosphiridines. Compounds excluded from the general correlation are uncomplexed (green) and complexed (red) species with exocyclic double bond.

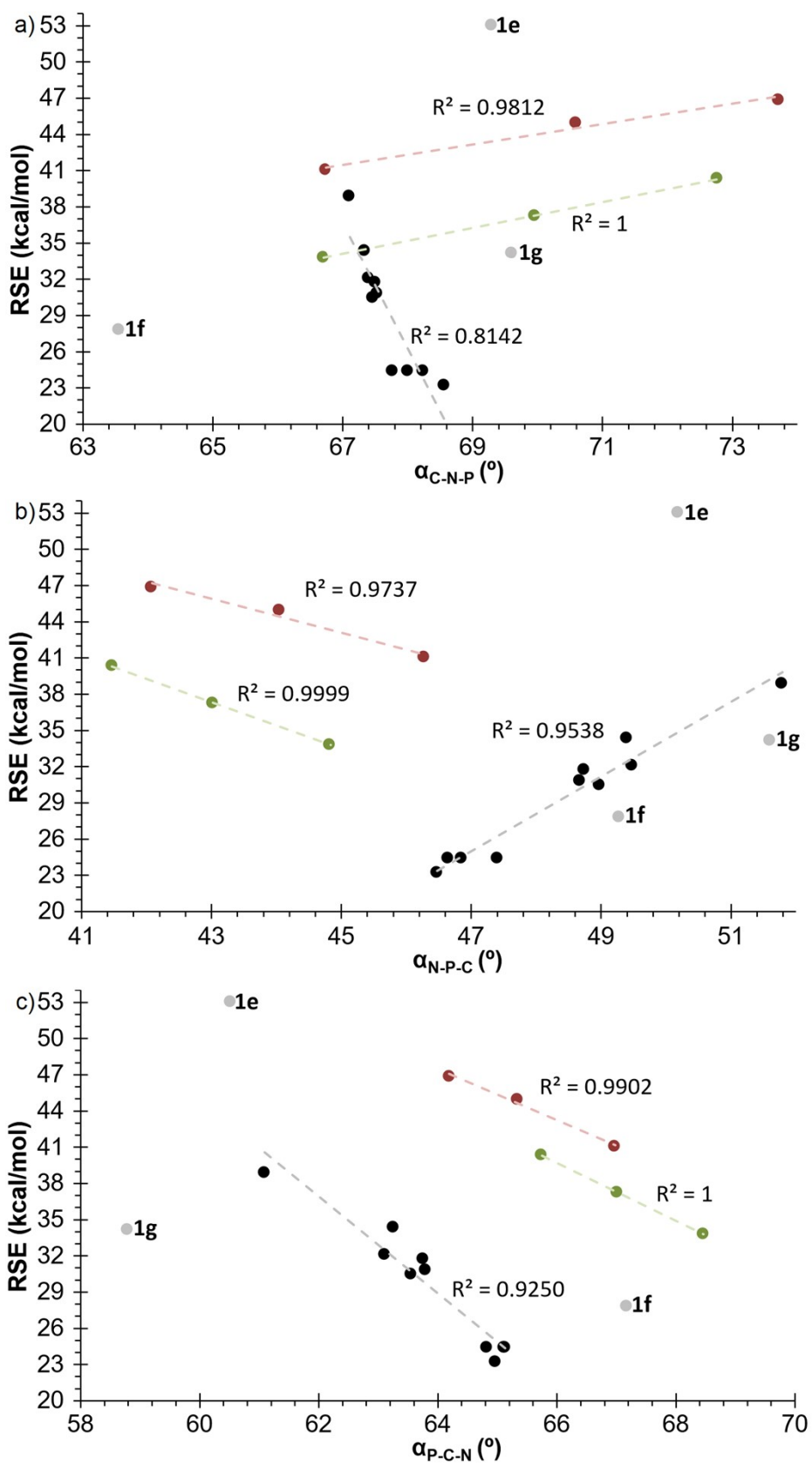


Figure S2. Plot of RSEs (kcal/mol) versus endocyclic C-N-P (a), N-P-C (b) and P-C-N (c) bond angles for the azaphosphiridines. Compounds excluded from the general correlation are uncomplexed (green) and complexed (red) species with exocyclic double bond.

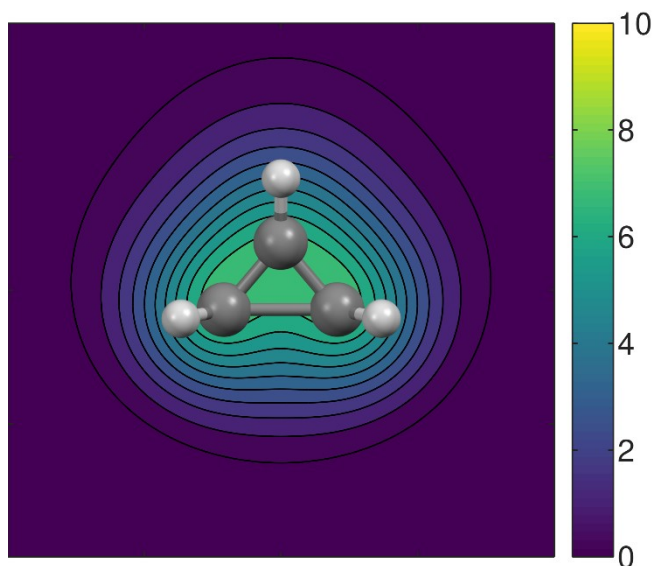


Figure S3. ISCP of σ_{zz} (ppm) in the plane parallel to the xy (ring) plane located at $\pm 2 \text{ \AA}$ (average) for cyclopropenide anion.

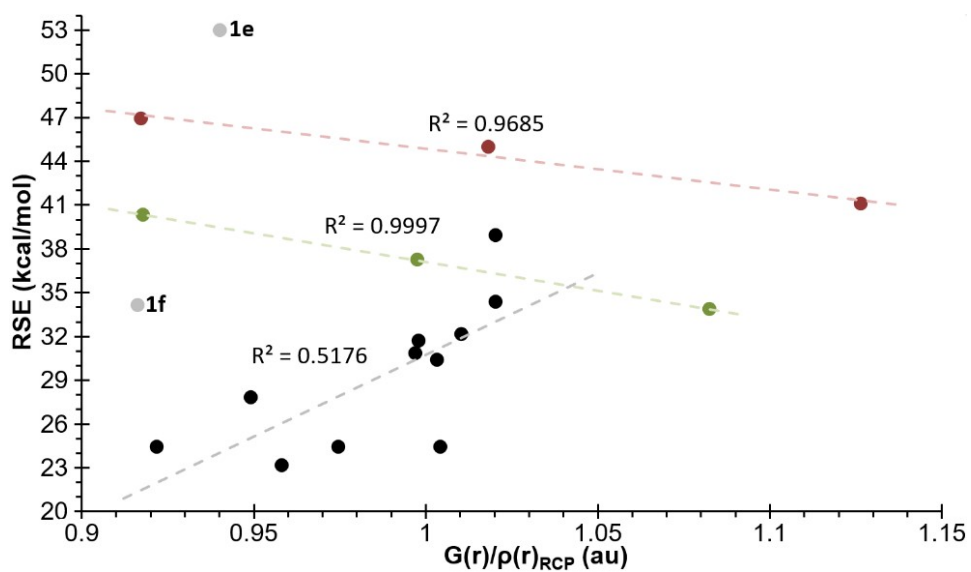


Figure S4. Plot of the RSEs versus $G(r)/\rho(r)_{RCP}$ for the azaphosphiridines **1**. Compounds excluded from the general correlation are uncomplexed (green) and complexed (red) species with exocyclic double bond.

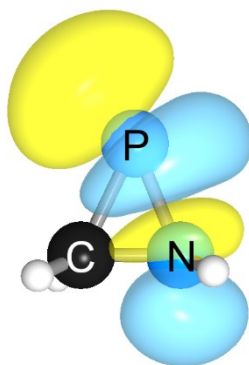


Figure S5. Computed (B3LYP/def2-TZVPP//B3LYP-D4/def2-TZVP) $\sigma^*(\text{P-N})$ natural bond orbital (isovalue 0.032 a.u.)

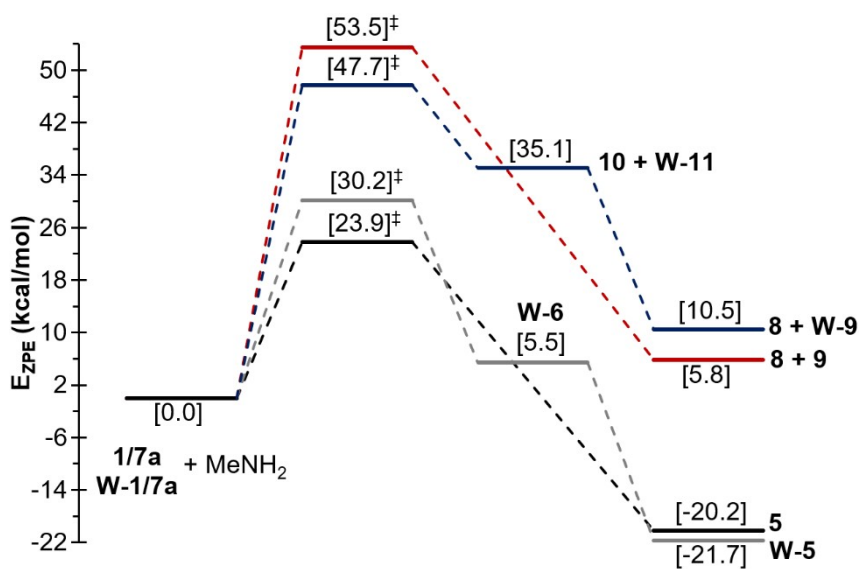


Figure S6. Computed (DLPNO-CCSD(T)/def2-TZVPP) zero-point corrected energy profile for the MeNH_2 -mediated P-C bond cleavage reactions depicted in Scheme 3: **1a** (black); **W-1a** (grey); **7a** (red); **W-7** (blue).

Calculated structures

Cartesian coordinates (in Å). Unless otherwise stated G correction (G-E) and ZPE (in hartrees) for TSs and minima were computed at B97-3c, electronic energies (in hartrees) are quoted using the default DLPNO-CCSD(T)/def2-QZVPP(ecp) level.

1a E = -435.969838470154 au
ZPE = 0.05151348 au
G_{corr} = 0.02616598 au

C	-2.39644304088927	0.25900448930267	0.03192364361377
H	-2.96739184426344	-0.03352021129884	-0.83884258351710
H	-2.76919103862742	-0.14589160242036	0.96649425457674
P	-1.71361865924691	1.96709087715978	0.11205868852180
H	-1.87135326401171	2.30304105643132	-1.26429789309328
N	-0.96726923041145	0.35469234883264	-0.18605749198390
H	-0.45229690254978	0.07430445199279	0.64280756188197

1b E = -475.200894576208 au
ZPE = 0.07883535 au
G_{corr} = 0.05140868 au

C	-2.35922896141590	0.25116984947588	0.03371844934378
H	-2.87199204682974	-0.10580021706927	-0.84994857535971
H	-2.74569756152309	-0.14417509575404	0.97008299806345
P	-1.79528643620219	2.00705508138020	0.10189133864327
H	-1.89242615971924	2.29642516382555	-1.29067535199789
N	-0.93991728847814	0.43968817159234	-0.09532556901919
C	-0.14289461099878	0.01460169251522	1.04748738357155
H	0.01558786974831	-1.06189528703810	0.97727991530771
H	0.82531991599896	0.50797807090961	1.01016364482444
H	-0.60005709058017	0.22603049016261	2.02352191662259

1c E = -475.214387829414 au
ZPE = 0.07943959 au
G_{corr} = 0.05195927 au

C	-2.42502790979949	0.24871067697653	0.04206624957341
H	-2.96601753180366	0.01119546519240	-0.86721252890825
P	-1.71622568895073	1.95424359624999	0.12923526793412
H	-1.85759730741761	2.30851538112121	-1.24478561316663
N	-0.99639057971318	0.32660901471136	-0.17730811670230
H	-0.49267874345645	0.03884587389415	0.65821173544339
C	-2.97344093067348	-0.38242042964899	1.28613406454351

H	-4.03521542554377	-0.16951910116330	1.39827879800577
H	-2.84919797466110	-1.46676330159784	1.25194353538896
H	-2.46356510798050	-0.01327783573553	2.17630133788803

1d E = -475.220187425988 au
ZPE = 0.08015475 au
G_{corr} = 0.05228810 au

C	-2.36542833573585	0.28060826201531	-0.06095651989376
H	-2.84783127331956	-0.00442410355793	-0.98739234788665
H	-2.75961319247341	-0.22314331269394	0.81487215144607
P	-1.82695101302707	2.01776713324845	0.16298304032707
N	-0.92927430852002	0.50374924393688	-0.17083423161990
H	-0.44309251809606	0.19494639993223	0.66450173506952
C	-1.92763195245944	2.68764320472614	-1.56072478376990
H	-2.87458177905053	3.20879482346603	-1.69527009663065
H	-1.12337138314839	3.40347911363972	-1.72049402160728
H	-1.84184900416964	1.89561940528711	-2.29980400543452

1e E = -436.327721745194 au
ZPE = 0.06091330 au
G_{corr} = 0.03541425 au

C	-0.08382603109948	-0.05295695867710	0.04458631108650
N	-0.04783093465993	0.00163019533928	-1.42711506465316
P	1.49810231355290	-0.06262976007307	-0.80065602305987
H	-0.44785874716977	-0.98431179864172	0.45660475644503
H	-0.31316493870917	0.84262099444176	0.61405356563717
H	-0.40552119865407	0.82118561302424	-1.90460036605848
H	2.23627679780949	-1.19436028557270	-1.15917693824060
H	2.28059079893002	1.09368514015929	-0.70683879115658

TS(**1e**→**1a**·H⁺) E = -436.276648250682 au
ZPE = 0.05886082 au
G_{corr} = 0.03317140 au
 $\bar{\nu}$ = -1077.38 cm⁻¹

C	-0.02462546793134	-0.07872032678849	-0.05670261937781
N	0.10916766410496	0.29154445109391	-1.40337540036143
P	1.86465248785222	0.09156187242595	-0.25847646619112
H	-0.28323393487371	-1.11937593103187	0.09052649505186
H	-0.44089550134105	0.62982854908288	0.64946654103216
H	-0.08776671537669	1.29745861209833	-1.49463130367814
H	2.05396026933293	-1.22212126274299	-0.75758295619711
H	1.52550925823256	0.57468717586226	-1.65236684027831

1a·H⁺ E = -436.368778885003 au
 ZPE = 0.06573794 au
 G_{corr} = 0.04021506 au

C	0.04258257648396	-0.08233382681010	0.02535502061651
N	-0.04350982006312	0.02607438851470	-1.44421495699513
P	1.69254239022082	0.11008552005353	-0.77636308150031
H	-0.26998580150632	-1.03550749331389	0.42164426056579
H	-0.34559216422612	0.77950700361758	0.54720499999353
H	-0.43372452662621	0.87945441356661	-1.82895669510627
H	1.88360689723539	-1.28285277845860	-0.97046930138910
H	-0.34337444151840	-0.79396015716983	-1.95898823618501

1f E = -437.106309045102 au
 ZPE = 0.06784289 au
 G_{corr} = 0.04192556 au

C	-3.28610611937425	-0.18151222025792	1.40395309198602
H	-3.73743886464030	-0.90662211458741	0.73052285004778
H	-3.95543116506217	0.04855031253555	2.23417951004099
N	-1.82040630733580	-0.33572208169024	1.67267560844839
H	-1.62987691619424	-0.35210648696063	2.66978265132874
P	-2.33302285169469	1.19063198252462	0.81982071924688
H	-3.13724578953044	2.17695641253633	0.07723544465018
H	-1.97561076040243	2.13047806175190	1.81711891937535
H	-1.42597128576566	1.00546473414780	-0.24023104512436

1g E = -817.022355940067 au
 ZPE = 0.13930131 au
 G_{corr} = 0.10515797 au

C	0.02651473923433	-0.36470556568161	0.09430419759627
N	-0.13824747168210	0.25949608229539	-1.27030090462939
P	1.45931054522900	0.11438246257617	-0.89430301894702
H	-0.40400339741413	-1.35648111626853	0.18928238830549
H	-0.17238387465133	0.27207102954747	0.95084863481579
H	-0.68646704792372	1.09027516912122	-1.43285685534499
H	2.00601676529418	-1.04314902515610	-1.45935174261548
O	2.49369090664960	0.68976029011628	0.30488800359340
O	2.14666931205332	1.24143534673667	-2.04266678726318
C	3.42641614623424	1.58239995771622	-0.17753477469128
C	3.21867023967946	1.88933744696273	-1.51892304599217
C	4.04260739241401	2.78504223978614	-2.16998634154110
C	5.08531953213447	3.36037796437608	-1.44377784358336
C	5.28620214310637	3.04899061680658	-0.10632917444345
C	4.44651284720475	2.14811637516267	0.55059497635630

H	3.87749011530776	3.02399115977655	-3.21072979744434
H	5.74676780468597	4.05969294939455	-1.93652760999976
H	6.10164116156244	3.50511515311713	0.43739506576848
H	4.58635822088127	1.89640872361432	1.59206540005984

1a^{=C} E = -473.971191461073 au
ZPE = 0.05521721 au
G_{corr} = 0.02821099 au

N	-1.91312697108647	-0.38193190767630	1.46606975592051
H	-1.54259641900052	-0.40839290241616	2.41105669452132
P	-2.28751686504602	1.29013582045730	0.84350685144172
H	-2.10889610019717	0.96260299083750	-0.53366950643280
C	-3.26739861391969	-0.13132476361302	1.35323933192717
C	-4.44128753449882	-0.68073359518878	1.59912520269143
H	-5.35443906477994	-0.17254588479842	1.33090076761085
H	-4.51855791147134	-1.65719841760212	2.06029934231979

1a^{=NH} E = -490.016314971438 au
ZPE = 0.04437060 au
G_{corr} = 0.01750295 au

N	-2.14947090166737	-0.29297530316093	1.58132823465075
H	-1.86865948757495	-0.41338980262118	2.54678104523218
P	-2.32287128106096	1.35389719818787	0.82710089085216
H	-1.92117221983897	0.94221060019390	-0.47854841135584
C	-3.43975014215146	-0.06416783417434	1.26301109935512
N	-4.55787114522860	-0.61410546503001	1.41682196934851
H	-5.30567833247766	-0.07534682339532	0.98962411191712

1a^{=O} E = -509.889243991761 au
ZPE = 0.03196846 au
G_{corr} = 0.00501272 au

N	-1.94521044599490	-0.23591544774268	1.53939825688012
H	-1.40746824763493	-0.51251660835125	2.35056609834749
P	-2.32077811553267	1.37505407440924	0.78687260666566
H	-2.03637903282262	0.97082047443246	-0.55366024802333
C	-3.25495369288922	-0.17020216849327	1.39052006767722
O	-4.28581071512565	-0.72783878425450	1.62528771845284

Fe-1a E = -2151.727358609185 au
ZPE = 0.08741436 au
G_{corr} = 0.04706231 au

C	-2.46356762906679	-0.28646318219113	1.73243446405134
H	-3.04099996181555	-1.15464506550797	1.44486698499880

H	-2.27318612482681	-0.19963229828125	2.79597339223548
N	-1.38761697586439	0.07984055186775	0.78466689683738
H	-0.53198402932154	0.36468954603694	1.24848446700112
P	-2.64048060832291	1.27917605778481	0.86790543341327
H	-3.36144778137087	1.01339519588261	-0.31096316954910
Fe	-2.55837585822908	3.28190959925600	1.74226539180908
C	-2.54174783631306	4.89925984501660	2.44803073019986
O	-2.53149440131224	5.95309514998881	2.90969901773575
C	-0.823054448478214	3.06853626742083	2.02425347187450
O	0.30654691453359	2.89550608983888	2.20444708585677
C	-3.12695538280356	3.93862894535114	0.18737609372770
O	-3.49893310954796	4.36620839417922	-0.81848469329567
C	-3.69594974241403	2.71019138429645	2.98317622051065
O	-4.42344075854260	2.33497060906022	3.79803415259301

Cr-1a E = -2045.723531943813 au

ZPE = 0.09581824 au

G_{corr} = 0.05315318 au

C	-3.20009477564138	-0.25758941916357	1.40292829465723
H	-3.58071193399952	-0.98784857486010	0.70180855737146
H	-3.83005958824386	-0.09241434981696	2.26946953373156
N	-1.73759207857819	-0.28675682373465	1.58367128890760
H	-1.46783859099533	-0.13295006691248	2.54933377849496
P	-2.28957354977101	1.18881724761823	0.82328516528608
H	-1.98650080567199	0.90506715422660	-0.52504443876890
Cr	-2.29552293666690	3.30528987940693	1.71780547655090
C	-0.41403250372348	3.30641912828328	1.71941055399653
O	0.73717155382100	3.31906456695335	1.72880611730476
C	-2.29469003199805	4.02076297536265	-0.02039636292431
O	-2.29337918995373	4.45472770068090	-1.08690133120231
C	-4.17372510710872	3.27077961184357	1.71414457672915
O	-5.32485933160519	3.24133227548773	1.71726206421470
C	-2.30775414681031	5.01338199644315	2.44317250280986
O	-2.31611392208114	6.07367254783185	2.89509982483046
C	-2.29331559048931	2.53248518264417	3.42181658790961
O	-2.29022727048283	2.02581433770532	4.45885601010063

Mo-1a E = -1070.013331083963 au

ZPE = 0.09379459 au

G_{corr} = 0.04998747 au

C	-3.21222671082498	-0.35717817955566	1.33801591066047
H	-3.60859967833660	-1.07803859017849	0.63589655917558
H	-3.82422416330398	-0.19915848706336	2.21851966045152
N	-1.74981418119620	-0.38701515144076	1.48317129861982

H	-1.45987703499252	-0.22516162140130	2.44182638430478
P	-2.32034484476128	1.09858623741461	0.74053013201191
H	-2.05821741930238	0.81128788764573	-0.61548539994310
C	-0.25094780252485	3.29309400368299	1.80610455363787
O	0.89822909431794	3.27310208991151	1.84897361536428
C	-2.21353006145368	4.17355373809629	-0.11520058019846
O	-2.16996447365974	4.63283896737352	-1.16873356552554
C	-4.32485132528631	3.37583369613359	1.69098028403749
O	-5.47486255971741	3.38673097000156	1.66602196459000
C	-2.27180690741703	5.16559883009764	2.57975599586387
O	-2.26419088906836	6.21320646722612	3.05936716586420
C	-2.36198819913320	2.45808745327674	3.56982080887157
O	-2.40268914352892	1.92100101777963	4.58913332517438
Mo	-2.28891349981045	3.34368605099961	1.74583008703933

W-1a E = -1068.811086833151 au

ZPE = 0.09379277 au

G_{corr} = 0.04967234 au

C	-3.28959325417874	-0.34262985087467	1.38567765388318
H	-3.73267836426794	-1.05726893795696	0.70544674410277
H	-3.85904700285924	-0.16440267261159	2.29056581228367
N	-1.82243499188609	-0.40537434870825	1.46812455309403
H	-1.48763355165207	-0.24606103133492	2.41265135954976
P	-2.39099339173102	1.08783920017964	0.74212158762433
H	-2.18766712567822	0.79615015281479	-0.62224560381372
C	-0.21848882608670	3.20373854914204	1.79206608311439
O	0.93023632039969	3.13480110325294	1.83256697996365
C	-2.15400790573389	4.14732049438786	-0.14182105941111
O	-2.09396255440054	4.58605296889240	-1.20474493810026
C	-4.29996821388609	3.47436504873051	1.69055569714733
O	-5.44920348927542	3.54586508753358	1.67233465041406
C	-2.15538644747524	5.17426501683356	2.55842306977947
O	-2.09700315383616	6.22498851324566	3.03094754611137
C	-2.36537584435759	2.46562374610961	3.57174461099344
O	-2.42580083608953	1.93332380177242	4.59423340679210
W	-2.25977592700514	3.34142496859131	1.73586620647148

B-1a E = -462.546820698529 au

ZPE = 0.08161784 au

G_{corr} = 0.05314072 au

C	-3.31085116106950	-0.12181641246533	1.43013334415072
H	-3.76058131051952	-0.83648853286641	0.75457622486497
H	-3.89416335333345	0.09713994877246	2.31701129782125
N	-1.84246949649180	-0.23398247559768	1.55173938785367

H	-1.52207232366757	-0.07385592980242	2.50113343494644
P	-2.34018861434988	1.25067741305543	0.79777499208911
H	-2.09021538227853	1.01218299274687	-0.56770987435979
H	-1.06662769216096	3.32125358501522	1.45146351463659
H	-3.00601571373823	3.66009713657529	0.98867112481215
H	-2.53402885543088	2.76410544230603	2.74682804170583
B	-2.21519997695966	2.98211390226050	1.60062527147905

O-1a E = -511.125702038646 au
ZPE = 0.05559847 au
G_{corr} = 0.02869880 au

C	-3.34861571119977	-0.12061890942280	1.40165066085165
H	-3.79161951944101	-0.84269823512843	0.72702520750569
H	-3.92705508782647	0.06141595867086	2.30124919116911
N	-1.84342909327130	-0.24315513854677	1.55442164519709
H	-1.52000638888586	-0.27585338044290	2.51265691593393
P	-2.31969680841867	1.24525705185987	0.90827614449965
H	-1.97104855599248	1.18284435697989	-0.45151981014527
O	-2.25761577496440	2.59437816603026	1.53490907498814

W-1a^c E = -1106.812495984085 au
ZPE = 0.09746053 au
G_{corr} = 0.05210278 au

N	-1.93986441279810	-0.42622329947792	1.47950452826274
H	-1.57330578863974	-0.40094818462346	2.42591319832744
P	-2.39038628983097	1.11503413624098	0.71851992907179
H	-2.06099850297702	0.82257884293402	-0.62256201476623
C	-0.21681063436627	3.20795959316229	1.79647968379240
O	0.93153218000278	3.13451080164900	1.84287465999127
C	-2.13245211853058	4.16834081542609	-0.14330576850382
O	-2.06106695591059	4.61577877356406	-1.20199739521842
C	-4.29912586595331	3.47425875312155	1.67034653912786
O	-5.44805224479759	3.53705529928013	1.64504161975484
C	-2.15787974723197	5.17892079325997	2.56054425079425
O	-2.10108525785455	6.22655059506153	3.03890358685480
C	-2.38064008004050	2.45892552534124	3.55851633583607
O	-2.44672276930873	1.92430088209011	4.57768229218334
W	-2.25665313203802	3.34840195694008	1.72579467327704
C	-3.31718576458620	-0.27444870442967	1.31559686778553
C	-4.46635749091880	-0.83961849395154	1.62870804517854
H	-5.39726105663039	-0.40585283252481	1.29873122416962
H	-4.50617106758938	-1.74945673306369	2.21320282408089

W-1a^{NH} E = -1122.856521716639 au

ZPE = 0.08634748 au

G_{corr} = 0.04086244 au

N	-2.09736132166119	-0.38448835164009	1.43953469741407
H	-1.64190828043477	-0.54516817828930	2.33047810428917
P	-2.47717865082822	1.17371437353626	0.68474302398301
H	-2.09987873069060	0.88987286828934	-0.64737112338041
C	-0.20684015100607	3.13114949715395	1.76451640608328
O	0.93611934012139	2.99597557410092	1.79608956779394
C	-2.09099415009165	4.20912064582520	-0.14404225464944
O	-2.00667660320432	4.66174819887991	-1.19938426692330
C	-4.27009939680409	3.62780272774857	1.69356467218746
O	-5.41291824980698	3.76439877550606	1.68604367728812
C	-2.02420100343326	5.19639810328723	2.56785045834568
O	-1.89703964286402	6.23422331138736	3.05287520820965
C	-2.38585409365170	2.48776607016908	3.55095757815532
O	-2.46445567319517	1.95723248292706	4.57053683349972
W	-2.23766210442215	3.38007626034925	1.71941794026358
C	-3.44101961215058	-0.26807912526296	1.29848589558292
N	-4.47809090486917	-0.86739285053530	1.66443027849497
H	-5.32641053100739	-0.41746230343262	1.33477854336222

W-1a⁰ E = -1142.729919808355 au

ZPE = 0.07394523 au

G_{corr} = 0.02834780 au

N	-1.88323581326459	-0.34685057133778	1.50394934048660
H	-1.21304520041655	-0.65807316302486	2.19913439506319
P	-2.48490376818128	1.14223002668277	0.74098480351867
H	-2.10288961551865	0.89794016690440	-0.60053702422136
C	-0.28685865225271	3.14996493642224	1.81350951201130
O	0.85727033629241	3.02623896889715	1.86455695712639
C	-2.16376493884368	4.15222612573420	-0.14501970366334
O	-2.07381361624471	4.57784804749314	-1.21100665278895
C	-4.35718811181435	3.59926665518211	1.68895535771727
O	-5.49778039697842	3.74164881572145	1.67435002892242
C	-2.13401322558989	5.20783379148204	2.54279423639522
O	-2.01770806652868	6.25888260131342	3.00051728181390
C	-2.47809587934798	2.51564767954410	3.58708887642540
O	-2.56219247569203	2.01341109156655	4.62018557852522
W	-2.31788039229148	3.36700237151422	1.73609261613533
C	-3.19652288908955	-0.48294181890772	1.40949605614221
O	-4.12464504423775	-1.16741698518750	1.71189949039045

1a^{-P-C cleav} E = -912.460272112268 au

ZPE = 0.15462185 au

$G_{\text{corr}} = 0.11838858 \text{ au}$

N	-2.88912845619132	1.10310848662045	1.52179654667689
H	-3.23882741684223	1.15997359195865	2.46110080673201
P	-1.93552263436760	2.41789762535408	1.01178083423700
H	-2.64184278763220	2.81139577994615	-0.17125132470251
C	-0.53917852899390	1.60234255684099	0.10261455019456
H	-0.86457931756001	0.83820501284270	-0.60056446672180
H	0.00631520427227	2.36694880976971	-0.45048543645388
H	0.14146392287462	1.14980881857049	0.81937292264361
C	-3.48354329070196	0.07745219504612	0.69594095629418
H	-3.25828346559811	0.28558936581875	-0.34770191007528
H	-4.57148184478131	0.05272618843228	0.78837386697991
P	-2.81464268537733	-1.59368550350267	1.23061393154223
H	-1.48429560250460	-1.32782255842954	0.77303551076304
N	-3.39717457236903	-2.63585675084759	-0.00478718457774
H	-3.54851610945824	-3.57426870449242	0.32750733041277
C	-2.87628217964879	-2.59225981813841	-1.35968487984119
H	-1.80608121476543	-2.82416822662791	-1.42378898312801
H	-3.41739771303435	-3.29674465079246	-1.99073837308350
H	-3.02515436732029	-1.60190684836937	-1.78490723789231

1a-*C-N cleav* $E = -570.940770260271 \text{ au}$

ZPE = 0.14594003 au

$G_{\text{corr}} = 0.11274459 \text{ au}$

P	-1.63360206524379	1.04530233072075	0.37180088791029
H	-1.82475700235719	1.98740805069230	-0.68986095011260
C	-2.92347829561968	-0.16569053415901	-0.23189497322728
H	-2.90211667431032	-0.26141021198940	-1.31730019905808
H	-2.67237619318806	-1.15315698202796	0.18554085636234
N	-0.18193822943837	0.26492445784670	-0.11048863237231
H	0.59634438522240	0.53006428466367	0.47062545208178
C	0.18160618560947	0.11747025680156	-1.50889875182175
H	0.26897325119333	1.07290451676174	-2.04103317241158
H	1.13181080766496	-0.40918704215557	-1.59241880249796
H	-0.56485368517829	-0.48156796566013	-2.02613293651770
N	-4.22314714553414	0.34477869652162	0.15621075636071
H	-4.26576314718791	0.42450598910173	1.16423357113067
C	-5.32841997676302	-0.46497749250897	-0.32216182269612
H	-6.26665870926368	-0.06219145023409	0.05584017626150
H	-5.36834390264592	-0.42213557373245	-1.41051096441354
H	-5.26686862295975	-1.52592369064249	-0.03444795497836

1b-*P-C cleav* $E = -990.919970276494 \text{ au}$

ZPE = 0.20979105 au

$G_{\text{corr}} = 0.17071948 \text{ au}$

N	-2.98047560631924	1.60808749144047	1.21045891352609
P	-1.73224843409659	2.66590560911192	0.69843823311502
H	-2.09734629479431	2.89359006320290	-0.67307254995641
C	-0.35552767674228	1.49094447517150	0.30918488549178
H	-0.65726903966060	0.65093885944744	-0.31317119526372
H	0.42656296956988	2.04154655208297	-0.21323840330198
H	0.05957109669876	1.10571680798338	1.23692036045488
C	-3.49499450122040	0.54737855107020	0.36963232983910
H	-2.98006485259138	0.54334794688316	-0.58798555670432
H	-4.56057187893696	0.68234933077734	0.16033679586119
P	-3.29347146105789	-1.08737494295999	1.27224575627636
H	-1.87850307304647	-1.16519974827534	1.05440540699154
N	-3.88762248140377	-2.21546229792823	0.11257356883780
C	-3.17310583700953	-2.40719133834167	-1.13392892184843
H	-2.26096298652927	-3.00773907766057	-1.00790196376380
H	-3.81096944378785	-2.91702643179126	-1.85822177597384
H	-2.88906627145800	-1.45160526539808	-1.56558366822752
C	-4.42221870421891	-3.45473949754938	0.65142465837234
H	-3.64588180293516	-4.20517850479662	0.85450071314927
H	-4.95140042305970	-3.25616017014813	1.57959672120386
H	-5.12915832402728	-3.89193030963398	-0.05624382211137
C	-3.92532437203727	2.10424327995482	2.19533144539610
H	-4.79131468671224	2.59679745648987	1.73494274043073
H	-4.29312491911052	1.27966597137183	2.80647327941333
H	-3.43395018551297	2.81817094949544	2.85027846879198

1b-*C-N cleav* $E = -649.403294225575 \text{ au}$

$ZPE = 0.20074227 \text{ au}$

$G_{\text{corr}} = 0.16464015 \text{ au}$

P	-1.64848292769599	1.28969734111245	0.21229000322988
H	-1.94214056415446	2.00736906794063	-0.99519568447788
C	-2.86460318115473	-0.09691267790640	-0.12295801485418
H	-2.87850909541359	-0.34705179077107	-1.18105148999688
H	-2.51986716159011	-0.99089256392496	0.42019505456138
N	-0.15003850221080	0.53149996616111	-0.18040597416776
C	0.09036651500910	0.08283379535311	-1.53769945600924
H	0.27905470695146	0.91559504781781	-2.23058598299591
H	0.95890971636339	-0.57754677881040	-1.56479117997173
H	-0.75930133810749	-0.48052342438547	-1.91252565157121
N	-4.19322267800594	0.33991005923601	0.26532010063988
C	-5.23767221579780	-0.39534507922407	-0.42025625109154
H	-6.21045679257870	0.01249158975142	-0.14975629042626
H	-5.12058739616591	-0.29301659117565	-1.49756958599355

H	-5.24226936393856	-1.47093579511180	-0.17600274628982
C	-4.38145680545554	0.31075750392530	1.70297012196498
H	-4.34543244774580	-0.71240528287963	2.11381273472721
H	-3.60719468959469	0.89746898331967	2.19062066989537
H	-5.34603840063678	0.74526206790634	1.95844368634327
C	1.02585662846241	1.13104113042221	0.42773674976295
H	0.79797318097621	1.44192142263865	1.44392481767926
H	1.83434782742471	0.39877738461360	0.46912644910190
H	1.39730764505964	2.00690063399114	-0.12233334006013

1c^{P-C cleav} E = -951.705559791732 au
ZPE = 0.18258627 au
G_{corr} = 0.14496368 au

N	-2.46140760677971	0.95975603664391	1.67444860107930
H	-2.77813130329289	0.97959335511615	2.63019567145795
P	-1.76727509877011	2.43139858395458	1.14424190136075
H	-2.68907909529980	2.81275382852674	0.11411804514635
C	-0.44860005621174	1.83674784899591	-0.01398779413412
H	-0.79461744333417	1.08024937840246	-0.71570597011651
H	-0.07304524319969	2.68733729941537	-0.58226312015411
H	0.37291060951003	1.42408611094099	0.56604923462297
C	-3.20477902692299	0.03363813872424	0.83652806946296
H	-2.93568597035917	0.24102867255174	-0.19791620007014
P	-2.56921477752190	-1.67139958599507	1.31822734541502
H	-1.27189720770930	-1.45338280213062	0.75404013614407
N	-3.28378381147257	-2.69824212837157	0.14046688689474
H	-3.42442343446862	-3.63517019627743	0.48100052240432
C	-2.89909403902669	-2.64927974466049	-1.25814070950425
H	-1.83795937118659	-2.86980402981617	-1.42751114478057
H	-3.49215781035140	-3.35848582166933	-1.83478988250206
H	-3.09847595898144	-1.65933134605264	-1.66448270974653
C	-4.70717556145664	0.13589137979988	0.99428642676879
H	-5.00160041928984	-0.05967856779434	2.02603503394855
H	-5.05336944106081	1.13349523206156	0.72368971234839
H	-5.21350577281376	-0.59356362236585	0.36422877395411

1c^{C-N cleav} E = -610.183813541824 au
ZPE = 0.17372862 au
G_{corr} = 0.13909768 au

P	-1.67224829680299	0.98062025981392	0.39322590303069
H	-1.97178768252021	1.87012538135408	-0.68577832673233
C	-2.92596140321533	-0.31808871570277	-0.13564346609652
H	-2.89220453911523	-0.42745644045329	-1.22087186788330
N	-0.18114257854391	0.30196806086951	-0.12716969269838

H	0.59647399958233	0.61657519853765	0.42929251041981
C	0.14454087911766	0.15706853835060	-1.53386201667923
H	0.15406977339620	1.10776364228661	-2.08122980192211
H	1.12164439844597	-0.31235273147260	-1.64573358487404
H	-0.58246958513120	-0.49302198528830	-2.01750883977815
N	-4.20700279103419	0.29405780796003	0.18687708735646
H	-4.32511345519212	0.31788730733806	1.19191412495590
C	-5.36370937702697	-0.31573496462326	-0.44388146026407
H	-6.26312996140168	0.21138650064925	-0.12969133729809
H	-5.28460948988213	-0.20652448554853	-1.52531642885101
H	-5.50532672369464	-1.38341297336943	-0.22654692415562
C	-2.63823629209498	-1.65986998981470	0.51645637487396
H	-2.66466862924226	-1.57159520448387	1.60366742234152
H	-3.36792730985998	-2.41261531367048	0.21887479666583
H	-1.64786076578427	-2.02001822273248	0.24313608758870

1d-P-C cleav E = -990.959141157149 au
ZPE = 0.21142845au
G_{corr} = 0.17157787 au

N	-1.71289686116435	0.73223455250796	-0.33888598281495
H	-0.77126798191711	0.46338884099569	-0.07873446233961
P	-2.15385870207486	2.36345376991504	-0.00317293953670
C	-1.56042194267779	2.64126493872904	1.74013557391192
H	-0.51423522185880	2.36060549569894	1.87227488223371
H	-1.67391787333905	3.69054687754673	2.01145633206047
H	-2.16849919471602	2.05644986436511	2.42744572455705
C	-2.67221231149890	-0.32351650844770	-0.06501180172710
H	-3.66666490478832	0.03786919255387	-0.33370873030479
H	-2.71166763448483	-0.62763959994424	0.98913304804503
P	-2.23898630448973	-1.83937709138091	-1.08814559633779
N	-3.46241113369491	-2.97514191792425	-0.67902822291516
H	-4.40996075067156	-2.61987400407899	-0.66620351633588
C	-3.20820562929554	-3.92505707622739	0.39079239289674
H	-3.26997440696675	-3.50167475821432	1.40052696278696
H	-3.91659987149447	-4.75148740359481	0.32933493393482
H	-2.20927082865381	-4.33838188047845	0.26744331336466
C	-0.77683051907464	3.21391496015920	-0.89348997150931
H	0.20308231420641	2.82768881459985	-0.60890333882490
H	-0.90486353436698	3.08583547100487	-1.96500307947903
H	-0.80292714759456	4.27906484135096	-0.67042812593882
C	-2.89168379172271	-1.24205579515787	-2.70499030876933
H	-3.96406757368088	-1.04569941018424	-2.66522622855852
H	-2.38143651921351	-0.31605156697335	-2.95944147931025
H	-2.69772195476609	-1.97719617682075	-3.48107260908921

1d-C-N cleav E = -610.190688790488 au
ZPE = 0.17457964 au
G_{corr} = 0.13966566 au

P	-1.57610211423776	0.99048458806967	0.48738734941007
C	-2.90813722319291	-0.10158290228509	-0.23416084569185
H	-2.91749520172315	-0.04042018474773	-1.32466445612887
H	-2.66022878561377	-1.14087167541047	0.03009524986403
N	-0.17090993816602	0.19263024839112	-0.09799565729818
H	0.61623297932756	0.31693567237139	0.51679018244237
C	0.20816839451464	0.13207635778454	-1.49812249275183
H	0.51330577025742	1.09460047010779	-1.92368804904252
H	1.03336391963947	-0.56838251579367	-1.62423229754567
H	-0.62208222576682	-0.24375283662448	-2.09225982965341
N	-4.19681334524346	0.35156981912934	0.25653226869034
H	-4.19753432057658	0.31080721214856	1.26814284397068
C	-5.31233661025921	-0.41622933497435	-0.26571602871659
H	-6.23915808796671	-0.07174588388993	0.19043146894632
H	-5.39549190477931	-0.25454655157290	-1.34045414622086
H	-5.22819058076721	-1.50148781391592	-0.10038269446295
C	-1.82520432308865	2.46346860503441	-0.61064959735282
H	-2.83806161005482	2.82367848079736	-0.44282420080736
H	-1.12815744337850	3.25632820203947	-0.34812258434894
H	-1.71823086892421	2.23322306334087	-1.67017907330193

1e-P-N cleav E = -834.632419795535 au
ZPE = 0.11867507 au
G_{corr} = 0.08574383 au

N	-3.06294947897864	1.67439233734289	-0.24563991354928
H	-3.80574298307813	1.32866215696339	-0.83519957751645
H	-2.85117635027644	2.65473106752625	-0.36128219112393
P	-2.30178215800124	0.74174334036015	0.83725056011492
C	-0.77089402927899	-0.14448046421687	0.24490563370782
H	-0.10589341126074	0.58379410044181	-0.21938829711267
H	-1.08722153096583	-0.83359342825990	-0.53639996596631
N	-0.14598163619607	-0.84983956848342	1.36315294527581
H	0.38647176684988	-0.25765231826084	1.98917727762446
P	0.42564439274702	-2.40980206794875	1.26254215861835
H	-1.90222948356660	1.52533555931916	1.92706647242173
H	-3.17176454104810	-0.24551494300501	1.31541469922600
H	1.50098964996980	-2.62720372277715	0.38082120212578
H	-0.61797720850527	-3.24239787618002	0.84437676192420
H	0.83116061158937	-2.77875016282169	2.54868089422955

1e-C-N cleav E = -532.153387664690 au

ZPE = 0.12899485 au

G_{corr} = 0.09744468 au

C	-2.82374674323272	1.59507004822995	-0.51163281667189
H	-3.21400595669789	0.75952656903416	-1.08595220429833
H	-2.30571787584776	2.27883468194024	-1.18092997504279
H	-3.66591478524399	2.10530328768719	-0.05628245696091
N	-1.95231558699044	1.09066170793487	0.56369590270298
H	-1.72163530764957	1.77268251174121	1.27151866224506
P	-0.88501762892075	-0.14330854224915	0.35354690784300
H	0.33995364303407	0.15688015876731	-0.27828507526971
C	-0.39372221832794	-1.12759024120077	1.83402226142018
H	0.11100085800848	-0.48763394953347	2.55442088784282
H	-1.29106448176788	-1.52234591510273	2.30493536157559
N	0.45077439200951	-2.11514169628008	1.22634586041815
H	1.41021191669683	-2.09171555183819	1.52881997834009
H	0.08927040873590	-3.05343300336785	1.26923729836619
H	-1.51280198380583	-1.02224755576268	-0.53108409251044

1e-C-P cleav E = -818.585394336126 au

ZPE = 0.12957379 au

G_{corr} = 0.09674024 au

P	-2.78776342003712	1.62621016141882	-0.63973894615345
C	-1.78655207675599	1.20364838142157	0.87356151758482
H	-1.27664808216839	2.11487565142388	1.18703360042688
H	-2.50697938229160	0.95917506302892	1.65263859358107
N	-0.87544124923009	0.10383004303911	0.61285233271104
H	-0.01588815246191	0.37545498539309	0.15250682169495
P	-0.71329720847711	-1.21616705965605	1.63759367664369
C	0.44537107181324	-2.39474266856471	0.95930231396763
H	1.44339202682935	-1.96398715698257	0.91190400174738
H	0.47713365485388	-3.25570800707762	1.62761966568256
H	0.12327517371913	-2.72056213900786	-0.02612128993419
H	-1.94655927557177	1.96868063971276	-1.70469964038345
H	-3.63158502845127	2.71547194014525	-0.38204490276318
H	-3.56886956067744	0.53770714618076	-1.04370733937601
H	-0.33011351855898	-0.84528166097655	2.93878010409378
H	-1.99817769253393	-1.75417469949881	1.77317211047648

1a-H⁺-C-N cleav E = -532.360325915007 au

ZPE = 0.14771401 au

G_{corr} = 0.11569210 au

C	-2.74410491698946	1.72962858719282	-0.52547677436749
H	-2.92826124669529	1.18022677998519	-1.44176753139899
H	-1.99398776834710	2.49609529034396	-0.68069874213171

H	-3.66485043348426	2.17806260388502	-0.16740900288296
N	-2.24925215950984	0.76228089370335	0.53620158064750
H	-2.09898512250320	1.27964219537842	1.40342711935892
P	-0.72841153819286	-0.14911446239472	-0.05629199264046
H	0.05840974917124	1.02273663544095	-0.01064206035358
C	-0.10485281160318	-0.87509806608220	1.58912353682566
H	0.72098997139318	-0.30424475038020	2.00163537803135
H	-0.89452781978924	-0.91969150999196	2.33538245843217
N	0.39122071127919	-2.29244673327202	1.39662380264880
H	1.20041407338464	-2.34302250352032	0.77297741392023
H	0.68927821561052	-2.69263950466525	2.29134102934025
H	-2.99656877634185	0.09209515630716	0.72188994152981
H	-0.32145609738245	-2.91723102193018	1.01228641304047

1a·H⁺-C-P cleav E = -818.382817641193 au

ZPE = 0.12288835 au

G_{corr} = 0.09002012 au

P	-2.20485721283268	2.09290078374285	-0.85257253253868
C	-1.66175907144247	1.27635234745420	0.75707728573526
H	-1.05406942868509	1.90410755460076	1.39945115005669
H	-2.53836461983133	0.95711475309691	1.31241434204101
N	-0.86452017039643	0.03467387205403	0.45312889272491
H	-0.00531518901570	0.28737886088643	-0.03373208585010
P	-0.50905318803078	-1.02007139893035	1.97658523014310
C	0.73224618627405	-2.14995852618748	1.23009199545962
H	1.52306670488200	-1.65770183196442	0.66985493908142
H	1.19906878231335	-2.68324602995693	2.05848899846854
H	0.24403658643280	-2.89874283253207	0.61220693426851
H	-1.20943423895425	3.10052499826404	-0.87179432524581
H	-3.18267247639903	2.90766714077992	-0.23744166729614
H	0.39243896647221	-0.04650470968214	2.47756670473823
H	-1.39736632078663	-0.53069832162576	-0.20891613178657

1a·H⁺-N-P cleav E = -834.629473233048 au

ZPE = 0.12662979 au

G_{corr} = 0.09354091 au

N	-2.58867952412983	2.06059115487485	-0.25999153569634
H	-3.35744588266310	1.46591320019756	-0.57550504132038
H	-3.01386775468493	2.96497298539822	-0.03571435369961
P	-1.78531462719113	1.38476558787144	1.30452787649003
C	-0.73306418462174	0.02858269934271	0.48336762806888
H	0.10767821303755	0.41135957269543	-0.08729974124039
H	-1.36670782993770	-0.55878693107555	-0.17755675452055
N	-0.18744125364987	-0.90867536172051	1.51791565955298

H	0.43557463026315	-0.41221564374337	2.15583011194159
P	0.87764870332548	-2.30797670446781	0.72147121363967
H	-0.79447258741333	2.39634817085259	1.29195857279634
H	-0.28167020486709	-3.07907618613503	0.45085083108581
H	1.08645309545078	-2.90945994842146	1.98860784959081
H	-1.96863314479571	2.21995171735699	-1.05659596023131
H	-0.93433078812251	-1.30091108302605	2.09274485354246

1f-P-C cleav E = -914.743510339303 au

ZPE = 0.18959690 au

G_{corr} = 0.15244090 au

N	-1.83035577618694	0.77120716501070	0.38077559935418
H	-1.22892566034341	0.47819166428294	1.14623109450904
C	-0.71655157640319	3.10378556739707	0.94557265236696
H	-0.47898800760394	3.84028203400208	0.18161537928063
H	-0.74015854374440	3.62347975187794	1.90097250192324
H	0.03986483920629	2.32801098275784	0.94619075303446
C	-2.88489228687307	-0.18070665882698	0.21781938163948
H	-3.36291124700921	-0.06595717632580	-0.75227203543339
H	-3.68745879188152	-0.11114766692210	0.98429310156842
N	-3.61321110225730	-2.50410372574124	-0.78349324198572
H	-4.50285931173777	-2.10052645613356	-0.50935779672113
C	-3.73501690515142	-3.94444461533419	-0.85374281779084
H	-3.87615882730614	-4.44125588845236	0.12253147472933
H	-4.56722009310266	-4.23171583161854	-1.49530089371181
H	-2.83116057155068	-4.36797642348501	-1.29568177728034
P	-2.42028071208250	2.48583714720565	0.59466505262806
H	-2.91659300582299	3.87059232535463	0.72363072812605
H	-2.97683646900699	2.41559039485707	-0.70425486362590
H	-3.35272472680655	2.10451854844181	1.61479078880586
P	-2.27141880493367	-1.95408838302552	0.30848771283278
H	-1.15951751893820	-1.49840698327946	1.18174879104308
H	-2.61732569105417	-2.89862878166049	1.33205620667116
H	-1.33062116940937	-2.51795497038247	-0.58233994196356

1f-C-N cleav E = -572.085277513093 au

ZPE = 0.16401948 au

G_{corr} = 0.13047498 au

C	-2.79527076075088	-0.01599083231414	-0.37083533116050
H	-2.77844291593905	0.17686822375213	-1.44454973966664
H	-2.49573516267984	-1.06532831173400	-0.21856656301870
N	-0.21057292272636	0.58037482227972	-0.30289329394819
H	0.62991045535834	1.07915016794771	-0.06029703283954
C	-0.09862432554026	-0.30153096362834	-1.45139247938962

H	-0.53181993336019	0.11931539102152	-2.36192454553770
H	0.95608956899648	-0.48622547883106	-1.64441070216684
H	-0.56496668834339	-1.26741149621888	-1.27040882096470
N	-4.11272262312952	0.28795923804813	0.12969400640287
H	-4.13765865179236	0.14671683307771	1.13247061261168
C	-5.17763918843029	-0.47335990261300	-0.49507448134171
H	-6.12905103304549	-0.22663537073193	-0.02508568916383
H	-5.25196502974729	-0.20218031222595	-1.54805404004622
H	-5.04085416454029	-1.56504582420549	-0.44515620660483
P	-1.58578120583478	1.17869047992017	0.52221373354469
H	-0.62247278375081	2.03349439644978	1.22759082297896
H	-2.40531432314728	2.29559810013268	0.17810955920222
H	-2.14671312159669	0.77690940987323	1.78833714110861

1g^{-P-C cleav} E = -1580.044769112147 au

ZPE = 0.28765626 au

G_{corr} = 0.24162512 au

C	-1.75270511733331	-0.02827890073645	-0.53163751144363
N	-0.38255548713872	0.02024470850172	-0.93631461521955
P	0.93393204686601	-0.39897479297498	0.01849372272501
H	-2.26100988301784	0.93279001356729	-0.66236244011621
H	-0.20073571716530	0.13947509373230	-1.91849822541664
O	1.93914464686263	0.63193629959619	0.90854824192836
O	1.94814294252460	-0.03866601337963	-1.44443226040636
C	3.02027825643623	1.11486626289021	0.21068884688522
C	3.00603302478527	0.73005563566962	-1.12835116143374
C	4.01417060614875	1.14228000201048	-1.98041375502459
C	5.03271331298742	1.94089617850991	-1.46053833496279
C	5.03799388769064	2.31811936094067	-0.12519388299944
C	4.01844112794382	1.90305522760538	0.73376174166516
H	4.00465289586687	0.84470487776320	-3.01949763520760
H	5.83015812225309	2.26889881184779	-2.11360654484879
H	5.83682971532809	2.93683293714886	0.25934472290675
H	4.00374832525824	2.18804692237636	1.77627312125837
P	-2.79499716517153	-1.27917252970064	-1.41426396981761
H	0.11296047231317	-0.44434174708562	1.18368043159272
C	1.50142199795039	-2.12941863642919	0.04765287592888
H	0.84545836537682	-2.73012747177907	0.67020701541164
H	1.53168427794898	-2.53656670466418	-0.95612223250197
H	2.50783897459903	-2.14956080164810	0.46189317545534
H	-1.81027455571738	-0.27597588734051	0.52601715368368
H	-3.93093161638902	-1.19496224247151	-0.55018745024733
O	-2.56431456950414	-2.82798893017220	-0.70612955202449
O	-1.67954160630350	-1.78265752176040	-2.70362473285056
C	-1.03132334697554	-2.93287816893004	-2.40995006934015

C	-1.54148803252680	-3.54484025209658	-1.26725908171361
C	0.00221036974104	-3.51106809871420	-3.11836974083824
C	-1.04734728158783	-4.74384193509430	-0.80626742345267
C	0.51717135212425	-4.72131728229445	-2.65272493407139
H	0.39800328094719	-3.02939342061742	-4.00078999780230
C	0.00215291716377	-5.32914264396067	-1.51629156475771
H	-1.46003378824421	-5.20550907631412	0.07935118585576
H	1.33207028837987	-5.18805771939180	-3.18855593420435
H	0.41569981362174	-6.26663669737895	-1.17195051729929
H	-3.44573503404289	-0.58915530722481	-2.47200637729575

1g^{-P-N cleav} E = -1596.108285529583 au

ZPE = 0.27712551 au

G_{corr} = 0.23177380 au

C	1.62576370499299	0.01700622201563	-0.84872618497859
N	1.82658667457371	0.96159547036021	0.22250823587589
P	0.19200520319976	0.52927649504485	-1.95869183184036
H	1.43792989628614	-0.97070894702571	-0.43278389056827
H	2.53770413885204	-0.04723821687312	-1.44631127025618
H	0.63495250777695	1.86802258719822	-2.06777325480698
O	-0.84396274955610	0.26768165450982	-0.66426971540534
O	-1.24987175139422	0.99569048545542	-2.95304798261669
C	-2.15150571230946	0.64377938732039	-0.88452264238694
C	-2.36330982611959	1.05490154240729	-2.19689922766652
C	-3.62290619667053	1.46383918994884	-2.59571298887455
C	-4.64876822218441	1.45082383220487	-1.65054281041832
C	-4.42071929644393	1.04043778975555	-0.34445418523721
C	-3.14925177197643	0.62867944334808	0.05882360489717
H	-3.79559478891698	1.78695170581339	-3.61248852454254
H	-5.63896703749212	1.77060355388238	-1.94580483770099
H	-5.22949027892382	1.04467633909287	0.37280796080321
H	-2.94086852175003	0.31397410733219	1.07037932350751
P	1.14097715492739	0.84718149147811	1.74898461509267
N	0.61056648297936	-0.49527168094290	-3.20250390139161
H	-0.04344323889159	-0.64784777628221	-3.94873360046331
H	1.29734447527476	-1.21472411506663	-3.06687792364692
H	0.83864072849410	-0.52920331007625	1.57095649135264
H	2.06612273335461	1.89932926086936	-0.05747975841109
H	2.08713713693009	0.67423731778704	2.77646847168170
O	-0.41533551864547	1.02319377043453	2.37585261412909
O	1.34964286786178	2.64180617643225	1.87866393125097
C	0.26735830142038	3.22098290425589	2.43362425097151
C	-0.74593155484373	2.31186178351202	2.72758666989072
C	0.09310825908820	4.56550249652421	2.70427605276744
C	-1.93961917767865	2.70156885449869	3.28648031679258

C	-1.11190181762271	4.97253990905800	3.27688331405484
H	0.87794437684018	5.27310682734304	2.47738157468104
C	-2.11504735298185	4.05841759429989	3.56449092985709
H	-2.71097613823925	1.97548790214489	3.50048238069626
H	-1.26204495196321	6.02054942374231	3.49830784634137
H	-3.04311922824827	4.39390467819645	4.00576839656874

1g^{-C-N cleav} E = -912.806246243515 au

ZPE = 0.20722106 au

G_{corr} = 0.16862202 au

C	0.14120925384888	-0.94021747045770	0.35628237436665
N	0.13946117694648	-0.17602352561837	-2.13506559392561
P	1.26201747718595	-0.12158045443612	-0.90273960715912
H	-0.16139200728053	-1.89381135443940	-0.07979371538145
H	2.21751538896711	-1.15600392537400	-0.82845208649671
O	1.42649306133449	1.19268587576639	0.16460097688849
O	2.44668892784982	0.71315127190876	-1.99499905333525
C	2.20755953932595	2.22185369922369	-0.30257453830467
C	2.77227282326348	1.93476443443154	-1.54385995769235
C	3.58180278017269	2.86730065945239	-2.16755110224018
C	3.81304048578782	4.08104073047482	-1.51983415096549
C	3.24425460498663	4.35587601151161	-0.28456483838885
C	2.42371951622243	3.41591076570490	0.34332552735529
H	4.02521799767496	2.64702595426128	-3.12837978053484
H	4.44778265002336	4.81796367090424	-1.99332127891476
H	3.43473844289133	5.30286719706993	0.20099266292449
H	1.97153533502141	3.61225224986191	1.30541963992958
H	-0.78586664380848	-0.43448000500908	-1.83887677768201
C	0.20628283177373	0.39914951763408	-3.47155883015861
H	0.15221757102358	1.48755835608261	-3.46377022414443
H	1.12350325314255	0.10864725601223	-3.96976688929975
H	-0.63363661437903	0.01486454766950	-4.04743652908919
N	0.92231248291213	-1.21189127075505	1.55104775233603
H	1.10181203865465	-0.35028483856905	2.04695859633977
H	0.42262934062455	-1.82739851352685	2.17800493305066
H	-0.76340871416606	-0.33676991978435	0.51595621052236

1a^{=C_P-C cleav} E = -950.477322694369 au

ZPE = 0.15869830 au

G_{corr} = 0.12156388 au

N	-2.23287758000062	0.84274669528253	0.85853669973724
H	-1.74563785845330	0.43915667635671	1.64507619904561
C	-0.55339151072743	2.96882154289269	1.17746517783995
H	0.10509449183063	2.73013397448951	0.34660483726731

H	-0.48323433384206	4.03835451845112	1.37154052151157
H	-0.20968437421827	2.43787192737868	2.06402339614236
N	-3.62697198349540	-2.70052310524740	-0.10041614149251
H	-4.36761913624259	-2.54918686410298	0.56794204206440
C	-3.50978416243161	-4.07185917697880	-0.55905725083404
H	-3.20572396456823	-4.77995199966074	0.21988431273026
H	-4.46251164614818	-4.40722363718528	-0.96891279086583
H	-2.77130238836242	-4.11962701260496	-1.35681726837936
P	-2.29891015915936	2.56264102960070	0.71361864840344
P	-2.23584014538937	-1.73235572217030	0.04404301455892
H	-1.93385419583642	-1.74226174055690	1.45899787725449
H	-2.86127687983425	2.90203226846619	1.98503170409864
C	-2.99143953337630	-0.04915589961876	0.10888881940624
C	-4.06281980708235	0.26213209625475	-0.62604600127891
H	-4.51629728044713	-0.48380148321627	-1.25917314450439
H	-4.48080584221531	1.25909323216953	-0.63681782270539

1a^{=C-C-N cleav} E = -608.957355163218 au

ZPE = 0.15040540 au

G_{corr} = 0.11637243 au

N	-0.58332277288394	0.31842820495220	-0.62842339651448
N	-4.30782720345532	0.10404478660248	0.75574689903397
P	-1.63305526244233	0.72833762300695	0.65020755521045
H	-2.26957149524811	1.93467830647290	0.19870727489026
C	-4.37030466330545	0.70439181068386	2.07792620516833
H	-3.76397938257579	1.60699249272043	2.11581785807713
H	-5.39661126744688	1.00184748809487	2.27978207426657
H	-4.03304597342785	0.03914344413871	2.88078812832856
H	-5.03758801668710	-0.58081656522472	0.61863449778039
C	0.83661808695585	0.58841207138945	-0.49205207771749
H	1.11376993720832	1.63491756100173	-0.66268853033699
H	1.15648010247876	0.32020051012301	0.51252834735014
H	1.39740107483758	-0.02930200063006	-1.19362917917943
H	-0.93471915107238	0.45293922323851	-1.56476564644366
C	-3.08823137494342	-0.34711999899223	0.25829276524994
C	-2.95252465897412	-1.46400796380833	-0.46677292719175
H	-2.00267527937440	-1.73341592410525	-0.89780277109078
H	-3.79341781964340	-2.12264095966449	-0.65102328688117

1a^{=NH-P-C cleav} E = -966.529185711248 au

ZPE = 0.14826006 au

G_{corr} = 0.11137951 au

N	-1.93900532632782	0.80207782888408	0.51628783754163
H	-1.10047738437750	0.44808968487449	0.94956653083393

C	-0.62440039041669	3.07542378811750	1.09837257625634
H	0.01407676542278	3.04318224100372	0.21885705964834
H	-0.68545781085324	4.11171164397861	1.42561236120574
H	-0.16017242563516	2.49785413813537	1.89719990591271
N	-3.63912697000041	-2.71789475720906	0.10001825694620
H	-3.99894469741359	-2.67265724552507	1.04184711414536
C	-3.83159279355888	-4.01299677446191	-0.53243916684519
H	-3.28336411670790	-4.82900450106334	-0.05103988422296
H	-4.89130069252476	-4.26662367744773	-0.53244664962869
H	-3.5040521651194	-3.95617579058760	-1.56794786173850
P	-2.33213858324389	2.50512492427383	0.65089360493305
P	-2.22915467279248	-1.81857522586193	-0.23831167379402
H	-1.45367595471119	-1.92000225899945	0.96844647473218
H	-2.84240237745863	2.52752352859992	1.98743385187252
C	-2.89466084649539	-0.11398011683058	0.16653158040425
N	-4.11431845577869	0.23453902437040	0.03534294385223
H	-4.67052190061457	-0.54569072425125	-0.31031907205513

1a^{=NH_C-N cleav} E = -625.005306949168 au

ZPE = 0.13862108 au

G_{corr} = 0.10430749 au

N	-0.43565090672810	0.14148772202574	-0.33579162468415
N	-4.24478629426405	-0.03595382211694	0.73078721255054
P	-1.60369388898627	0.75042310736348	0.73117520377319
H	-2.09096988443994	1.97656399111150	0.12861200889585
C	-4.35672361335101	0.56738991688205	2.04392080456391
H	-3.91945138800700	1.56380206757659	2.05234729926579
H	-5.41099115517876	0.67821583069209	2.28304202813632
H	-3.87967320504109	-0.02157581123695	2.83014995479493
H	-5.00135234414840	-0.63982021978946	0.45164232185590
C	0.87565761504301	0.75075192324070	-0.36900148625461
H	0.90529770208588	1.73027360214466	-0.86398498687748
H	1.24675665734941	0.88415174582177	0.64712072823887
H	1.57098608143500	0.09154568648121	-0.88730626401720
H	-0.80871536097914	-0.16193005253072	-1.22725841818069
C	-3.06955080356856	-0.21119622742365	0.05320645525713
N	-2.88241693955723	-0.92795038999799	-0.98904784824169
H	-3.72308513166374	-1.42991227024409	-1.27944321907663

1a^{=O_P-C cleav} E = -986.405400693603 au

ZPE = 0.13621371 au

G_{corr} = 0.09933156 au

N	-2.11156143551578	0.59522968952896	1.64809986506449
H	-1.45575728896183	0.14091352068000	2.26501047194279

C	-1.08960732288272	2.84754492700852	0.34133228978597
H	-1.50237187211847	2.60637741428923	-0.63400192430714
H	-0.94789713083713	3.92660182164447	0.39181855071984
H	-0.12744713073019	2.35540329243773	0.45510564173596
N	-3.05627341628783	-2.51321479878519	-0.51984444599890
H	-3.77694718620022	-1.92444898718802	-0.91738652909387
C	-3.20771670698364	-3.92482565299503	-0.81677526798328
H	-4.09066265720617	-4.38833430597391	-0.35971736608669
H	-3.27399342167963	-4.06325030920104	-1.89498005632974
H	-2.33038140813928	-4.46803673992312	-0.46876640395030
P	-2.32149369414860	2.35115110297411	1.63563998490516
P	-2.57944734020482	-2.04725338354232	1.04655735644123
H	-3.79201491601366	-2.05569650789647	1.83349432655815
H	-1.46315735852661	2.52423002483149	2.75691721436381
C	-2.76861178147679	-0.18004487468732	0.75190072339680
O	-3.43816388208655	0.27990520679793	-0.16065266116430

1a^{O-C-N cleav} E = -644.887965443286 au

ZPE = 0.12727227 au

G_{corr} = 0.09318706 au

N	-0.41919172275156	0.14511594398369	-0.32719777648302
N	-4.21289655857764	-0.07798541456154	0.68521000600654
P	-1.52888432202532	0.59734179269685	0.87149967326145
H	-1.97314505782635	1.93391745556765	0.52833120125429
C	-4.43364524251245	0.65388220297106	1.91268566284766
H	-4.65024201783309	1.71035881214618	1.74011044178702
H	-5.26735191580490	0.21167922413636	2.45153293050031
H	-3.55421274901881	0.58208357723197	2.54936823691586
H	-5.01714442066979	-0.40076817614378	0.16840993048513
C	0.94894912703066	0.61219551102240	-0.25169208593684
H	1.07898396077749	1.66717426961841	-0.52344091274035
H	1.32527795030819	0.48358797823632	0.76246456640052
H	1.57505392071248	0.01418026291187	-0.91262205178286
H	-0.80519588195421	0.07703207233660	-1.25940512319482
C	-3.04735302426087	-0.14909584542018	-0.00031353181098
O	-2.95762247559379	-0.67342392673389	-1.10134910750990

Fe-1a^{P-C cleav} E = -4344.004664451329 au

ZPE = 0.22750801 au

G_{corr} = 0.16843671 au

N	-2.10112602621531	0.91814145721596	0.75045467384583
H	-1.75421732900783	0.75019880586931	1.68373414357328
C	-0.50673087102174	3.14220259565149	0.71075615172407
H	0.19920969728580	2.72032404995249	0.00362238555987

H	-0.48729223043406	4.22585729254865	0.63145694234359
H	-0.21648513628199	2.85394202924792	1.71890831993598
C	-3.03688316632883	-0.06938336458213	0.27959972789015
H	-3.33509011522323	0.18195438482815	-0.73369945144707
H	-3.94911314368810	-0.14196811297520	0.88255635075804
N	-3.61101847968750	-2.70201432476413	0.02323135892672
H	-4.30813333016815	-2.56739941996823	0.74054625689017
C	-3.58424306501537	-4.05887931107362	-0.50575696477652
H	-3.19555139858520	-4.79575957725216	0.20028927364377
H	-4.59535964650034	-4.34125737591210	-0.78965877353446
H	-2.96873169124836	-4.08374128945882	-1.39820838356722
P	-2.17926219037202	2.55596199907213	0.30633237084351
P	-2.24090797412681	-1.73315007240224	0.17962806200338
H	-1.78740142039606	-1.85531065819970	1.52735877242218
H	-2.93225396840087	3.18801250423990	1.33116236587695
Fe	-2.95325403491437	2.98128640722893	-1.69962253295571
Fe	-0.65361619881679	-2.00428727792522	-1.29786417966904
C	-4.53740578054973	2.40646378882682	-1.15585584349427
O	-5.57895723562319	2.05726867501029	-0.78787727561464
C	-2.63696610469478	4.70166088584049	-1.42708183027702
O	-2.44037024579738	5.82890919303721	-1.25859896810501
C	-3.58977045618654	3.23909438019671	-3.32947269474976
O	-4.00461051054268	3.40621285757755	-4.38979763494912
C	-1.59342768673424	2.05947001884212	-2.37824047804277
O	-0.69330468736101	1.50920882133742	-2.84807779339212
C	0.29542265412328	-0.71223063141904	-0.54323677151988
O	0.98902543680764	0.08842631343425	-0.07696149358048
C	-1.86345792562762	-1.61061988520442	-2.53608347712242
O	-2.64727038272776	-1.34141974499394	-3.34217936483404
C	-0.34703609188757	-3.61873051685214	-0.63788354326961
O	-0.12593645462208	-4.66624538669268	-0.19720772382325
C	0.56494942397654	-2.23191928425661	-2.55686238694582
O	1.35747368659460	-2.37973195602549	-3.37851337056711

Fe-1a-C-N *cleav*

E = -2286.709504449469 au

ZPE = 0.18253944 au

G_{corr} = 0.13688639 au

C	-3.30726816071206	-0.14963744680073	0.55950968773500
H	-3.06608193382707	-1.15850799413493	0.22299898731572
H	-3.87958816168100	-0.25103016992510	1.47842070981740
N	-0.57987107084082	-0.45277487536479	0.27412516575988
N	-4.09969933054160	0.53225081039143	-0.42062644172124
P	-1.65196394554080	0.62440198710882	1.02885987031405
H	-1.69713422897942	1.78969218569942	0.20926824377905
Fe	-1.19845396332040	1.06889663852175	3.13853447169549

C	0.08464004458504	2.13947409219716	2.55414770169477
O	0.91077064410179	2.85263295532394	2.16595630143049
C	-2.82499290835338	1.74247067905041	3.32555371181858
O	-3.88497837675286	2.18588936481209	3.47102772928762
C	-0.77240834166809	1.41383471586709	4.81849982717190
O	-0.48969250048405	1.64030745892654	5.91213058498268
C	-1.00003712829441	-0.67388294361480	3.40923205417455
O	-0.86616081611845	-1.80551730389118	3.60659090320472
C	-4.68921030786457	1.78497254896734	0.02091142030039
H	-3.96613895186580	2.54384996214471	0.34393739235106
H	-5.28444630109930	2.20431482466348	-0.78673099013449
H	-5.35377140673576	1.59131596808999	0.86044669890452
H	-3.59842983555179	0.65029694553762	-1.29052918031528
C	0.86361903647390	-0.31186493928197	0.41355197219111
H	1.27356224387756	0.56214495249905	-0.10015417787843
H	1.11305245394843	-0.23345004916159	1.46660998525101
H	1.34280062966237	-1.20627926390709	0.02205725584973
H	-0.85488437241717	-0.70269112371876	-0.66578077498054

Cr-1a-P-C cleav

E = -4131.990607062913 au

ZPE = 0.24457818 au

G_{corr} = 0.18103495 au

N	-1.87264911045263	0.75288894824305	0.54058870584652
H	-1.38872533787513	0.49245777377156	1.38871823232886
C	-0.12225815317594	2.83541654515095	0.40302145402054
H	0.41008878961151	2.44777175617160	-0.45866539323170
H	-0.00955500333984	3.91648223027172	0.43006006612201
H	0.30510754551818	2.41474732060833	1.31076182970208
C	-3.00667263474258	-0.08445568704884	0.24672019624312
H	-3.44576078203062	0.22008347169188	-0.69559374417830
H	-3.79754392443223	-0.04914594512084	1.00514766872763
N	-3.97136227884228	-2.52234201488264	-0.40535482248260
H	-4.72789866874493	-2.19789889332737	0.18206849252266
C	-4.08532800269275	-3.94889963372544	-0.68658932342785
H	-3.89906191248983	-4.58752781884599	0.18153973475108
H	-5.08658400771380	-4.15140314982302	-1.05892694276998
H	-3.38733641580360	-4.22716522256750	-1.46786416471853
P	-1.89584458040676	2.43562268725554	0.25001038438595
P	-2.46983564752784	-1.84294925800610	0.01189747767838
H	-2.26843697615116	-2.17373533602509	1.38892516761226
H	-2.35441509309522	2.99008873797042	1.47763982495541
Cr	-3.09631484513072	3.29085477470156	-1.54995390041462
Cr	-0.59409111168501	-2.29351840568659	-1.25814363875119
C	-4.65711079728444	2.75284035658014	-0.67020720850083
O	-5.61467645001236	2.41057708408057	-0.12270004881532

C	-3.08906868024990	4.91086533766990	-0.60859685084100
O	-3.08578339724020	5.91403107893034	-0.03949888130594
C	-3.11005861818175	1.72548279047118	-2.58483048317733
O	-3.15352938113213	0.79990909141113	-3.27059201466970
C	-1.48540313543480	3.76268762123195	-2.39202105462324
O	-0.50151111341763	4.05637848743840	-2.91285416601878
C	-4.08474332820269	4.11859444026513	-2.88254421925908
O	-4.70526653631019	4.64047449134818	-3.70274918851372
C	-0.36816082671350	-0.52846161244199	-1.85220523237790
O	-0.13301869526495	0.52369790463935	-2.26071988699625
C	-1.66984671291820	-2.61709636003971	-2.76772998537646
O	-2.31403861448278	-2.79837065321934	-3.70404437994521
C	-0.69714424900724	-4.07772414293528	-0.69347793337076
O	-0.72438156955781	-5.17782167267590	-0.34666037411598
C	0.94213793129596	-2.74019216107228	-2.19667657342598
O	1.89888770857723	-3.02733605464938	-2.77328081246506
C	0.38506939765687	-1.83165178780713	0.26152644366973
O	0.96151631908398	-1.50584753000248	1.20905873520723

Cr-1a-*C-N cleav*

E = -2180.702469706802 au

ZPE = 0.19122809 au

G_{corr} = 0.14448632 au

C	-3.00449252105425	-0.32960624430115	0.23346572959393
H	-2.50620990008796	-0.99850022982203	-0.46614589442494
H	-3.35650980062530	-0.94277366148959	1.07032667713739
N	-0.41548457174046	0.41198907233642	-0.21427293955403
N	-4.05491146803909	0.39431435152280	-0.44804921511861
P	-1.66719911403976	0.80898524702940	0.87770929839306
H	-2.20666434132927	2.03448032672621	0.39480085875079
C	-5.01569802616337	1.00229734455306	0.45892848065257
H	-4.53899457997620	1.79928136113871	1.02678088330427
H	-5.82260452500831	1.45232137950131	-0.11438057738565
H	-5.44769314428008	0.29608786323461	1.18123893215869
H	-4.53289150256985	-0.23024898359039	-1.08346151865657
C	0.89263994000012	1.04611624564890	-0.11018144856623
H	0.87772581237598	2.13012949016571	-0.25638585494076
H	1.32493223425355	0.84166512851459	0.86272290420918
H	1.55115137467248	0.60655091777979	-0.85603136941824
H	-0.74933964060822	0.41461941246639	-1.16979118068829
Cr	-1.17209843650092	0.85010287163968	3.15376923930643
C	-2.51656501267321	2.13754491815070	3.33151417589281
O	-3.35253694441871	2.92761876926172	3.42860212554019
C	0.06746167186460	2.22377560140739	2.85450304722860
O	0.81695804895836	3.08943884527214	2.71170922662904
C	0.12547582812730	-0.48294241425399	2.89865817975847

O	0.91257998839353	-1.31326641065258	2.75938636980420
C	-0.78120312760953	0.93509669943910	4.96297755835328
O	-0.53353208731209	0.99148018740692	6.08892635694259
C	-2.43230379826461	-0.48448223318748	3.52098400569377
O	-3.20638216634443	-1.29718242589848	3.79084734940392

Mo-1a-*P-C cleav*

E = -2180.570670592234 au

ZPE = 0.24030525 au

G_{corr} = 0.17444454 au

N	-1.86065812416993	0.76063989302463	0.62663054392532
H	-1.40924481137540	0.50348640031381	1.49356983313984
C	-0.09114177479186	2.84128878210709	0.45988979288316
H	0.43779968307017	2.44469164400881	-0.39972452236848
H	0.01846737565992	3.92311298762976	0.47167164028340
H	0.34164782316207	2.43414591556528	1.37121437953409
C	-3.01084838533234	-0.05215091758289	0.31654681802165
H	-3.41429776532039	0.25162033298824	-0.64271362767220
H	-3.82114896547215	0.01913980271890	1.05156774038868
N	-4.02232698881336	-2.51448602346208	-0.20249224522898
H	-4.74327696506585	-2.23577569241568	0.44896731860882
C	-4.13271641442138	-3.92214041442779	-0.56496781371565
H	-3.91275654422432	-4.60988701990857	0.25639168969458
H	-5.14283665820303	-4.11479323655636	-0.91885109976421
H	-3.45346544661657	-4.14146538609461	-1.38102858647160
P	-1.86582911191795	2.44025683045560	0.31338738916650
P	-2.50520613585141	-1.82384355212261	0.12682636119081
H	-2.24719525287882	-2.09575230691326	1.50771661188228
H	-2.32240375870291	3.01906386440329	1.53127253029214
C	-4.84534346011315	2.74260199843493	-0.71247524226653
O	-5.80616693540782	2.39685421200946	-0.17589888213422
C	-3.16704968302794	5.08687569346215	-0.62860954192800
O	-3.18657333739973	6.09187365242130	-0.06587380821125
C	-3.11826483429298	1.60267988126968	-2.72462328882122
O	-3.13823957115452	0.65651189484372	-3.38065451669336
C	-1.37380356753266	3.84456926601037	-2.51860111638586
O	-0.37703509850419	4.13817652052737	-3.01166703118670
C	-4.17356727597889	4.18476924136150	-3.11751917364784
O	-4.77592811187588	4.69116294926684	-3.95973066449640
C	-0.29243606928388	-0.43291221853865	-1.89618109981656
O	-0.06007873260345	0.63109527144989	-2.27165836359201
C	-1.76036789280821	-2.66786142719589	-2.90814431436938
O	-2.43844319315373	-2.82599794813959	-3.82330333365421
C	-0.69217153008165	-4.30108943397950	-0.71523747107518
O	-0.74127159719322	-5.40565021212198	-0.39053066140999
C	1.07692234826465	-2.83607523454098	-2.36129083820535

O	2.01527063563739	-3.12156023349164	-2.96695015504368
C	0.56543003509870	-1.91885092359039	0.33782536968262
O	1.16224730933926	-1.62138742414622	1.27978564303526
Mo	-3.13461480864212	3.32169835559685	-1.63592320743769
Mo	-0.55168527802013	-2.35622618464079	-1.29340989613252

Mo-1a-*C-N cleav* E = -1204.992043390577 au
 ZPE = 0.18904613 au
 G_{corr} = 0.14018246 au

C	-2.95215600557907	-0.28180580537955	-0.02109625876627
H	-2.51703766182052	-0.73288757100124	-0.91158286317912
H	-3.09272338581094	-1.08536251708702	0.71305738528388
N	-0.33631340241840	0.44824610371644	-0.33018003682894
N	-4.16687513130689	0.41145817046770	-0.38634693665353
P	-1.65249216870276	0.87327301025159	0.66936527067134
H	-2.17900135478929	2.08265736356573	0.13145558509326
C	-5.00010737538893	0.78011170854442	0.74677845482094
H	-4.49579690120427	1.53491846268958	1.34624974996568
H	-5.92563732904848	1.22188176780289	0.38549508487014
H	-5.24615402752961	-0.05928480360769	1.41004572630877
H	-4.69609611165012	-0.16390202926951	-1.02741461939838
C	0.99408267055656	0.99092614420868	-0.09123293339797
H	1.07011387668072	2.07162456741378	-0.24249984970445
H	1.30127016197480	0.76973813595138	0.92455641290644
H	1.69709894288590	0.49819060738763	-0.75953404902294
H	-0.57619418710097	0.47554201057841	-1.31235590609788
C	-2.60668162597132	2.43024799779303	3.27181364864413
O	-3.38327435286506	3.27878848633614	3.34573489865794
C	0.20587154489330	2.34074680674165	2.87972338938911
O	1.01357735593179	3.15520506893976	2.76869429154620
C	0.10063582721811	-0.58491272331678	2.94704879590524
O	0.85025062103002	-1.45400238218289	2.85253773358293
C	-0.93050515564608	0.99933240761025	5.10914671792197
O	-0.74650041263433	1.03790305480627	6.24730327777426
C	-2.70432240561850	-0.43976455228255	3.44047406939899
O	-3.52771242884825	-1.21883789398221	3.65078147231229
Mo	-1.24170938723719	0.93486183330401	3.13113288799582

W-1a-*P-C cleav* E = -2252.110845399768 au
 ZPE = 0.22131713 au
 G_{corr} = 0.15551698 au

N	-1.71223230643165	0.74073988099703	0.42177399179715
H	-0.83972281058423	0.40794090704413	0.03725168454886
C	-0.29790391290679	3.05806782559354	0.61491321809585

H	0.25435247983514	2.87254509123357	-0.30246680875062
H	-0.32610745658539	4.13297831083192	0.77384352676352
H	0.20196952212191	2.58191020151063	1.45389123088521
N	-3.78917303354470	-2.48925800401441	-0.27796225029776
H	-4.49873032250529	-1.99046590935427	0.24473808062383
C	-4.03662965323808	-3.91340990269563	-0.43134557363881
H	-3.93940530137034	-4.48084987187280	0.49958580819979
H	-5.04151206787521	-4.05546214638276	-0.82073371087095
H	-3.34458896643907	-4.33303207023380	-1.15606066020411
P	-2.01675746594840	2.47083774517900	0.41858877951823
P	-2.24046976615497	-1.93133244744691	0.06852368517270
H	-1.93476190378255	-2.31329270145376	1.41339037280450
H	-2.49640798833729	2.59684551486337	1.73941406303029
C	-5.07390341257807	2.99811695726102	-0.31253664865920
O	-6.02351645832397	2.78812445934828	0.30111577230384
C	-3.21866264413853	5.21685004300929	-0.50873513052127
O	-3.10469563801356	6.24144578845771	0.00962703378663
C	-3.50834870165435	1.53784481900817	-2.25499361139742
O	-3.55111998843029	0.47647304479888	-2.70037812814982
C	-1.69937506006430	3.78039649197599	-2.48336098288909
O	-0.74384330452208	4.01132713685434	-3.08598532340646
C	-4.51309884445455	4.18920699069206	-2.88006795720753
O	-5.15703404594272	4.64861625937005	-3.71931180732216
C	-0.28581873508787	-0.46730903857133	-2.20573921986509
O	-0.18784548189067	0.61591201900423	-2.59719644004676
C	-1.77467970397681	-2.76744836976893	-2.98752534337182
O	-2.55513955543225	-2.97475538291330	-3.80516820612187
C	-0.43267525157542	-4.33280259855205	-0.90766446555072
O	-0.44243219596496	-5.43309553472707	-0.56713640524070
C	1.12701045828086	-2.84304776251736	-2.77152616869702
O	1.99595614041033	-3.12003135782589	-3.47723548837645
C	0.92597165995986	-1.93917602957716	-0.03525131977475
O	1.65508851961810	-1.66712221099188	0.81821475544079
W	-3.38755645905058	3.39327967312678	-1.40779054414281
W	-0.38767323913975	-2.38082780885006	-1.52507291487709
C	-2.72602649386542	-0.14809465787575	0.48238201207018
O	-3.87154323041583	0.13829668546513	0.78603131433900

W-1a-C-N *cleav*

E = -1277.738219748889 au

ZPE = 0.17020066 au

G_{corr} = 0.12014446 au

N	-0.51998673001718	0.17208778901321	-0.35854151439973
N	-4.31171443877165	-0.33823899999622	0.54277028072007
P	-1.74382679013491	0.77335756729421	0.61713839349221
H	-2.32768705570151	1.89583495499924	-0.05501738154315

C	-4.84752243920458	0.76305583151431	1.31599116553814
H	-4.33491334332816	1.68895419800788	1.07786208770961
H	-5.89366096476198	0.89499074261036	1.05459668626712
H	-4.77505421765322	0.59035884476154	2.38750336688432
H	-4.93796292460161	-1.08767140818240	0.28921991062884
C	0.71523221575902	0.89388813016043	-0.58476091099138
H	0.59869071630641	1.78134933825814	-1.21500687423657
H	1.14266475503142	1.20976865410944	0.36289236119255
H	1.43158533042743	0.22657877623993	-1.05785702824996
H	-0.85175003699343	-0.40604157297968	-1.11798630266086
C	-2.65661864159497	2.52132513223755	3.22342095613828
O	-3.50088812215052	3.30084767750612	3.34266655849954
C	0.07119321724741	2.68815138883164	2.44289518033178
O	0.75776271495284	3.56064663751688	2.12977373357822
C	0.35957836508424	-0.19482836976938	2.79235175180566
O	1.21844734442123	-0.95156238112785	2.67540396282680
C	-0.62432891993128	1.44740397151099	4.93166288604502
O	-0.31273669458291	1.61326830875270	6.03102583176392
C	-2.40185054803559	-0.35445642848190	3.57622689876460
O	-3.10742274044921	-1.21036412528997	3.89387080658437
W	-1.15903975043520	1.16259058556787	3.01494346174088
C	-3.05050296219405	-0.52155978890657	0.11477259575796
O	-2.70532855868785	-1.47101883415854	-0.57254329418837

B-1a^{P-C cleav}

E = -965.647309504553 au

ZPE = 0.21665475 au

G_{corr} = 0.17642487 au

N	-2.76106508658806	0.95796059894750	1.21266924511258
H	-2.35056653339997	0.68081721855039	2.08966951996143
C	-0.36043612613971	2.24512675410999	0.26984765268636
H	-0.11555025329815	1.49146786501691	-0.47139185114328
H	0.00106777997598	3.21376289470168	-0.07035754896137
H	0.12413511181218	1.99060664974693	1.20929552337378
C	-3.49802649882939	-0.05864437611648	0.50440369558939
H	-3.76998800978131	0.31389365539000	-0.47926629988434
H	-4.42818463396391	-0.30533335220520	1.02336601897614
N	-3.64501829253812	-2.59200971416110	-0.56999160702691
H	-4.51022325043378	-2.76456280591181	-0.08080629597133
C	-3.20316595217903	-3.71556824619573	-1.38933182999984
H	-2.90723626915038	-4.59146469211979	-0.80606143518897
H	-4.00943563960819	-3.99885827340412	-2.06262812807815
H	-2.35620347212451	-3.40666136225927	-1.99204636640577
P	-2.17044447769964	2.33890536500554	0.43762347091310
P	-2.53342366907046	-1.61225657830287	0.22819859066782
H	-2.41231611942731	-2.07805877440770	1.56971747531260

H	-2.30913902161582	3.30844145457117	1.45338421052334
H	-2.78860549206948	1.90024962739543	-1.96530794798839
H	-4.26677830291858	2.81640917825614	-0.90976182424823
H	-2.61373133267830	3.83820546349034	-1.46640079417668
H	-0.98262034880461	-0.89968243810644	-1.64695483651933
H	-0.21718511938414	-0.78553441921175	0.22682108976508
H	-0.37764462547704	-2.56952723446985	-0.65351333308129
B	-0.82438655168270	-1.44879659645196	-0.58374074323957
B	-3.08903595292544	2.76300375814205	-1.17313357096816

B-1a^{-C-N cleav}

E = -597.538405624394 au

ZPE = 0.17675871 au

G_{corr} = 0.14103255 au

C	-2.92926073699092	-0.28723733556363	-0.12242435293063
H	-2.85928330134013	-0.44225875901490	-1.19991749533704
H	-2.74402752269445	-1.25823969390692	0.36050306236476
N	-0.15134994814383	0.16078930438847	-0.13441256762771
H	0.60424068338542	0.30021360908591	0.51826762758289
C	0.24257333068745	0.23683303301659	-1.53202942626150
H	0.46869084064041	1.25401631707336	-1.86789837769554
H	1.12116139295471	-0.38339974282816	-1.69547424936354
H	-0.55052211323715	-0.15697851108597	-2.16373435214559
N	-4.19892728072600	0.32898603847299	0.18827319491934
H	-4.26072287018091	0.48491325244035	1.18609207632782
C	-5.33939297885528	-0.44530752683156	-0.26968474476200
H	-6.25781837431619	0.04512776432519	0.04583829059723
H	-5.34407991272959	-0.48210323020727	-1.35889156144885
H	-5.35571419002037	-1.48082718772090	0.09999945139860
P	-1.58704196394997	0.84501033615112	0.42026689883186
H	-1.83952579322280	1.97306931538628	-0.39891349861888
H	-2.64340618363562	1.61862684973403	2.57032463517098
H	-1.36228382527170	0.07093995233907	2.77853961665902
H	-0.65836237341258	1.95311646334742	2.49064108332622
B	-1.55508298894045	1.16507498139852	2.29593901901258

O-1a^{-P-C cleav}

E = -1062.820296972539 au

ZPE = 0.16424101 au

G_{corr} = 0.12612563 au

N	-3.11556128666159	1.10831066659478	1.38022402642146
H	-2.80083385398562	0.83012897423457	2.29781712956674
C	-0.57829994760439	2.05973661411872	0.40773198064952
H	-0.48218771211435	1.20411159222478	-0.25487984392316
H	-0.08805368322445	2.92761274752712	-0.02867830458873
H	-0.10558929110371	1.81984152004109	1.35935097062914

C	-3.68837978064387	0.06202957847941	0.56401270517372
H	-3.93850685965594	0.47907003004995	-0.40970060061980
H	-4.61774437582623	-0.30697454709751	1.00766364475257
N	-3.48732070195092	-2.48630806846359	-0.47012389066248
H	-4.41456977444072	-2.61925276999406	-0.09480973032914
C	-2.87649239792630	-3.69373840960637	-1.01306376006769
H	-2.71968138179094	-4.47533735102252	-0.26427645380665
H	-3.50118778010758	-4.09227010655332	-1.80969900514626
H	-1.91532993737206	-3.43022369708896	-1.44324733323366
P	-2.33727087533060	2.42321177463102	0.63835634553275
P	-2.53113065604105	-1.34071948192402	0.29550370617382
H	-2.28631105981964	-1.77133536958294	1.63810733606095
H	-2.34653023810416	3.33102369633753	1.73029183875452
O	-3.05084348009771	2.85688350353084	-0.59752316359203
O	-1.25132130619801	-1.05389270643649	-0.41840086774559

O-1a^{C-N cleav}

E = -646.122209272900 au

ZPE = 0.15073494 au

G_{corr} = 0.11625838 au

C	-2.95631887533155	-0.27057828322276	-0.20309636152799
H	-2.87642203987722	-0.44755138249653	-1.27857068479988
H	-2.77038737717834	-1.23347093490753	0.29868090381897
N	-0.18928556668304	0.13612164149303	-0.15934363285460
H	0.53553985662326	0.31790021723256	0.51987002679254
C	0.26148606478663	0.23184225627962	-1.54134407402884
H	0.47807866571358	1.25466147877060	-1.86795766671807
H	1.15984513268339	-0.36714947257656	-1.66960085744457
H	-0.49283476061097	-0.17947683052330	-2.20890431016878
N	-4.22845082629425	0.34884347185622	0.09390475398354
H	-4.25787109375992	0.57832619973188	1.07933133310154
C	-5.36771018718499	-0.47748175273322	-0.26274644339690
H	-6.28584135896194	0.02036668597530	0.04263444252750
H	-5.40570723484172	-0.60253774629189	-1.34480565200073
H	-5.35142821104370	-1.48088659348575	0.18811535023609
P	-1.63311988050579	0.87759169077542	0.31166856894612
H	-1.80522885316100	1.96992436896057	-0.58745546756975
O	-1.67679181437240	1.23576164516233	1.76179501110380

W-1a^{C-C-N cleav}

E = -1241.810811806963 au

ZPE = 0.19355199 au

G_{corr} = 0.14376769 au

N	-0.66291229030406	0.27888147711664	-0.53429048234479
N	-4.45956076384357	-0.07644164445437	0.24114913725439
P	-1.85291869894771	0.76770253480234	0.57308905736786

H	-2.50130275012076	1.89055215545963	-0.01881113529422
C	-4.96135853670311	0.88617105855710	1.20890191313096
H	-4.41135699359096	1.81956768595502	1.14112405280249
H	-5.99686976629020	1.11019567895058	0.96717586972364
H	-4.91147075343073	0.53534093883653	2.24277294270254
H	-5.09422518907385	-0.85257472521221	0.11848379063147
C	0.61150971187442	0.97847698982681	-0.60781461246084
H	0.53368883166932	2.01324305267212	-0.95457174755158
H	1.08372371511544	0.98431569026310	0.36840446946347
H	1.26740170777467	0.43561304225242	-1.28448595119594
H	-1.04674704206703	0.06290702719213	-1.44375931504127
C	-2.55919113094769	2.50089135276110	3.21398261191489
O	-3.36809617583542	3.31104473107825	3.36300755566821
C	0.16167686112168	2.55929355455640	2.38981422785036
O	0.88059146461151	3.41269782402290	2.09506881739928
C	0.29005380774727	-0.36332934440942	2.64404072701891
O	1.08449983734803	-1.18152978020937	2.47859338823592
C	-0.53912960829917	1.28305288586573	4.85540217928558
O	-0.19478135596860	1.39918438085016	5.95162419730080
C	-2.44476428286534	-0.37630526762420	3.50637323504850
O	-3.19175974203489	-1.19137688453717	3.83281253987179
W	-1.12797856952047	1.07876889856126	2.94327432788633
C	-3.14081082695778	-0.50626601045690	0.25643903295636
C	-2.75297660148409	-1.76329751954539	0.00839115916667
H	-1.71016901645850	-2.02205981108874	-0.06801818140516
H	-3.47639177251818	-2.55624899204252	-0.13521648738681

W-1a^{C-P-C cleav}

E = -2216.183917647167 au

ZPE = 0.24436919 au

G_{corr} = 0.17711744 au

N	-2.01217624229118	0.76231429067572	0.58162707136165
H	-1.19165033753599	0.45209194872262	1.07954479588483
C	-0.49321040506981	2.97637629473930	0.83044760373309
H	0.16827615282161	2.68706733310146	0.01944969680937
H	-0.47435059053090	4.05904995530171	0.91848834032471
H	-0.14521638129928	2.54324281937779	1.76574918281221
N	-3.59336763845369	-2.86961367122038	0.34104994554216
H	-4.12695121951371	-2.70133032796032	1.18072191526005
C	-3.64084427410258	-4.24998748584222	-0.11549916745377
H	-3.06217802166490	-4.94052184558725	0.50170096855139
H	-4.67840857072612	-4.57616936036859	-0.12239940609052
H	-3.27381965844403	-4.31200055514003	-1.13369428021191
P	-2.19956438880580	2.46376551667131	0.42171803354175
P	-2.23569865488689	-1.88621057282514	0.17424974613251
H	-1.60326477925699	-1.87678102362463	1.45682062470581

H	-2.85012930556496	2.81625100266202	1.63440892843896
C	-5.08169444528219	3.33821952079796	-0.82861629468501
O	-6.15030536659387	3.25609903234639	-0.39970374271153
C	-2.99744874321974	5.28213643308269	-0.58341094665084
O	-2.86838437234514	6.27019950709232	0.00005269490951
C	-3.38693972103315	1.75368238667189	-2.60538355536202
O	-3.48992434282760	0.77431388704946	-3.20043938717979
C	-1.33652933575907	3.80090903417122	-2.38008771386693
O	-0.29542559425488	4.00496859151950	-2.82828767916884
C	-3.97241273950712	4.51014341375750	-3.17285334190375
O	-4.41214485455744	5.08054073198934	-4.07460999171410
C	-0.44855712408433	-0.29962811081700	-2.06197516344880
O	-0.27599707864969	0.81280012825971	-2.31152084598101
C	-2.14707033339462	-2.49964973277288	-2.95889376823364
O	-3.03353108164882	-2.62240737750113	-3.68254749013443
C	-0.53525728390572	-4.29646686006083	-1.27010911660410
O	-0.44866772421624	-5.42900768868743	-1.06980591503783
C	0.76912830016820	-2.60083641159711	-3.10119648088449
O	1.54671531042696	-2.78349984263794	-3.93389159170827
C	0.86226203618259	-2.02557105431919	-0.24699232842772
O	1.64641305315882	-1.84567841985683	0.58186578676522
W	-3.20457889165109	3.52798393815612	-1.59463709456626
W	-0.58664665591691	-2.29014401755641	-1.64676386597564
C	-2.96785678959331	-0.20368052472392	0.31260790842067
C	-4.26652862786238	0.01025171364473	0.10159022482515
H	-4.90316010895624	-0.79715228336972	-0.22028999833004
H	-4.71332811935160	0.98565759667816	0.20421701831230

W-1a^{=NH₂-C-N cleav}

E = -1257.859322016114 au

ZPE = 0.18230180 au

G_{corr} = 0.13237373 au

N	-0.72166232950187	0.57740623643303	-0.70576695407789
N	-4.33599038075524	-0.30118135109102	0.53800000305608
P	-1.83165944038590	0.91937196621422	0.52722334128894
H	-2.54953122255075	2.02058458966895	-0.00106181845798
C	-4.92665043451048	0.83458611669590	1.21799528329657
H	-4.51696493791327	1.76558982119474	0.84113397137691
H	-5.99313241715820	0.84566774013538	1.01052252789496
H	-4.78323549104522	0.80486540897987	2.29746431255988
H	-4.88299237414737	-1.14789484063685	0.55535566931072
C	0.64988357918194	1.04562279663390	-0.59259235693690
H	0.67981310897054	2.13270685768170	-0.57504742494343
H	1.17878686166326	0.67796283992554	0.29003966539364
H	1.19439505680414	0.72114233310726	-1.47604432540712
H	-0.81406732899570	-0.40661152589433	-0.94639308136569

C	-2.56209102785004	2.59123880810778	3.15354403176923
O	-3.36439999436332	3.41553025049152	3.25789633686536
C	0.21800726862663	2.55408307167353	2.42274444095522
O	0.99648005670338	3.36214461395537	2.15604303471011
C	0.21431611326184	-0.35452673312153	2.64700574732025
O	0.97833183224450	-1.20380042014661	2.49696365040032
C	-0.62074784072043	1.30679967822894	4.85869230154488
O	-0.31302399767189	1.41136739414373	5.96682983388233
C	-2.51078279635180	-0.30596803778483	3.43147581554598
O	-3.26867198022597	-1.13094045729873	3.71191382453027
W	-1.16107157628606	1.13305702266357	2.92897983026419
C	-3.02920990013942	-0.47355550138745	0.20741951816029
N	-2.47140782573412	-1.52111648937822	-0.27038790061360
H	-3.11010422114904	-2.30642453919543	-0.38809559832368

W-1a^{=NH₂P-C₂cleav}

E = -2232.235553079767 au

ZPE = 0.23377503 au

G_{corr} = 0.16664760 au

N	-1.80232353353612	0.78472057987201	0.58313724468233
H	-0.84836405742188	0.51308177462060	0.40815230240716
C	-0.55458187141305	3.16129043596411	0.94228813632015
H	0.14607325910554	3.01012930205089	0.12520948794543
H	-0.66263368040016	4.23240029684063	1.09083502419111
H	-0.16860220951341	2.70984791273519	1.85240849032170
N	-3.58607561600776	-2.76041040924064	0.37867610328225
H	-3.96786821762819	-2.72515730941329	1.31266038146437
C	-3.84412391078834	-4.03188941521215	-0.28611358934865
H	-3.33699929429990	-4.87881249875922	0.17881270285250
H	-4.91582419719964	-4.21737659718748	-0.27715246390879
H	-3.53293952200892	-3.97330158827095	-1.32200922397229
P	-2.18931481029619	2.48398358657976	0.47871205728846
P	-2.13139146579791	-1.90888890544985	0.21168779445784
H	-1.52340859892149	-2.00617295894765	1.49217617657905
H	-2.88551145503680	2.61916742112325	1.69864648792619
C	-5.10685112331375	3.07828148012713	-0.65584023204024
O	-6.13237196713211	2.88039985619685	-0.17354451256740
C	-3.19426512195405	5.25103219810982	-0.55535109263903
O	-3.12800337068267	6.26132629117524	0.00040065661176
C	-3.37324017499382	1.63995838115282	-2.44568313607270
O	-3.42280566580808	0.61324579368791	-2.96658496004688
C	-1.46354254667998	3.82552174699076	-2.34700412085090
O	-0.43109936103773	4.05478082480598	-2.80861099064829
C	-4.18803670152017	4.33135129873331	-3.09132505602086
O	-4.70440929492864	4.83985510474658	-3.99020572773609
C	-0.32643548386953	-0.37844078856484	-2.09112136908120

O	-0.13620004503352	0.73086512435963	-2.34447914186980
C	-2.08141385313951	-2.48948151532043	-3.00369717503840
O	-2.93371493532017	-2.57986031303655	-3.77080487611063
C	-0.64674085498871	-4.36292362302491	-1.27335531827649
O	-0.66828864341022	-5.49733244090921	-1.07136265132032
C	0.79514001489234	-2.75016951890028	-3.10352086590648
O	1.56552350843967	-2.98607651786002	-3.92842744310024
C	0.95214230206744	-2.19652942103023	-0.28294655163931
O	1.78309640605402	-2.09007562936992	0.51068138732162
W	-3.28738709647125	3.45775897965729	-1.51766681854557
W	-0.54382002302151	-2.35702638846184	-1.65376607046371
C	-2.77354731576793	-0.15850639218295	0.40252085499819
N	-4.00269563162242	0.16482327866973	0.39202744200726
H	-4.59337435959327	-0.64877309705718	0.23373490654697

W-1a^{=O-C-N cleav}

E = -1277.738219748889 au

ZPE = 0.17020066 au

G_{corr} = 0.12014446 au

N	-0.51998673001718	0.17208778901321	-0.35854151439973
N	-4.31171443877165	-0.33823899999622	0.54277028072007
P	-1.74382679013491	0.77335756729421	0.61713839349221
H	-2.32768705570151	1.89583495499924	-0.05501738154315
C	-4.84752243920458	0.76305583151431	1.31599116553814
H	-4.33491334332816	1.68895419800788	1.07786208770961
H	-5.89366096476198	0.89499074261036	1.05459668626712
H	-4.77505421765322	0.59035884476154	2.38750336688432
H	-4.93796292460161	-1.08767140818240	0.28921991062884
C	0.71523221575902	0.89388813016043	-0.58476091099138
H	0.59869071630641	1.78134933825814	-1.21500687423657
H	1.14266475503142	1.20976865410944	0.36289236119255
H	1.43158533042743	0.22657877623993	-1.05785702824996
H	-0.85175003699343	-0.40604157297968	-1.11798630266086
C	-2.65661864159497	2.52132513223755	3.22342095613828
O	-3.50088812215052	3.30084767750612	3.34266655849954
C	0.07119321724741	2.68815138883164	2.44289518033178
O	0.75776271495284	3.56064663751688	2.12977373357822
C	0.35957836508424	-0.19482836976938	2.79235175180566
O	1.21844734442123	-0.95156238112785	2.67540396282680
C	-0.62432891993128	1.44740397151099	4.93166288604502
O	-0.31273669458291	1.61326830875270	6.03102583176392
C	-2.40185054803559	-0.35445642848190	3.57622689876460
O	-3.10742274044921	-1.21036412528997	3.89387080658437
W	-1.15903975043520	1.16259058556787	3.01494346174088
C	-3.05050296219405	-0.52155978890657	0.11477259575796
O	-2.70532855868785	-1.47101883415854	-0.57254329418837

W-1a^{=O}-P-C^{cleav}

E = -2252.110845399768 au

ZPE = 0.22131713 au

G_{corr} = 0.15551698 au

N	-1.71223230643165	0.74073988099703	0.42177399179715
H	-0.83972281058423	0.40794090704413	0.03725168454886
C	-0.29790391290679	3.05806782559354	0.61491321809585
H	0.25435247983514	2.87254509123357	-0.30246680875062
H	-0.32610745658539	4.13297831083192	0.77384352676352
H	0.20196952212191	2.58191020151063	1.45389123088521
N	-3.78917303354470	-2.48925800401441	-0.27796225029776
H	-4.49873032250529	-1.99046590935427	0.24473808062383
C	-4.03662965323808	-3.91340990269563	-0.43134557363881
H	-3.93940530137034	-4.48084987187280	0.49958580819979
H	-5.04151206787521	-4.05546214638276	-0.82073371087095
H	-3.34458896643907	-4.33303207023380	-1.15606066020411
P	-2.01675746594840	2.47083774517900	0.41858877951823
P	-2.24046976615497	-1.93133244744691	0.06852368517270
H	-1.93476190378255	-2.31329270145376	1.41339037280450
H	-2.49640798833729	2.59684551486337	1.73941406303029
C	-5.07390341257807	2.99811695726102	-0.31253664865920
O	-6.02351645832397	2.78812445934828	0.30111577230384
C	-3.21866264413853	5.21685004300929	-0.50873513052127
O	-3.10469563801356	6.24144578845771	0.00962703378663
C	-3.50834870165435	1.53784481900817	-2.25499361139742
O	-3.55111998843029	0.47647304479888	-2.70037812814982
C	-1.69937506006430	3.78039649197599	-2.48336098288909
O	-0.74384330452208	4.01132713685434	-3.08598532340646
C	-4.51309884445455	4.18920699069206	-2.88006795720753
O	-5.15703404594272	4.64861625937005	-3.71931180732216
C	-0.28581873508787	-0.46730903857133	-2.20573921986509
O	-0.18784548189067	0.61591201900423	-2.59719644004676
C	-1.77467970397681	-2.76744836976893	-2.98752534337182
O	-2.55513955543225	-2.97475538291330	-3.80516820612187
C	-0.43267525157542	-4.33280259855205	-0.90766446555072
O	-0.44243219596496	-5.43309553472707	-0.56713640524070
C	1.12701045828086	-2.84304776251736	-2.77152616869702
O	1.99595614041033	-3.12003135782589	-3.47723548837645
C	0.92597165995986	-1.93917602957716	-0.03525131977475
O	1.65508851961810	-1.66712221099188	0.81821475544079
W	-3.38755645905058	3.39327967312678	-1.40779054414281
W	-0.38767323913975	-2.38082780885006	-1.52507291487709
C	-2.72602649386542	-0.14809465787575	0.48238201207018
O	-3.87154323041583	0.13829668546513	0.78603131433900

CH₃NHCH₃

E = -134.929342431073 au

ZPE = 0.09143896 au

G_{corr} = 0.06601019 au

N	-1.70379473896227	1.26907364614147	-0.04466802614132
H	-1.45489258528378	1.75854819608520	0.80483907999752
C	-1.19970377945522	-0.08939844633464	0.01725454172512
H	-1.55966420103377	-0.57588782556224	0.92233731760452
H	-1.57924521044577	-0.65756905936409	-0.83242508250049
H	-0.10023111689112	-0.16695285229229	-0.00182898809891
C	-1.19748943949846	2.00260433205722	-1.18878163084742
H	-1.57702515605110	1.55270961845793	-2.10659082149117
H	-1.55574201630913	3.03023691638980	-1.15648673056179
H	-0.09791488606937	2.02309686442163	-1.26452875968606

CH₃PHNHCH₃

E = -476.448801946488 au

ZPE = 0.10045657 au

G_{corr} = 0.07116709 au

P	-2.14709556838504	0.95279959807840	-0.17799066568701
H	-1.81659075307559	1.62608213025266	1.04786443707590
C	-0.85954685399559	-0.36752573098293	-0.00223501689135
H	-1.12959825710559	-0.99828239642277	0.84388465019252
H	-0.85933188943887	-0.98410776823905	-0.89749666280726
H	0.14574434246869	0.01243175134884	0.16458120729784
N	-1.42750581017783	1.99824931260902	-1.33636920262953
H	-2.12355031210705	2.51989891005527	-1.84397533665568
C	-0.24357026068586	2.78383601260717	-1.03816278770784
H	0.05605914222603	3.35349948595879	-1.91737743093360
H	-0.38145111025337	3.48345281929269	-0.20418191504998
H	0.58570077053008	2.12703596544189	-0.78464627620400

(CH₃)₃N

E = -174.163628979555 au

ZPE = 0.11898977 au

G_{corr} = 0.09171436 au

N	-1.64144609910216	1.29482684082829	0.00010710128725
C	-1.20731730876542	-0.08678401743077	0.00000779216778
H	-1.59565500665794	-0.59794461206215	0.87951597988646
H	-1.59243703600037	-0.59680787102963	-0.88157297452036
H	-0.10843706977570	-0.19596624281435	0.00194611668865
C	-1.20499525253588	1.98639186330622	-1.19510420883879
H	-1.58985793702985	1.47959731726743	-2.07865600438958
H	-1.59182497239524	3.00422824773050	-1.19720824396694
H	-0.10592580758014	2.04115656267076	-1.28733877191958
C	-1.20937143925673	1.98484555394563	1.19779877440139
H	-1.59621679186488	3.00267633521737	1.19980825686117

H	-1.59745397755653	1.47690529121801	2.07928194687972
H	-0.11064663147914	2.03949812115268	1.29411998546285

(CH₃)₂NPHCH₃ E = -515.678572570570 au
 ZPE = 0.12790505 au
 G_{corr} = 0.09692091 au

P	-2.10673316798691	0.76463114759888	-0.26194110133432
H	-1.95762065952153	1.52822264078884	0.94867387381891
C	-0.71303025453267	-0.40226698748987	0.08670675706536
H	-1.00332038133723	-1.03031872907400	0.92826464516471
H	-0.56448904884885	-1.04349410883205	-0.77829156653024
H	0.22964221821689	0.08032798380415	0.33399354783888
N	-1.40964316708479	1.82940864827052	-1.42680938711479
C	-0.28391531955465	2.66207336254717	-1.05352069929110
H	0.18756589619019	3.07577187452982	-1.94659107048156
H	-0.57741138057426	3.50190476838652	-0.40732581523224
H	0.46770490699843	2.07980365055929	-0.52852752966501
C	-2.36817732887696	2.53040564689183	-2.26512236841989
H	-1.88396887225402	2.85134748005144	-3.18902744504879
H	-3.18764635607216	1.86550570581056	-2.52502896567025
H	-2.79153843476150	3.42293933615687	-1.78347235509964

(CH₃)₂PNHCH₃ E = -515.697499685354 au
 ZPE = 0.12907068 au
 G_{corr} = 0.09786390 au

P	-2.00135522157806	1.06206728163121	0.05534873607130
C	-0.78647982762154	-0.33091948069124	-0.04410562024287
H	-0.98402581742344	-1.02826165073496	0.76853034294639
H	-0.92577792467054	-0.85872838669624	-0.98403438864301
H	0.25264290935974	-0.01106611102269	0.03018310108294
N	-1.44250794286927	2.07694381626484	-1.21597730630035
H	-2.18705231210041	2.63164669534270	-1.60485634649277
C	-0.16520400934075	2.76568061723213	-1.21191938945746
H	0.02252905870952	3.19744409220161	-2.19469611356663
H	-0.08874133289292	3.56794059468732	-0.46923831698083
H	0.63867188011711	2.05855948943656	-1.01806525982933
C	-1.36445140332156	1.85119610920720	1.61601864653088
H	-1.87727757750643	2.79591238214302	1.78582913649888
H	-1.59045291451868	1.19776528959443	2.45763272916845
H	-0.28975093434276	2.03155608140411	1.60510960921440

CH₃PH₃⁺ E = -382.300394210182 au
 ZPE = 0.06472835 au

$G_{\text{corr}} = 0.03997554 \text{ au}$

C	-0.31694564992790	0.46424124561705	-1.51545132542782
H	0.13805160577031	1.01070829309096	-0.69373030548254
H	-0.05388560018587	0.93990937805053	-2.45641383782388
H	-1.39724853769652	0.46677757436664	-1.39792361627803
P	0.28281113217689	-1.23235183992768	-1.51260514220153
H	1.67145499896552	-1.30405278284091	-1.66082638977018
H	-0.02531952315798	-1.90163599329154	-0.32409175622493
H	-0.26755952594444	-1.99101224506505	-2.55037193679108

NH_2PH_3^+

$E = -398.345925350268 \text{ au}$

$ZPE = 0.05392175 \text{ au}$

$G_{\text{corr}} = 0.02936728 \text{ au}$

N	0.01804051736173	-0.83350130982440	-1.51518671736740
H	-0.04705209178613	-1.38689452438465	-0.67395328733329
H	-0.02105657383986	-1.38053433864310	-2.36217046386692
P	-0.48665383873271	0.71830714993882	-1.51711112116095
H	0.04393311159175	1.35560655909610	-2.64149474746250
H	-1.86964242531662	0.98287956576344	-1.53746542308245
H	0.00889013072185	1.34701557805380	-0.37209063972648

$\text{H}_3\text{CNHPH}_3\text{CH}_3$

$E = -477.589565029473 \text{ au}$

$ZPE = 0.11809318 \text{ au}$

$G_{\text{corr}} = 0.08845913 \text{ au}$

C	-1.33692043658828	-0.70377604920626	-0.21664711077460
H	-2.26695781360345	-1.12855711653188	0.15421947408768
H	-1.26877809759539	-0.79697580424413	-1.29444766419960
H	-0.52063032255924	-1.26070249223879	0.23813332378792
N	-0.77125888592034	1.67026733353119	-1.23383362195656
H	-1.42087131676226	1.36033755686117	-1.94831698745951
C	-0.64653652636385	3.11143920024332	-1.28107425939424
H	-0.35469482646425	3.44372022071715	-2.27677175032525
H	-1.56175438447491	3.66040610150410	-0.99868164526995
H	0.14094985300145	3.43379633493562	-0.59701772788808
P	-1.21694888099191	1.03344707033823	0.40196349385220
H	-1.47169970011175	0.52131798026470	1.76656903531517
H	-0.05672358984544	1.69037580069324	0.89533314630554
H	-2.39397004172036	1.83621616313234	0.52889681391929

$\text{CH}_3\text{PH}_2[\text{O}(\text{o}-\text{C}_6\text{H}_4)\text{-O}]$

$E = -762.959589828384 \text{ au}$

$ZPE = 0.14352100 \text{ au}$

$G_{\text{corr}} = 0.10937087 \text{ au}$

P	1.35508432755784	-0.26674074262201	-1.06248743259694
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O	2.58867986971520	-0.06562736713724	0.16442678434182
O	2.20812418731985	0.93871232042912	-2.00405666538989
C	3.36810278378473	1.02947940327913	-0.03761502023112
C	3.14890103268046	1.60795706499517	-1.28663996798580
C	3.86427731304019	2.71289502214882	-1.69722535988487
C	4.81171665313970	3.24028328763269	-0.81927889698745
C	5.03004993821395	2.66422168335313	0.42444487195524
C	4.30818685106579	1.54174073746255	0.83135980431161
H	3.68945956239185	3.14859771031136	-2.67060944276783
H	5.38096747260427	4.11022458572922	-1.11663626660604
H	5.76861370689562	3.08751398358834	1.09124544594115
H	4.47343294830569	1.08045483236705	1.79457466423608
H	1.21558759290064	-1.56020438496638	-0.48128225962343
C	-0.09714703415030	0.60318886940902	-0.40448462589430
H	-0.23911791552103	1.53783076543961	-0.93823322414907
H	-0.97758584291097	-0.02222714091490	-0.53768774133376
H	0.04166063348635	0.80318442317724	0.65349997577933
H	0.88913805948009	-0.69968904368196	-2.33762995311470

NH₂PH₂[O(*o*-C₆H₄)O] E = -779.027695787523 au

ZPE = 0.13387517 au

G_{corr} = 0.10039772 au

P	1.36223152132365	-0.27509960905699	-0.79418858795433
O	2.61229047170345	-0.03191610122988	0.30664458318396
O	1.86516387037324	1.24051394137290	-1.64288946810189
C	3.42596019663975	1.04181743184432	0.01352459555519
C	2.98397953085216	1.75502829706980	-1.09829679258338
C	3.67920643517185	2.87116223677716	-1.52607255154312
C	4.82088578671529	3.24834135580127	-0.81903952092336
C	5.25138919659843	2.52993962673106	0.28709461139479
C	4.54817439266134	1.40358700274588	0.71931569988495
H	3.34038365017260	3.42614592938431	-2.38937270103401
H	5.37752155391365	4.11718564817286	-1.14338927019691
H	6.13914614333885	2.83848835486054	0.82124554183804
H	4.86626713938066	0.83056257442392	1.57869397028340
H	0.97630275629636	-1.39412366933751	-0.00036263685553
H	1.76335883208660	-1.01897222824354	-1.91908708037244
N	-0.20196286761832	0.28922891682092	-0.84934206749786
H	-0.39140561546070	1.20937860162983	-1.20439248713512
H	-0.88852186414891	-0.09826124976689	-0.22852368794237

H₃CPH(BH₃)NHCH₃ E = -503.044067874976 au

ZPE = 0.13144394 au

G_{corr} = 0.09966598 au

C	-1.31064882809241	-0.75352198460543	-0.12183940665378
H	-1.62656730782795	-1.31330182950452	0.75492667992496
H	-2.00286952553531	-0.95133600464575	-0.93720905929720
H	-0.31422944243842	-1.07920929259610	-0.40575699124929
N	-0.96365771931950	1.76720143871546	-1.17970562909893
H	-1.63964943995093	1.56337462955017	-1.90117357209421
C	-0.48681584637567	3.14574785762473	-1.21115612800358
H	-0.09156295747456	3.36115690067020	-2.20178215819352
H	-1.25852885907379	3.88391230675253	-0.97434828939083
H	0.32068879671393	3.25804617899330	-0.49545271201890
P	-1.24307756167721	1.01196767301064	0.30440480813424
H	-2.59484909539316	1.25614996198013	0.67531210361197
H	1.07724009184501	1.20041679434344	1.25365380567013
H	-0.18451856153964	2.63621949855711	1.94678867551309
H	-0.36886733171506	0.73777833846753	2.58857439298284
B	-0.02044963214532	1.46832951268654	1.68548422016302

H₃CNHPH(CH₃)Fe(CO)₄ E = -2192.222090578422 au

ZPE = 0.13705289 au

G_{corr} = 0.09442059

C	-1.43644116076069	-0.65081341383367	-0.18248279748581
H	-1.88973453140673	-1.18914178947414	0.64497540416392
H	-2.08223883933614	-0.73395439969605	-1.05460048308584
H	-0.47094781939707	-1.09613003195470	-0.40239963495967
N	-0.71230355833187	1.77917557831565	-1.16906414852902
H	-1.31054430883787	1.53585512294988	-1.94568262225087
C	-0.20406255299201	3.14209524165496	-1.25095250050017
H	0.23802791578200	3.29141212149332	-2.23319291058535
H	-0.96656775956217	3.90799981521186	-1.08744225466309
H	0.57726678741718	3.27664085885667	-0.51041296051777
P	-1.18514215822619	1.08681853606785	0.29893413328871
H	-2.52908685972688	1.48528277273915	0.54148331771719
Fe	0.14149825165058	1.47301304355158	2.00887238883404
C	-0.73878780693733	0.23874911372755	2.92251975207606
O	-1.30945464262662	-0.56535775451252	3.52910512549102
C	1.49934588510277	0.96082488774141	0.98915259363546
O	2.39303032366695	0.62580259526212	0.33553548578730
C	1.23835812697966	1.80663681876101	3.35372193100748
O	1.95487180171926	2.02515314208551	4.22865328076813
C	-0.49322427323013	3.12572306250920	2.06371392707562
O	-0.92020778094669	4.20097425854333	2.10929552273263

H₃CNHPH(CH₃)Cr(CO)₅ E = -2086.214030412871 au

ZPE = 0.14558114 au

G_{corr} = 0.10056399 au

C	-1.49325765889687	-0.63501372335564	-0.28549967351392
H	-1.87103368904584	-1.19440433166879	0.56611225730217
H	-2.22496981459206	-0.68517235764781	-1.08950418034108
H	-0.56382490062341	-1.09029767702449	-0.61350992136943
N	-0.80064063782483	1.80146277419094	-1.26572446801966
H	-1.41853630717336	1.49542639013959	-2.00538165601451
C	-0.53455790775105	3.23223572420166	-1.34557802238979
H	-0.20852623075850	3.47307628964909	-2.35467796730632
H	-1.39766109274404	3.85827244595238	-1.09927381156284
H	0.27456371936298	3.49481026039895	-0.67351125940716
P	-1.17480217586650	1.08682966208790	0.23386162321312
H	-2.51376738925772	1.48326659212708	0.52703882830369
Cr	0.26962143003511	1.43676061371119	2.01810049070266
C	-1.16203709149594	0.99495001953475	3.14114655755912
O	-2.04751171905128	0.71420702567701	3.82558911780339
C	0.78081651476728	-0.36392503394202	1.97425519596985
O	1.10177657639824	-1.47183660695144	1.95481727998700
C	1.36766094564740	1.72547613911080	3.48464846650915
O	2.04779177968610	1.90941053722621	4.39851943000503
C	1.69080530441774	1.81964850396032	0.85405265298790
O	2.58047228981009	2.04101522534445	0.15562386693258
C	-0.25705690153456	3.23497138146750	2.05503371159362
O	-0.58169891350897	4.34152927581034	2.09635270105541

H₃CNHPH(CH₃)Mo(CO)₅ E = -1110.503335344629 au

ZPE = 0.14344476 au

G_{corr} = 0.09730156 au

C	-1.47611182134283	-0.66887433243179	-0.39976113990358
H	-1.84959172122647	-1.25349677267515	0.43699996338459
H	-2.18483607370130	-0.74220836663512	-1.22236936635011
H	-0.51970547400847	-1.07869883719083	-0.70969096959546
N	-0.88273026885632	1.81955259733115	-1.33202941263271
H	-1.51718573077965	1.55622231299383	-2.07404214258955
C	-0.57815847950208	3.24419757819296	-1.36146701292484
H	-0.23272343635967	3.51045023604232	-2.35784472760352
H	-1.42606521887466	3.88611576567749	-1.10347164748352
H	0.22846017806734	3.45742850507384	-0.66867606459228
P	-1.23975542346282	1.05805242200375	0.14865304590436
H	-2.59882621399887	1.38459228155510	0.43734307141546
C	-1.27837737081487	1.01564053629909	3.28805762325284
O	-2.17454053495442	0.76166098543033	3.96648123988639
C	0.80477187483728	-0.51681593845587	2.04410031788387
O	1.09751445650461	-1.63130701023345	2.03266048294051
C	1.47959224066157	1.74186378118228	3.65634802211884

O	2.16188273032447	1.91326901502667	4.57016609031094
C	1.83830100545854	1.83234878062365	0.80708363120587
O	2.72160018981463	2.03488358077055	0.09660436586823
C	-0.24591774786245	3.40959366392449	2.09866249637368
O	-0.55264943334533	4.52012840138293	2.12923353847137
Mo	0.28867840342178	1.44809995411175	2.06944980465862

CH₃NHP(BH₃)CH₃ E = -503.044067874976 au

ZPE = 0.13144394 au

G_{corr} = 0.09966598 au

C	-1.31064882809241	-0.75352198460543	-0.12183940665378
H	-1.62656730782795	-1.31330182950452	0.75492667992496
H	-2.00286952553531	-0.95133600464575	-0.93720905929720
H	-0.31422944243842	-1.07920929259610	-0.40575699124929
N	-0.96365771931950	1.76720143871546	-1.17970562909893
H	-1.63964943995093	1.56337462955017	-1.90117357209421
C	-0.48681584637567	3.14574785762473	-1.21115612800358
H	-0.09156295747456	3.36115690067020	-2.20178215819352
H	-1.25852885907379	3.88391230675253	-0.97434828939083
H	0.32068879671393	3.25804617899330	-0.49545271201890
P	-1.24307756167721	1.01196767301064	0.30440480813424
H	-2.59484909539316	1.25614996198013	0.67531210361197
H	1.07724009184501	1.20041679434344	1.25365380567013
H	-0.18451856153964	2.63621949855711	1.94678867551309
H	-0.36886733171506	0.73777833846753	2.58857439298284
B	-0.02044963214532	1.46832951268654	1.68548422016302

CH₃NHPH(O)CH₃ E = -551.629909096137 au

ZPE = 0.10522781 au

G_{corr} = 0.07445607 au

C	-1.32824465206779	-0.73841354526788	-0.11105403645954
H	-1.63563263289116	-1.29612251195001	0.76984545695497
H	-2.05942817126770	-0.90155298506320	-0.90159571806864
H	-0.35558564815976	-1.09740341431134	-0.43618558319394
N	-0.84878022149506	1.74684175950690	-1.14814529489054
H	-1.39058809816796	1.42015468136353	-1.93495010531806
C	-0.57691093614276	3.17901638653240	-1.17014104113808
H	-0.03735568787158	3.43414396318834	-2.07996050240013
H	-1.47811929509539	3.79758680799424	-1.11264048794299
H	0.06032271920257	3.42183512008389	-0.32532461977506
P	-1.19312699325885	1.01578801381959	0.33025125388257
H	-2.53434486715573	1.35952908786935	0.67503099413142
O	-0.22974263562882	1.37852864623417	1.40905670421802

Cl ⁻	E = -460.245974231702 au (PWPB95-D3/def2-QZVPP)		
Cl	0.00000000000000	0.00000000000000	0.00000000000000
1a·Cl⁻	E = -896.786260686427 au (PWPB95-D3/def2-QZVPP)		
	ZPE = 0.05216749 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
	G _{corr} = 0.02244421 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
C	-0.04742246102130	0.00539347451449	-0.00050517495067
N	-0.06444775165922	0.04613880847950	1.47016989224658
P	1.63007105517793	-0.10858791442641	0.66347146355313
H	-0.36047051249507	0.92701539929004	-0.48327451556798
H	-0.42852637560642	-0.88022409094449	-0.50734054760691
H	-0.31516933067347	-0.87387265548714	1.82470000450982
H	1.88113340358628	1.27580002166357	0.78305078746725
Cl	3.32862741269125	0.32008687691045	-1.47016104965123
MeOH	E = -115.705093802237 au (PWPB95-D3/def2-QZVPP)		
	ZPE = 0.05097303 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
	G _{corr} = 0.02818780 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
O	3.42005820706976	0.70829159176762	-1.53064250698150
H	4.29299142540571	0.37649794920285	-1.29795292685576
C	2.87993686643162	-0.10883812859079	-2.55999919534789
H	1.89679543161075	0.29464559274215	-2.79955479744597
H	3.49190320663572	-0.08839483088110	-3.46907836153437
H	2.75674933284643	-1.15003454424074	-2.24043763183452
1a·MeOH	E = -552.231420300403 au (PWPB95-D3/def2-QZVPP)		
	ZPE = 0.10396199 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
	G _{corr} = 0.07035690 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
C	0.06211460293424	-0.28015026333854	0.04928518146833
N	-0.02070546873250	0.08774405786596	1.46014916008983
P	1.64935896902711	0.16954571822851	0.83705254223218
H	-0.41664992506893	0.42026510211890	-0.62528210332291
H	-0.06335727092611	-1.32297811749762	-0.22703684027375
H	-0.13264894524502	-0.72666188289241	2.05616812605675
H	1.63974738506643	1.55785000723576	0.54689049861134
O	3.60025043459682	0.55809705770563	-1.47880739225075
H	4.01962833550790	-0.20780734303008	-1.07276596187762
C	2.89346104506214	0.13385657091380	-2.63817830174775
H	2.41521855010729	1.01852600928674	-3.05628264713933
H	3.56456086845704	-0.28855149995954	-3.39350324089961
H	2.11703002921352	-0.59995137663710	-2.39791653094668
MeNH ₂	E = -95.830635920835 au (PWPB95-D3/def2-QZVPP)		

ZPE = 0.06369288 au (RIJCOSX-B3LYP-D4/def2-TZVP)

G_{corr} = 0.04075224 au (RIJCOSX-B3LYP-D4/def2-TZVP)

N	2.85398337461213	0.18990779577050	-1.14451470046720
H	2.90840056329581	1.10758881018167	-1.57022436571458
H	3.77105920328024	-0.01403951260016	-0.76541208274485
C	2.46390013572353	-0.81776118389355	-2.13056465003198
H	1.46865051254159	-0.58144111447536	-2.51157948576524
H	3.13992368243117	-0.91619016110401	-2.99173961650923
H	2.39933674811552	-1.79208125387910	-1.64263723876691

1a·MeNH₂

E = -532.357781263142 au (PWPB95-D3/def2-QZVPP)

ZPE = 0.11696332 au (RIJCOSX-B3LYP-D4/def2-TZVP)

G_{corr} = 0.08371225 au (RIJCOSX-B3LYP-D4/def2-TZVP)

C	-0.25299133114436	-0.08856205357460	0.16581320957158
N	-0.27185067007517	0.13260957818435	1.61279893379940
P	1.38492537395194	-0.06964709334408	0.96323495593354
H	-0.57700581349437	0.76342982121128	-0.42157595552202
H	-0.59236848865751	-1.04556949836576	-0.22034505026397
H	-0.55879783940574	-0.70244540605871	2.11399781654850
H	1.66065885585911	1.31653040116999	0.84233059349888
N	3.22861102286155	0.18247098103506	-1.34664367654685
H	3.37714961049852	1.09507231155452	-1.76019410916894
H	4.12775912178418	-0.15276242573065	-1.02260288097085
C	2.63701053472293	-0.74544183063844	-2.31035054807542
H	1.66834717901739	-0.35905757318471	-2.63036434116826
H	3.24554592398543	-0.92747063334857	-3.20543168507198
H	2.45704280009610	-1.70259232890966	-1.81879975256360

NHC^{Me2}

E = -304.717435647324 au (PWPB95-D3/def2-QZVPP)

ZPE = 0.12621482 au (RIJCOSX-B3LYP-D4/def2-TZVP)

G_{corr} = 0.09541650 au (RIJCOSX-B3LYP-D4/def2-TZVP)

C	3.25058276064910	0.38361824223080	-1.05185995327593
N	3.97471297756839	-0.69912030650608	-1.45039821413048
C	4.04695983382006	-0.81916796933514	-2.82927351983870
C	3.34619616629389	0.22075336636520	-3.33317581915384
N	2.87544827500106	0.93227915484514	-2.24085943822340
C	4.59666778748512	-1.61988278054794	-0.52042777481889
H	4.20392008314739	-2.63013587679257	-0.65360609744763
H	5.67958508798795	-1.63998787988883	-0.65982702816466
H	4.36981314331929	-1.27569701743176	0.48483132792276
C	2.06958425721058	2.13245773259343	-2.33849999632690
H	1.13191116481111	1.92894800385188	-2.86000344065865
H	1.85351061951162	2.46698178523050	-1.32761026571401
H	2.60768255788415	2.91876968809576	-2.87212363762556

H	4.57653062189765	-1.61317635116961	-3.32685372545426
H	3.15004534821973	0.50419509466991	-4.35282107422634

1a·NHC^{Me2}

E = -741.247584229193 au (PWPB95-D3/def2-QZVPP)

ZPE = 0.17926291 au (RIJCOSX-B3LYP-D4/def2-TZVP)

G_{corr} = 0.14077525 au (RIJCOSX-B3LYP-D4/def2-TZVP)

C	-0.14517456926552	-0.09548256416776	-0.12127707480012
N	-0.41206699304811	-0.10089800662795	1.32034308174792
P	1.34644160952901	-0.09881862823051	0.91627529659376
H	-0.45241638280852	0.81307170802371	-0.62901048267460
H	-0.34110645985941	-0.99864214093583	-0.69362720013318
H	-0.70175419518688	-1.02101331354656	1.63773457990259
H	1.51705999583227	1.29935867927421	1.05837670650015
C	3.26880045959214	0.39082505919942	-1.05972759349477
N	3.97955691264553	-0.69901779517990	-1.45137813017618
C	4.03682643980065	-0.82588566550096	-2.82910219967042
C	3.33994240443302	0.21710713399544	-3.33318132185869
N	2.88649059544741	0.94081858094034	-2.24255931576549
C	4.59687901530595	-1.62073165257087	-0.51793171507786
H	4.27366692473131	-2.64295853192052	-0.72168818274375
H	5.68535695277620	-1.57069882024437	-0.58563606525486
H	4.28310661752323	-1.34132135110938	0.48356549735576
C	2.07620144918092	2.13873493136739	-2.33779067784743
H	1.11519438892810	1.91974399243170	-2.80703223386452
H	1.90633565739970	2.50789216030650	-1.33054553197731
H	2.58986253856203	2.90501113955674	-2.92121127746072
H	4.55803563643267	-1.62558447942469	-3.32600594364767
H	3.13689469204824	0.49690018436384	-4.35228396565259

PMe₃

E = -461.019742945137 au (PWPB95-D3/def2-QZVPP)

ZPE = 0.11211235 au (RIJCOSX-B3LYP-D4/def2-TZVP)

G_{corr} = 0.08285788 au (RIJCOSX-B3LYP-D4/def2-TZVP)

P	1.28344255897223	2.35678218686099	-1.10000505643911
C	0.01047396988936	3.57852663955078	-1.65997879598774
H	-0.17228725370579	3.45093929827315	-2.72839137860924
H	-0.92946860569870	3.39107433759241	-1.13789910036096
H	0.31614258334457	4.61220137640891	-1.47557021059140
C	2.77492833221830	3.07574079281376	-1.92777254793939
H	3.67010063602304	2.55567125309731	-1.58218881891374
H	2.70073012546024	2.92742648296167	-3.00649859179568
H	2.88807764570468	4.14453803872471	-1.72575298449139
C	1.56413766399037	2.98192406881363	0.61963087939705
H	0.68524095131773	2.77268207624197	1.23196067922259
H	2.41119933968315	2.45713958258269	1.06493071226004

H	1.76300190280079	4.05701368607798	0.64408236424898
1a-PMe₃			
	E = -897.547610442017 au (PWPB95-D3/def2-QZVPP)		
	ZPE = 0.16491036 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
	G _{corr} = 0.12725679 au (RIJCOSX-B3LYP-D4/def2-TZVP)		
C	0.45527621034238	-0.55511351515692	-0.10012243291128
N	-0.03199721506826	-0.09439302052122	1.19882587113687
P	1.53229153778183	0.64774447496810	0.74788845593032
H	-0.14335400504412	-0.23292811697622	-0.94453780683538
H	0.83492712993887	-1.56922531882569	-0.18646333299089
H	0.10486156786664	-0.79425877850171	1.92178008755460
H	0.98760990554621	1.83950012220087	0.20495351589361
P	3.86791855959354	1.19859400727044	-1.51153301217060
C	3.80583835630526	-0.53603294719090	-2.14425299369126
H	3.50536512205131	-1.20313456645389	-1.33547815538457
H	3.05662148431906	-0.61015343930685	-2.93421885839286
H	4.76983934995713	-0.86768127692911	-2.53884895164424
C	4.64811256448061	2.03697368514674	-2.96494245898802
H	3.94061995006308	2.06001653804786	-3.79552664676335
H	4.88879456208980	3.06890127950687	-2.70413920596460
H	5.56157921477808	1.53359211754289	-3.29326150985853
C	5.33101923137880	1.07504607528096	-0.39156333119299
H	5.60728159411937	2.07129439534412	-0.04186289962452
H	5.06497708338963	0.47751371248475	0.48137649191908
H	6.19503047611061	0.62229195206889	-0.88522139602132
2a			
	E = -419.177095591712 au [B97-3c]		
	ZPE = 0.03777636 au		
	G _{corr} = 0.01262503 au		
P	1.11402852137814	0.13490485590304	-0.06829584942243
H	1.52995663521492	-1.24218676787874	-0.16821523932102
C	-0.67178958410455	-0.04612082574472	-0.50094978536230
H	-1.38720859958685	-0.06505047720365	-1.30524389251618
C	-0.51106900264964	-0.09058217963020	0.77846620281237
H	-1.00562956025203	-0.17031789544572	1.73142496380957
2b			
	E = -435.232321775046 au [B97-3c]		
	ZPE = 0.02682316 au		
	G _{corr} = 0.00177926 au		
P	1.12127808253353	0.14186791072493	-0.03113975548909
N	-0.59093617831063	-0.20899297088975	0.70975028128918
H	1.52579612215874	-1.21949161317531	-0.23354186361542
C	-0.60147713914128	-0.05681988971328	-0.52668680265038
H	-1.36492509724036	-0.05866321694659	-1.29703389953429

3 E = -116.560864972907 au [B97-3c]
 ZPE = 0.05509883 au
 G_{corr} = 0.03115746 au

C	-0.61380222368123	0.10647851721218	-0.49138662482348
H	-1.12265515370099	0.53360618388373	-1.33719052386684
C	-0.43703436504509	0.03559586399161	0.78199901240868
H	-0.69058828919387	0.36036361848981	1.77547112734744
C	0.42575419657953	-0.86661909970679	-0.03892703746271
H	0.21782578605493	-1.93537029241451	-0.06953694743615
H	1.48131267898673	-0.63344965145603	-0.17247441616694

4 E = -115.672376105543 au [B97-3c]
 ZPE = 0.04469754au
 G_{corr} = 0.02107458 au

C	-0.57960799141514	0.07637576252931	-0.53174183047480
H	-1.10089185844321	0.49043751501522	-1.38174538282460
C	-0.39363539358906	0.00182886004123	0.80801022691743
H	-0.65818651948833	0.31292256247144	1.80747047202781
C	0.36724491975476	-0.74887552063737	-0.02423743199313
H	1.15303388318097	-1.47407767941982	-0.17368938365272

4' E = -115.863493618381 au [B97-3c]
 ZPE = 0.03718688au
 G_{corr} = 0.01309423 au

C	0.03799089225278	-0.47545492928618	-0.19321905897564
H	0.21011789943305	0.37988612912060	0.50385450865935
C	0.49028974789499	-0.19892374606297	-1.46302127655766
H	1.32525195958578	0.34096193699137	-1.93407945621858
C	-0.83856316836099	-0.44995743870579	-1.71711028829752
H	-1.34226677080560	0.42498364794296	-2.19448838860994

TS(1a→5) E = -531.703568309930 au
 ZPE = 0.11471536 au
 G_{corr} = 0.08187042 au
 $\bar{\nu} = -491.02 \text{ cm}^{-1}$

P	-1.68456671820849	2.99230470376262	0.79621971369114
H	-0.45827908847321	3.69348345018574	1.09076916647332
N	-1.06483685175629	1.99020459839082	-0.53758220359972
H	-0.91955709623808	0.97990638051383	-0.39784337714440
N	-0.99581806436198	-0.81047724899600	0.31764349867896
H	-0.40487328015218	-0.73965721580750	1.13663171751965
H	-0.66754719014464	-1.61339942480680	-0.20329884588068

C	-2.39059351549833	-0.99788037957076	0.72540338131640
H	-2.71961227553202	-0.11317483818800	1.26596432028382
H	-3.01468314858872	-1.08909768079524	-0.16141649585665
H	-2.56711541747900	-1.87483187584373	1.35615393001489
C	-1.92834299796764	2.40310034850632	-1.47464979708991
H	-2.59698559997948	1.71171547696617	-1.98545108919866
H	-1.87942073561912	3.41638937568218	-1.83425010920821

5
E = -531.703568309930 au
ZPE = 0.11709536 au
G_{corr} = 0.08635859 au

N	-0.95598072281666	2.17131054452182	-0.17641771546483
H	-0.07366047489905	1.83362102184515	0.17722695910235
N	-2.57677013430687	0.42240508827749	0.59529001638037
H	-3.01678003910356	0.25089925294614	-0.29982299478596
C	-1.58057347472659	-0.59202384534555	0.88108891139506
H	-2.03848873905372	-1.57758764749516	0.82813251209432
H	-0.71155028233930	-0.58893817848204	0.20808322617450
H	-1.21105985925249	-0.45910735548574	1.89864627331152
C	-2.09450647904975	1.78433508230293	0.65760393177245
H	-1.81459037227976	1.99849131824755	1.68996444833531
H	-2.92697616334478	2.43638276745449	0.39924604507834
P	-1.19347480540083	2.12765821189853	-1.87883568549380
H	-0.07107347490947	2.90618306509064	-2.26644412652310
H	-0.56648443851706	0.90187955422363	-2.28498217137658

TS(1a→W-5) E = -1164.464532031608 au
ZPE = 0.15931819 au
G_{corr} = 0.11019576 au
 $\bar{\nu} = -388.36 \text{ cm}^{-1}$

N	-1.03432024563267	2.62539451488865	0.01085521091803
H	-0.67378531053069	2.68830726669880	0.95488288052700
N	-0.99895226222798	-0.03308334251400	0.07160181813773
H	-0.63720691637608	-0.06375230928465	1.01669038291305
H	-0.22070916262871	0.14609282266527	-0.55061741887942
C	-1.73596742160669	-1.24789794394798	-0.27191722302258
H	-2.59083820796376	-1.34608532460047	0.39160777843674
H	-2.10383652200475	-1.16504706495607	-1.29077558265847
H	-1.12654423188776	-2.14806599343033	-0.19259932690163
C	-2.02964352068081	1.66337612177294	-0.09329712156730
H	-2.70451953748787	1.42640112375632	0.72439865432969
H	-2.39986620048741	1.45596703218404	-1.08425066511617
P	-2.28594997970043	3.93993039705385	-0.22941366043937
H	-1.69918762475453	4.47727828782574	-1.40695078412989
W	-2.12431357876586	5.49160328886896	1.79947146754958

C	-4.15896049231203	5.45376978390646	1.98699223803749
O	-5.30712144423167	5.42839309385423	2.09987360491159
C	-2.00128942628994	3.82078108454616	2.93353242302413
O	-1.92402237067452	2.81709910201050	3.51470524776921
C	-1.96375294683394	6.70201904428463	3.38256154480453
O	-1.85085382018479	7.40258508197230	4.29860368339306
C	-0.10232385231999	5.50019933336785	1.55308624923824
O	1.04438857821544	5.49158349619746	1.40949723536284
C	-2.27707501540373	7.06996702169028	0.50452824472766
O	-2.36495532722733	7.93947919118611	-0.24794233136652

W-5

E = -1164.547142554756 au

ZPE = 0.15928748 au

G_{corr} = 0.11154844 au

N	-1.70503429372746	2.32755342423750	0.55314776607500
H	-1.35932578962888	2.23396616695614	1.49611227284876
N	-0.99490776141283	0.13069517056266	-0.04748393756118
H	-0.79481937680590	-0.12894858225105	0.91148944613843
C	-1.28366220311564	-1.07207662181401	-0.81347242074096
H	-2.21132835629868	-1.58712379093933	-0.52312133131442
H	-1.36078374213181	-0.82027310561169	-1.87049749670523
H	-0.45890129430483	-1.77199428496264	-0.70397808561443
C	-2.09062296799492	1.07080044888230	-0.06914285980729
H	-3.01140017159208	0.66777200820151	0.39563212046097
H	-2.33381459660852	1.28008859599055	-1.11202194816370
W	-2.10121684109125	5.60822020124752	1.85712535949257
C	-4.09677684619964	5.95857748555829	2.10364829994176
O	-5.22658054626009	6.14371644229492	2.23874978138679
C	-2.14437294805241	4.30261497131135	3.41927041184514
O	-2.16711970123239	3.54541084225703	4.29145913446969
C	-1.65673931986998	7.12786741349583	3.09936672463638
O	-1.40051062905968	7.99828300120542	3.81269664867952
C	-0.11073568611035	5.22614484178728	1.58267732948667
O	1.01175969381314	5.01480824856694	1.43399398476603
C	-2.06679433733624	6.87311935431595	0.25041699412352
O	-2.04965223277235	7.57392391722134	-0.66383978260791
P	-2.63946659465662	3.71864359196555	0.34180974123779
H	-2.52811672883387	3.90315715970532	-1.05474092611725
H	-3.99448943871671	3.27961493981523	0.33237507304333

W-6

E = -1164.506566400411 au

ZPE = 0.16196131 au

G_{corr} = 0.11457516 au

N	-0.11502812496318	2.05896922174988	0.82240065414508
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H	0.31243124267904	2.26365100352132	1.71545179773828
N	-1.59441393556061	0.76149350112880	-0.41062141094957
H	-0.87196495980561	0.21342833736538	-0.86866939943357
H	-1.53798031299079	1.77547799180972	-0.84174700746201
C	-2.93753756023218	0.17412778527657	-0.55333869058950
H	-3.01470829014434	-0.74043393302352	0.02714933007010
H	-3.66705113750088	0.89461744169080	-0.19899724824594
H	-3.12154737898750	-0.03966618529005	-1.60134827724344
C	-1.15087876678316	1.08499594976741	0.98778982246811
H	-0.79137874269610	0.18108466525424	1.47633470275182
H	-2.05555276840962	1.42988426996578	1.50332921304200
P	-0.79501079118208	3.49394468138963	-0.02900766850597
H	0.44820152302816	4.00706264045871	-0.46886416185128
W	-2.03548415849040	5.06048667089784	1.58173230371126
C	-3.64447966279364	3.89777128002340	1.19988078712494
O	-4.51046477614611	3.16669754407169	0.93882533391550
C	-1.54195397265979	3.84681828628239	3.12436264524060
O	-1.23150962344642	3.10612425374982	3.96220949192805
C	-3.03735594783749	6.29558333796977	2.80309769344236
O	-3.60677452071514	7.01229327598995	3.51313388345278
C	-0.25709670193054	6.04257434118979	1.80243814535782
O	0.77625756576541	6.54841864477442	1.89571196881318
C	-2.48545022610589	6.22655330721157	-0.04018047523884
O	-2.73983800457375	6.87422823937556	-0.96090306216883

7 E = -492.485501999802 au
ZPE = 0.09076137 au
G_{corr} = 0.06197777 au

C	-0.75414833415319	0.84892768885077	-0.47620272611328
H	-0.23201464163362	1.35018082816167	-1.29289809984491
H	-1.82500932456837	0.87439408431913	-0.71705829879275
P	-0.51134165253773	1.92915906196232	1.01939579678637
H	0.91227535473111	1.82499543326872	1.00757013397999
N	-0.20594148473297	-0.48921304483146	-0.29667732826430
H	-0.77746988038931	-0.98113329134639	0.37880817300922
H	-0.27074736121741	-1.01218870492201	-1.16173199177188
N	-0.90788558798496	0.79255077336079	2.26290938525539
H	-0.19276845862412	0.12518446412691	2.50907043178261
H	-1.28130867888943	1.22128026704954	3.09323546397355

TS(7→8+9) E = -588.097754110000 au
ZPE = 0.15222256 au
G_{corr} = 0.11019576 au
 \bar{v} = -124.38 cm⁻¹

P	-1.68133057505053	1.20226035912283	1.83435031858612
H	-2.35793324140537	0.42243798557482	2.83671782071158
N	0.44962938871634	1.42168734693520	-0.17680286625483
H	0.59012891137692	1.17295386474093	0.84318972112148
H	0.02697090669900	0.69756883580174	-0.80274146102837
N	0.02082977879179	0.97125233885151	2.45657800713216
H	0.22256756783324	1.55673537940726	3.25720737509428
H	0.19491760901127	0.01586511037186	2.74336386126294
C	0.45602284421595	2.67173618479813	-0.49007474266407
H	0.14782452557836	2.99451849009365	-1.47429066612662
H	0.73839591427025	3.40495905168700	0.25128182296625
C	-0.83542926893004	-1.94644252173237	-1.10634785652313
H	-0.21143927209135	-2.27321598980369	-1.93670484596054
H	-0.24742099822799	-2.03894333388954	-0.19455955591599
H	-1.68216045653263	-2.63503649999004	-1.02379334677585
N	-1.21400510469379	-0.54612810857298	-1.28326050040225
H	-1.82324209445639	-0.44008368206728	-2.08469299259059
H	-1.72868591510481	-0.22103459132921	-0.45922145263258

W-7

E = -1125.340390765710 au

ZPE = 0.13322074 au

G_{corr} = 0.08662072 au

C	-0.63010302151916	0.71557495731923	-0.47533133567022
H	-0.00771745606040	1.12718546734874	-1.26899852430468
H	-1.67261379310040	0.91043004504148	-0.74812106241053
P	-0.26818770849998	1.72215773808414	1.02825143527335
H	1.13594537521023	1.52639809920217	1.08036993676848
N	-0.29612745904549	-0.67987716730477	-0.24958917672433
H	-1.06354496353370	-1.14445589563506	0.21520979456094
H	-0.13979313251384	-1.15977108010901	-1.12486279584616
N	-0.89205346852223	0.72533162037963	2.25982615814439
H	-0.34267666646683	-0.09407057347182	2.47333770027476
H	-1.14467404605886	1.22030421415435	3.09936254090173
W	-1.09619778871992	4.06523707575153	1.05297305381499
C	0.82817785527783	4.71345652117634	0.84376479298064
O	1.92271763098703	5.05525837546198	0.72343053338029
C	-0.88004961475552	4.08784745323704	3.07931143872128
O	-0.75769120458298	4.08113219968327	4.22765397417883
C	-2.99027917564824	3.32827861002366	1.24638318147962
O	-4.05754996142993	2.90317403375568	1.34824498275160
C	-1.78578668488932	5.95848021184867	1.08565667575211
O	-2.18411932886260	7.04176185706902	1.10937697303651
C	-1.29794036049900	4.01920889452051	-0.97801964788079
O	-1.41057701676663	3.99280992246315	-2.12614153918283

TS(W-7→8+W-9)

E = -1220.963961711267 au

ZPE = 0.19679245 au

 $G_{\text{corr}} = 0.14572650$ au $\bar{\nu} = -339.17$ cm^{-1}

P	0.67795034860762	2.41723049682439	2.53247537973489
H	1.23105720725150	2.91196304981977	3.75452713905380
N	0.20669701305166	-0.27797911712800	0.80873779928488
H	-0.39448274931735	-0.03533537222980	1.62078869713456
H	0.78606992852132	-1.09280665732631	0.92999596998243
N	-0.34063204461055	1.08803652970363	3.17062932295365
H	0.14699117114027	0.56456299276737	3.88791161951715
H	-1.20678945559677	1.41647060204842	3.57628734430013
W	-0.95704727802297	4.23063019031936	1.68218526403613
C	0.52479683174465	5.56936534496556	2.13418231054337
O	1.38192686992368	6.30056076864995	2.38345179807177
C	-1.59357372821305	4.24850895638547	3.62478820073883
O	-1.93612835623164	4.21107711674603	4.72729734791295
C	-2.30367035556098	2.79432315125941	1.21733932262709
O	-3.04957947228902	1.95252594097025	0.92670217544827
C	-2.23982879427677	5.67916354037044	1.16801632932931
O	-2.99441034641631	6.51561701113321	0.89542660608433
C	-0.27797524160443	4.11447820979630	-0.21864680711676
O	0.08215795601956	4.02295394341902	-1.32256951097958
C	0.71421797807366	0.75682349273904	0.17689431062733
H	1.69321786015297	0.71988044098586	-0.26607250281350
H	0.18781470806959	1.68774958715267	0.20712337572127
C	-1.47746404631340	0.19330522192303	-1.93888008111641
H	-1.42443909824772	-0.80588670976730	-1.51021359288102
H	-2.09070845850092	0.79739728374772	-1.27719623982598
H	-1.97610986631591	0.12897233854812	-2.90882749148355
N	-0.13670652189402	0.76077377576596	-2.00660097661179
H	0.43903264632329	0.27880426304192	-2.68414207913152
H	-0.15439355546756	1.74085867736712	-2.25800451114259

8

E = -190.579322430401 au

ZPE = 0.12439328 au

 $G_{\text{corr}} = 0.09659572$ au

N	0.32578899973715	-0.44522599421649	0.45687312618640
H	-0.33762728285857	-0.43655605669543	1.21181399354815
H	1.17060306508135	-0.92428035086337	0.71674876081891
C	0.48996617887501	0.75544215617424	-0.23650853271206
H	1.52838642271527	1.05096524287050	-0.36460120016316
H	-0.07712890121033	1.58868390684550	0.16998378868189

C	-1.51888574464006	0.35337990186528	-1.77620943965354
H	-1.74258764913465	-0.52712717384415	-1.18649863910304
H	-2.04023949745592	1.21800391309711	-1.38050846543498
H	-1.80273405030325	0.19049111662782	-2.81005184228123
N	-0.05090855796984	0.60073746806660	-1.69899972897393
H	0.44404931305947	-0.18611736794585	-2.11709121268540
H	0.19587899410438	1.42968788801823	-2.23974271822801

9 E = -397.972174826894 au
ZPE = 0.04334741 au
G_{corr} = 0.01919221 au

N	-0.32021258022485	1.13904389614211	3.17579061190115
H	0.12159243987078	0.46602913160567	3.78170893564524
H	-1.24456911148950	1.35868773286438	3.50656924285857
P	0.56932955064152	2.51994869866455	2.66216636077824
H	1.48501119252861	2.75181355487027	3.74087094737937
H	1.55817252867344	1.85781133585302	1.88511429143742

W-9 E = -1030.820377542090 au
ZPE = 0.08654284 au
G_{corr} = 0.04306880 au

N	-0.23838971926741	1.11008157283290	3.29977682251323
H	0.33249864811898	0.46525970825980	3.82442794556304
H	-1.05393592088241	1.38566641934061	3.82192947212342
W	-0.97180821994265	4.21947866011759	1.74293842953554
C	0.44911856413941	5.58473056624967	2.27657164105942
O	1.25778518126657	6.34577123343357	2.58562248665932
C	-1.74819152550047	4.30373859310276	3.62509650180205
O	-2.18250007649316	4.33683191460378	4.69448711039780
C	-2.36886294105712	2.82201391201140	1.21732956388045
O	-3.16048798981125	2.03936971086894	0.92073755425577
C	-2.20097761885940	5.69705546571451	1.14331973079389
O	-2.90730911164079	6.54366552001728	0.80282387953034
C	-0.16295035116584	4.09545312310953	-0.13103009182404
O	0.30049176851942	4.01361442765177	-1.18256508767111
P	0.52884849961634	2.39552693848343	2.50065247963456
H	1.62957603030392	2.78168969425352	3.31180869662508
H	1.27989428265588	1.69618767994887	1.53205586512120

10 E = -190.201418384942 au
ZPE = 0.10880507 au
G_{corr} = 0.08157312 au

N	0.23271763774128	-0.47490677766388	0.52147426553602
H	-0.18233391689093	-0.22042104351498	1.40528960973760

H	1.09194370607786	-0.96559449124603	0.71951335782109
C	0.46215106188836	0.69268678474685	-0.33999474922453
H	1.52417174610690	0.94433788194115	-0.39065978830926
H	-0.05159877744939	1.55449853949590	0.08893615359040
C	-1.43196254894293	0.30406543224164	-1.80915663606757
H	-1.77584383017849	-0.56783225539653	-1.24253186965220
H	-1.97646620739569	1.17732168278857	-1.44645370783608
H	-1.69692185173270	0.16811378220774	-2.85624518287096
N	-0.00251026453968	0.55346675593751	-1.70225636019799
H	0.50369219531541	-0.20176516153793	-2.14885684252651

11 E = -397.352066769894 au
ZPE = 0.03199272 au
G_{corr} = 0.00809469 au

P	0.73843343317001	2.44132058544812	2.62418155499403
H	0.98873474743574	3.06414897510314	3.93078757320447
N	-0.35820085596533	1.07844175599909	3.14324058953733
H	0.09928241869176	0.46409016864382	3.80769759383437
H	-1.19561720333218	1.42602982480584	3.59725712842978

W-11 E = -1030.271111614472 au
ZPE = 0.07532189 au
G_{corr} = 0.03192412 au

P	0.60911871619369	2.35988379555731	2.47361370818303
H	1.18130603442978	3.04048546859460	3.61419059378014
N	-0.44542866632228	1.18117508775069	3.26914835573622
H	0.09664018318950	0.44911034788100	3.70888659399224
H	-1.06345133668383	1.57667325833854	3.96532561127818
W	-1.02216323174816	4.27558660728734	1.67113697434582
C	0.43666932618321	5.59407020481902	2.17627537531360
O	1.28827944745584	6.32990939676573	2.46486061366895
C	-1.61279138723682	4.18120929969138	3.60539807882720
O	-1.90246691477265	4.05436447772133	4.72548263602012
C	-2.36302818269253	2.82598237933808	1.16897359434676
O	-3.12453749353591	2.00578875126267	0.86737880100188
C	-2.28027416439711	5.72016146225651	1.14560385616374
O	-3.03262102364990	6.57155616007025	0.86739869967008
C	-0.19030663685424	4.09270010455470	-0.17416867961051
O	0.31116335044142	3.95817529811080	-1.21257776271749

10 + W-11 E = -1220.963961711267au
ZPE = 0.19679245 au
G_{corr} = 0.14572650 au

P	0.67795034860762	2.41723049682439	2.53247537973489
H	1.23105720725150	2.91196304981977	3.75452713905380
N	0.20669701305166	-0.27797911712800	0.80873779928488
H	-0.39448274931735	-0.03533537222980	1.62078869713456
H	0.78606992852132	-1.09280665732631	0.92999596998243
N	-0.34063204461055	1.08803652970363	3.17062932295365
H	0.14699117114027	0.56456299276737	3.88791161951715
H	-1.20678945559677	1.41647060204842	3.57628734430013
W	-0.95704727802297	4.23063019031936	1.68218526403613
C	0.52479683174465	5.56936534496556	2.13418231054337
O	1.38192686992368	6.30056076864995	2.38345179807177
C	-1.59357372821305	4.24850895638547	3.62478820073883
O	-1.93612835623164	4.21107711674603	4.72729734791295
C	-2.30367035556098	2.79432315125941	1.21733932262709
O	-3.04957947228902	1.95252594097025	0.92670217544827
C	-2.23982879427677	5.67916354037044	1.16801632932931
O	-2.99441034641631	6.51561701113321	0.89542660608433
C	-0.27797524160443	4.11447820979630	-0.21864680711676
O	0.08215795601956	4.02295394341902	-1.32256951097958
C	0.71421797807366	0.75682349273904	0.17689431062733
H	1.69321786015297	0.71988044098586	-0.26607250281350
H	0.18781470806959	1.68774958715267	0.20712337572127
C	-1.47746404631340	0.19330522192303	-1.93888008111641
H	-1.42443909824772	-0.80588670976730	-1.51021359288102
H	-2.09070845850092	0.79739728374772	-1.27719623982598
H	-1.97610986631591	0.12897233854812	-2.90882749148355
N	-0.13670652189402	0.76077377576596	-2.00660097661179
H	0.43903264632329	0.27880426304192	-2.68414207913152
H	-0.15439355546756	1.74085867736712	-2.25800451114259