Electronic Supplementary Information

Mechanism of C–P bond formation *via* Pd-catalyzed decarbonylative phosphorylation of amides: insight into chemistry in the second coordination sphere

Wen-Yan Tong,[a] Thu D. Ly,[b] Tao-Tao Zhao,[a] Yan-Bo Wu*,[a] and Xiaotai Wang*,[b,c]

[a] The Key Laboratory of Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan, 030006, Shanxi, People's Republic of China.

[b] Department of Chemistry, University of Colorado Denver, Campus Box 194, P.O. Box 173364, Denver, Colorado 80217-3364, United States

[c] Hoffmann Institute of Advanced Materials, Shenzhen Polytechnic, 7098 Liuxian Boulevard, Nanshan District, Shenzhen 518055, P. R. China

Email address: wyb@sxu.edu.cn
Email address: Xiaotai.Wang@ucdenver.edu

Contents **Pages**

- Fig. S1 Optimized structure of *N*-benzoylglutarimide S2
- Fig. S2 Optimized structure of **1cat** S2
- Fig. S3 Optimized structures of **2a**–**2d** S2
- Fig. S4 Reaction pathway through **2b** S3
- Fig. S5 Reaction pathway through **2c** S4
- Fig. S6 Reaction pathway through **2d** S5
- Fig. S7 IRC plot S6
- Cartesian coordinates, electronic energies, and Gibbs free energies S7–S99

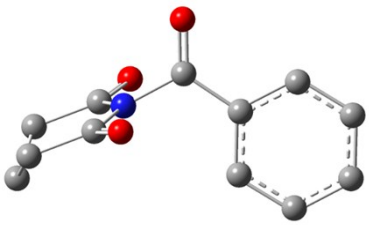


Fig. S1 Optimized structure of *N*-benzoylglutarimide. Color scheme: C grey, N blue, and O red (the same below). Hydrogen atoms are omitted for clarity (the same below).

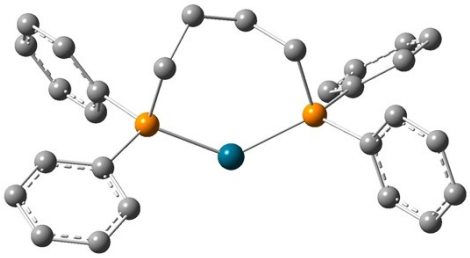
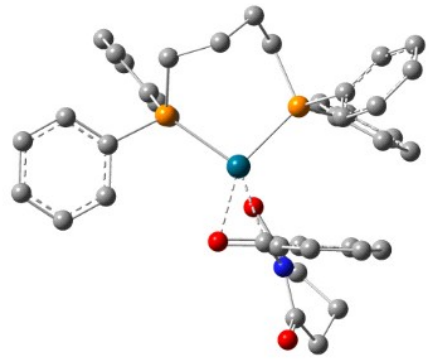
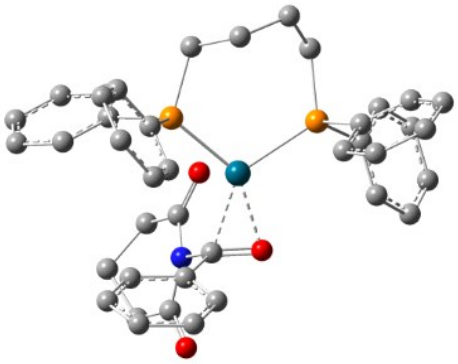


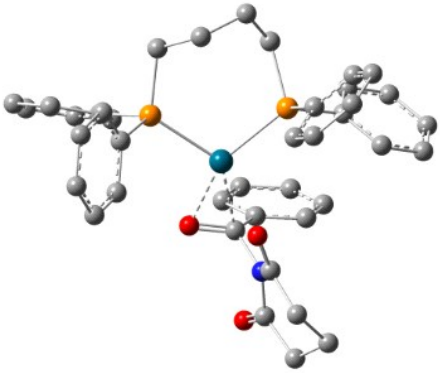
Fig. S2 Optimized structure of **1cat**. Color scheme: Pd green and P yellow (the same below). Bond angle P–Pd–P = 126.45°.



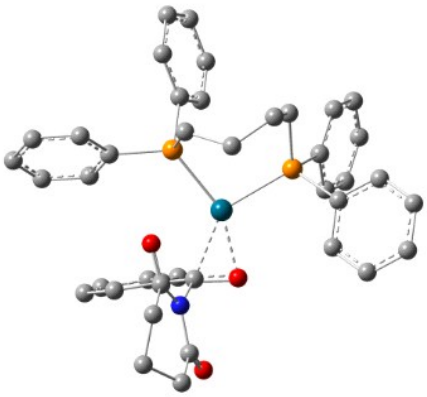
2a



2b



2c



2d

Fig. S3 Optimized structures of **2a**–**2d**.

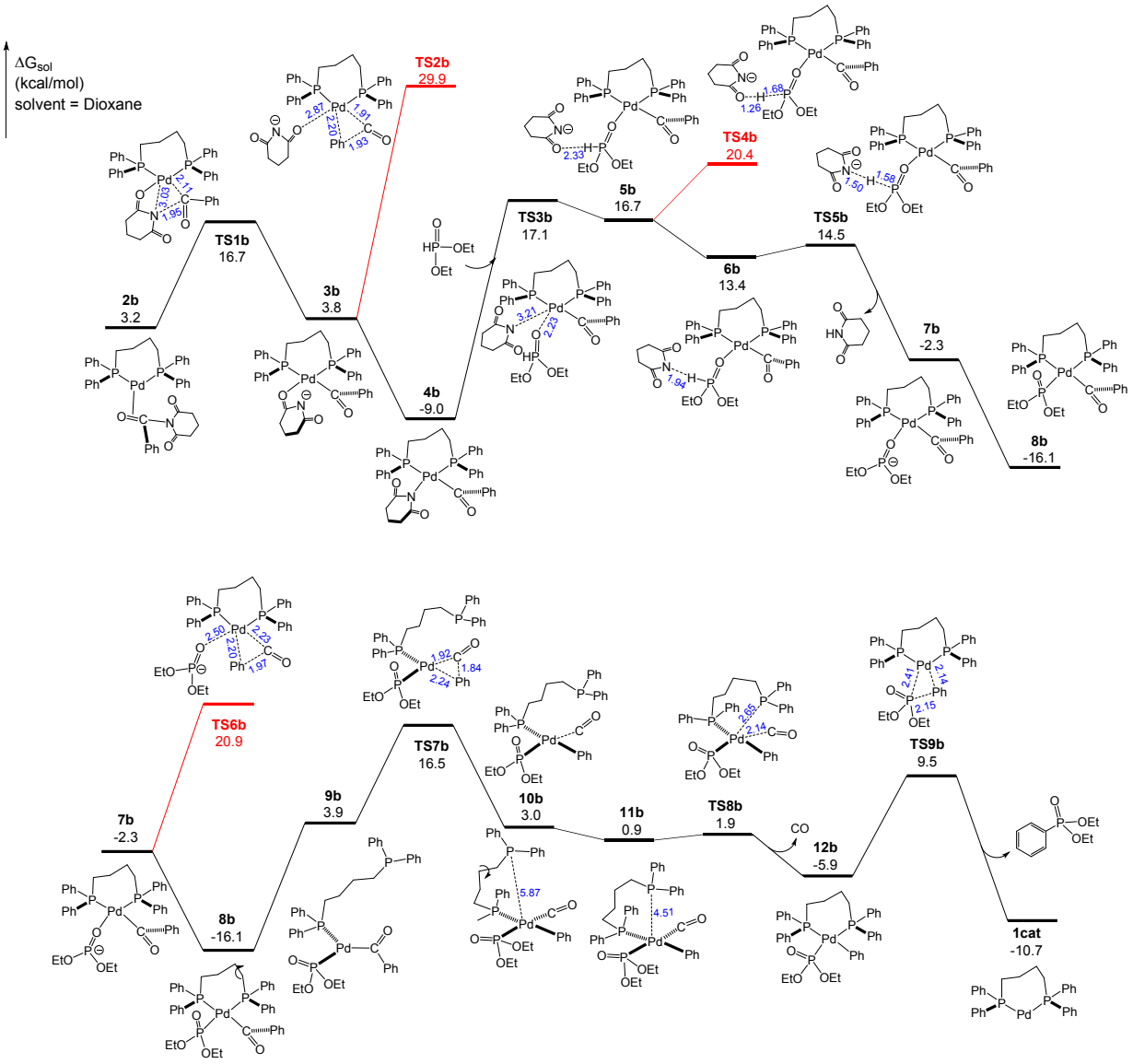


Fig. S4 Reaction pathway through **2b**.

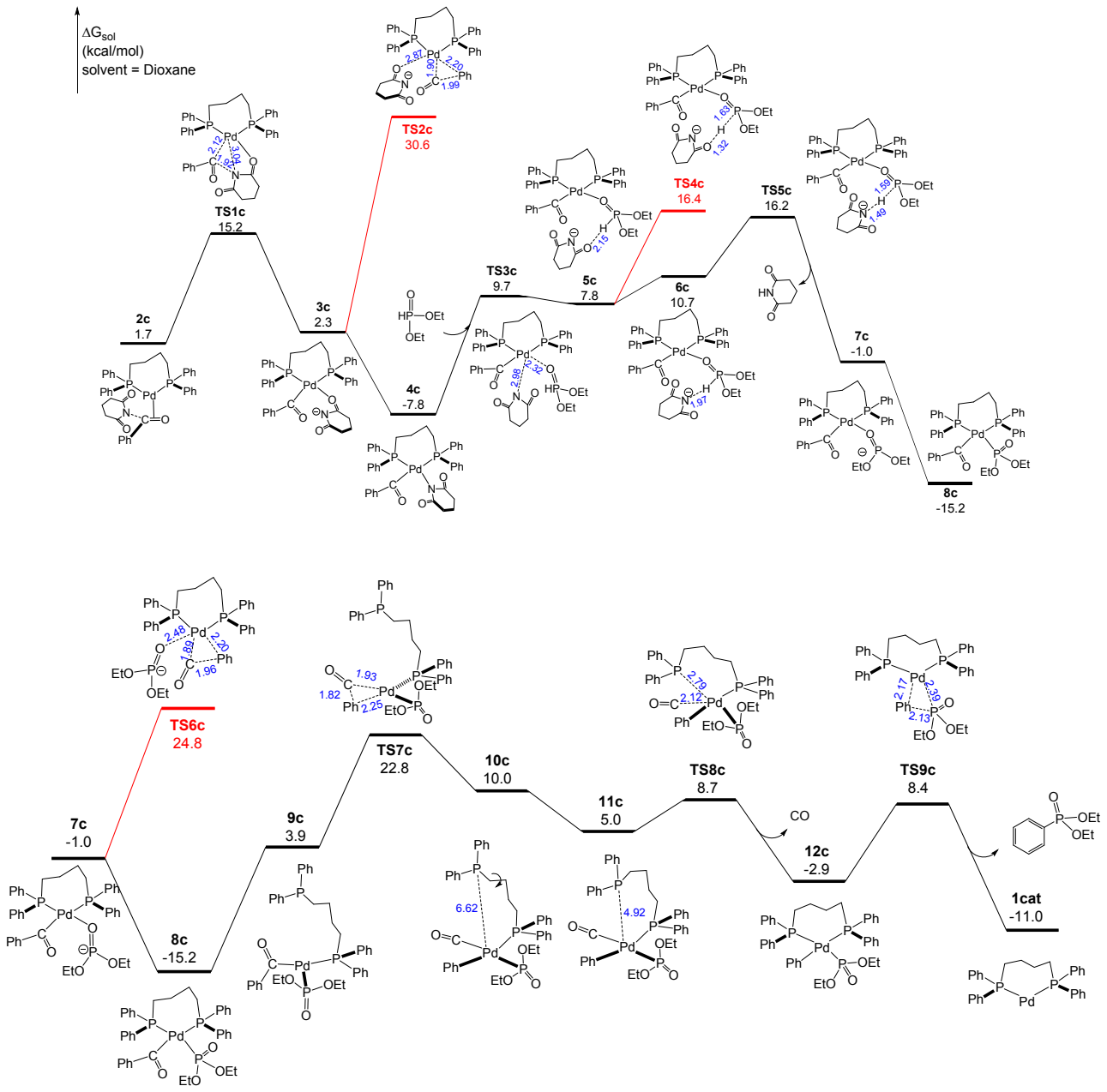


Fig. S5 Reaction pathway through **2c**.

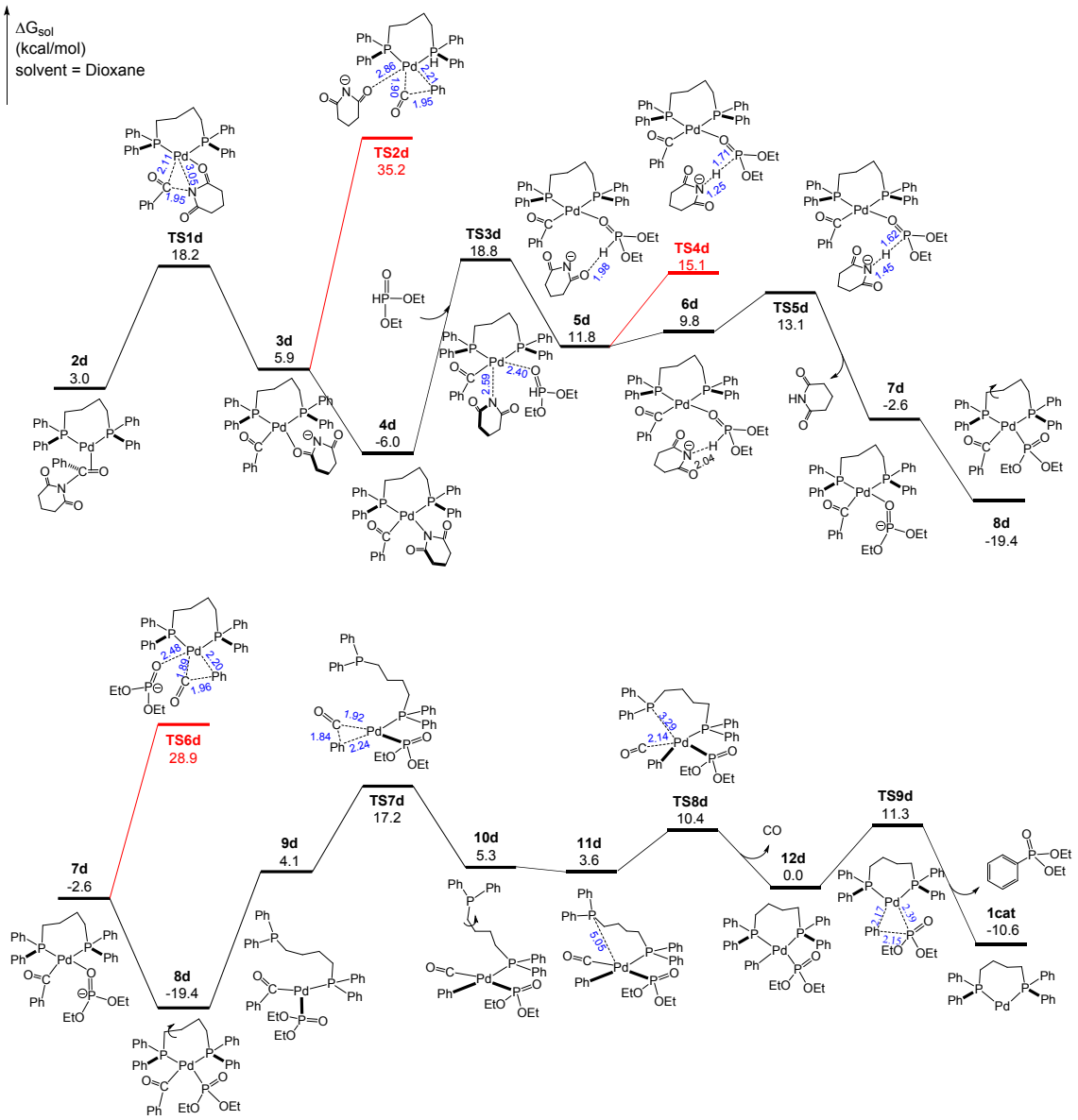


Fig. S6 Reaction pathway through **2d**.

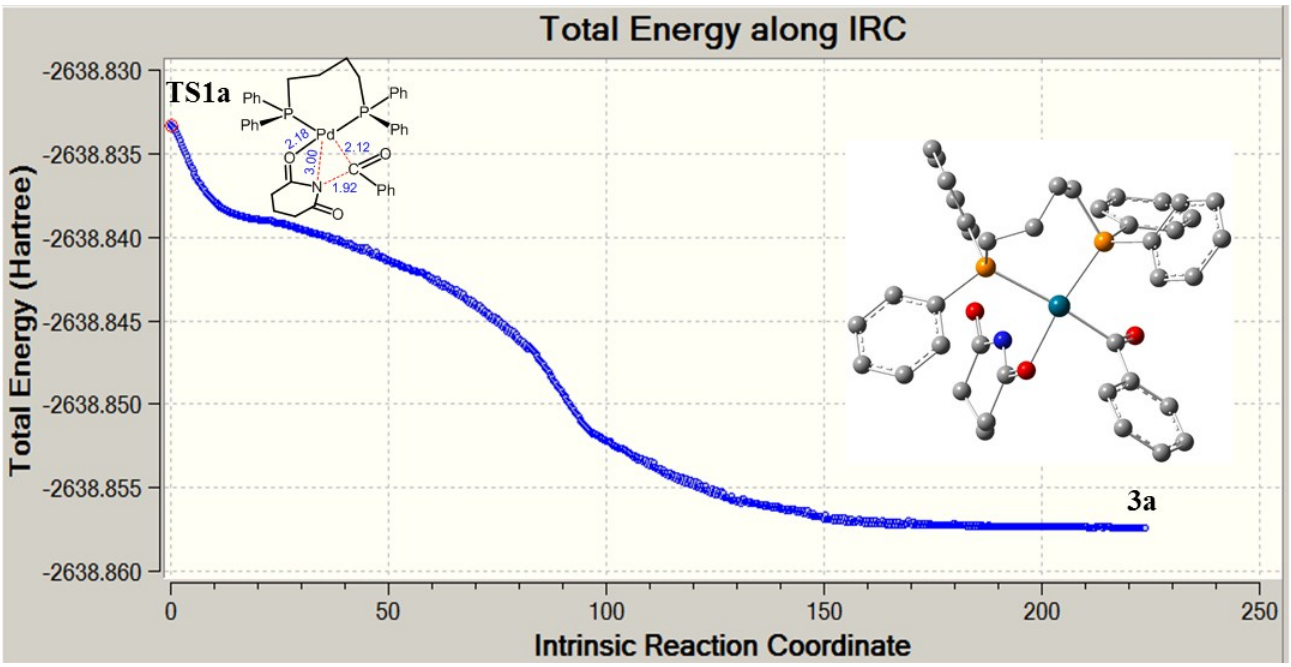


Fig. S7 B3LYP/6-31G(d,p)-computed IRC plot showing the **TS1a→3a** connection.

Cartesian Coordinates, SCF Energies (a.u.), and Free Energies (a.u.) at 298.15 K and 1 atm

dppb

SCF energy: -1766.516766

SCF energy in solution: -1765.94321278

Free energy in solution: -1765.52622978

P	2.12281200	-0.08929700	-0.23714400
C	-1.86805400	-1.83672200	0.72573900
H	-2.02562200	-2.00496800	1.79950200
H	-2.62614400	-2.44588500	0.21704300
C	1.20768400	-0.55043400	1.33956200
H	1.86940800	-0.41479700	2.20487600
H	0.37357700	0.15170200	1.44648500
C	-0.45459800	-2.31633700	0.32646600
H	-0.19250900	-1.93838600	-0.66949200
H	-0.50394700	-3.40952600	0.22925400
C	0.67781000	-1.99780900	1.32385300
H	0.33188700	-2.24840300	2.33705500
H	1.51699900	-2.67585500	1.12111300
P	-2.25332500	-0.01523400	0.45139200
C	-2.42880400	0.10760400	-1.38900900
C	-2.54594800	-0.98036700	-2.26910400
C	-2.41972200	1.40339900	-1.93446500
C	-2.66176000	-0.77825100	-3.64674700
H	-2.54540200	-1.99732600	-1.88846900
C	-2.54801100	1.60818900	-3.30795400
H	-2.30469300	2.25903800	-1.27309300
C	-2.66800800	0.51554600	-4.16953600
H	-2.74739300	-1.63469800	-4.31090600
H	-2.54246000	2.61944500	-3.70624700
H	-2.75751900	0.67125500	-5.24140000
C	-4.02021100	-0.00914800	1.02513600
C	-5.09991700	-0.48316400	0.26334600
C	-4.27645100	0.48809700	2.31297000
C	-6.39653400	-0.46880000	0.77955900
H	-4.92858600	-0.85575200	-0.74268800
C	-5.57164400	0.49428600	2.83492000
H	-3.45423400	0.87901900	2.90820500
C	-6.63529500	0.01645500	2.06769600
H	-7.22212300	-0.83570100	0.17470600
H	-5.75037200	0.88101100	3.83502800
H	-7.64582500	0.02821100	2.46781300
C	2.73372900	1.61506600	0.15046300
C	3.63212600	2.20322500	-0.75960100
C	2.29872200	2.38494400	1.24025000
C	4.09433400	3.50455900	-0.57600500
H	3.97468300	1.63202500	-1.61960900
C	2.75318000	3.69529500	1.41886200
H	1.60044400	1.97103400	1.96037800
C	3.65397200	4.25834900	0.51586600
H	4.79368600	3.93403900	-1.28894300
H	2.40165400	4.27297000	2.27021600
H	4.00760100	5.27628200	0.65695500
C	3.67314200	-1.09107100	-0.02379500
C	4.64748000	-0.82297300	0.95275600
C	3.86655200	-2.18841000	-0.87714400
C	5.77672500	-1.63254200	1.07411600
H	4.52710300	0.03155800	1.61347600
C	4.99395900	-3.00509100	-0.75311200
H	3.13019200	-2.39934000	-1.64908100
C	5.95148100	-2.72759000	0.22265900
H	6.52287600	-1.40906200	1.83268500
H	5.12600300	-3.85108900	-1.42286200
H	6.83277600	-3.35668400	0.31779200

[Pd(dppb)] (1cat)

SCF energy: -1894.503537

SCF energy in solution: -1893.91329973

Free energy in solution: -1893.49594073

P	2.05438300	0.15684300	0.08484600
C	-1.56268100	-0.16012300	1.89785600
H	-1.22020800	0.82258700	2.24437400
H	-2.44586300	-0.41964900	2.49404300
C	1.66331500	0.38737400	1.91475700
H	2.59533600	0.58506300	2.46118400
H	1.09615400	1.32562500	1.93742400
C	-0.45162900	-1.22912100	2.08447200
H	-0.25840900	-1.74133200	1.13501100
H	-0.81927900	-2.00125600	2.77191500
C	0.88958800	-0.72403600	2.65781400
H	0.71565200	-0.35409300	3.67929400
H	1.54557200	-1.59753700	2.76345400
P	-2.04576900	0.05848700	0.09218200
C	-3.10969400	-1.43568000	-0.19106200
C	-4.36471000	-1.60459600	0.41599700
C	-2.62809600	-2.44654800	-1.03582900
C	-5.11472200	-2.75812600	0.18717200

H	-4.76626200	-0.82589700	1.05949300
C	-3.37572200	-3.60537800	-1.26042000
H	-1.66293900	-2.31428500	-1.51960800
C	-4.62050400	-3.76250900	-0.65002200
H	-6.08730300	-2.87247400	0.65935400
H	-2.98777200	-4.37966500	-1.91734500
H	-5.20723400	-4.65987600	-0.82874200
C	-3.29169400	1.42673100	0.14418800
C	-3.83594300	1.95914900	1.32364100
C	-3.69091800	1.98004300	-1.08489200
C	-4.75832400	3.00829400	1.27402100
H	-3.54524900	1.56148800	2.29105800
C	-4.62052100	3.01753000	-1.13574000
H	-3.25924200	1.59545000	-2.00628000
C	-5.15614900	3.53696800	0.04595400
H	-5.16622000	3.40975800	2.19834700
H	-4.91858000	3.42872200	-2.09673200
H	-5.87327600	4.35273300	0.00887300
C	3.25639400	1.55382400	-0.14316600
C	4.64479000	1.43872200	0.02198900
C	2.72309100	2.80428000	-0.49946200
C	5.47594300	2.54696300	-0.15708000
H	5.08500000	0.48075200	0.28130700
C	3.55223300	3.91437800	-0.66326600
H	1.65096400	2.89810000	-0.66026900
C	4.93294300	3.78781200	-0.49451700
H	6.55054900	2.43812200	-0.03274700
H	3.12085400	4.87409300	-0.93621400
H	5.58192900	4.64851500	-0.63353600
C	3.11324900	-1.35887700	0.04193700
C	3.92482600	-1.77971600	1.10895000
C	3.08651500	-2.13847100	-1.12550100
C	4.69133900	-2.94265300	1.00765000
H	3.96539400	-1.19921900	2.02634700
C	3.85861800	-3.29642100	-1.23182800
H	2.44543900	-1.83237100	-1.94884200
C	4.66150100	-3.70206300	-0.16394500
H	5.31137800	-3.25494200	1.84414600
H	3.82638300	-3.88526100	-2.14479600
H	5.25716900	-4.60780700	-0.24148200
Pd	-0.00037800	0.21278700	-0.94092400

[Pd(dppb)(OAc)]$^-$

SCF energy: -2123.048568

SCF energy in solution: -2122.45066392

Free energy in solution: -2121.99418392

P	-2.04118100	0.07442600	-0.44124500
C	1.24551700	-0.68633000	-2.44311700
H	0.87974500	0.21769800	-2.94440300
H	2.08538600	-1.05099800	-3.04846400
C	-1.89846800	-0.04272300	-2.32471900
H	-2.88723300	0.07253200	-2.79122400
H	-1.30679900	0.83306000	-2.61898400
C	0.12464300	-1.75410000	-2.36098600
H	0.00242400	-2.08119500	-1.32227600
H	0.42902300	-2.64506600	-2.92782000
C	-1.25456900	-1.32149500	-2.89979000
H	-1.17893800	-1.18307900	-3.98992000
H	-1.94916800	-2.15879100	-2.74905600
P	1.77853900	-0.11461900	-0.73284300
C	2.95627700	-1.46498200	-0.20867200
C	3.31676900	-2.56600700	-1.00046300
C	3.46520400	-1.38717200	1.10302000
C	4.17050000	-3.55800800	-0.50783800
H	2.93459900	-2.66472700	-2.01223500
C	4.33116000	-2.36933800	1.58373700
H	3.16688300	-0.55950400	1.74742200
C	4.68640500	-3.46044500	0.78429300
H	4.43219300	-4.40539400	-1.13920500
H	4.71885300	-2.28727200	2.59689600
H	5.35189300	-4.23093900	1.16851600
C	2.98088700	1.25070200	-1.13323700
C	3.48856400	1.51451000	-2.41548900
C	3.35929200	2.09241200	-0.07027900
C	4.35309600	2.59022300	-2.63631900
H	3.21776700	0.87964200	-3.25448200
C	4.23619500	3.15555400	-0.29352300
H	2.96309600	1.90373500	0.92872600
C	4.73219000	3.41314800	-1.57451800
H	4.73320400	2.78033700	-3.63858300
H	4.52292100	3.79292000	0.54014500
H	5.40619000	4.25039600	-1.74509200
C	-3.36850400	1.37996600	-0.31821300
C	-4.09949000	1.47493300	0.88208300
C	-3.59169800	2.36294000	-1.29735400
C	-5.03310300	2.48814500	1.08191800
H	-3.92147800	0.74657400	1.66956500
C	-4.51741500	3.39100200	-1.09179600
H	-3.03881300	2.33752300	-2.23157000
C	-5.24770900	3.45633700	0.09400000
H	-5.58866600	2.53082800	2.01635900

H	-4.66707200	4.14067900	-1.86654100
H	-5.96822000	4.25525200	0.25377400
C	-3.07202400	-1.45128900	-0.11229700
C	-4.31308600	-1.69625500	-0.72322900
C	-2.57133000	-2.40340700	0.78779900
C	-5.03137300	-2.86031100	-0.44504100
H	-4.72760900	-0.96416600	-1.41242200
C	-3.28633900	-3.57218500	1.06579300
H	-1.61743900	-2.20682300	1.27350100
C	-4.51749700	-3.80335900	0.45003100
H	-5.99343100	-3.03152200	-0.92413900
H	-2.88224400	-4.29741200	1.76848900
H	-5.07763500	-4.71013900	0.66830900
Pd	-0.05152400	0.28181900	0.60961500
O	0.18708700	0.69909900	2.82155900
C	1.27448500	1.01840500	3.40588900
C	1.12964600	1.22315900	4.92996700
H	0.69807100	0.32563600	5.38928300
H	2.09484800	1.44554800	5.39496300
H	0.43368800	2.04817600	5.12619600
O	2.40720500	1.18484200	2.90012000

[Pd(dppb)(sol)]

SCF energy: -2202.162834

SCF energy in solution: -2201.47954945

Free energy in solution: -2200.95026545

P	1.81510900	-0.71918600	0.66694000
C	-1.88865400	-1.84271800	1.69902200
H	-1.57312400	-1.37924800	2.64177000
H	-2.84312500	-2.34525800	1.89542500
C	1.29725100	-1.64472200	2.22377400
H	2.18953000	-1.89522500	2.81262400
H	0.72261800	-0.92023000	2.81284200
C	-0.83193900	-2.86662400	1.20938300
H	-0.57819800	-2.67256900	0.16127700
H	-1.27541400	-3.87006100	1.23009900
C	0.47165800	-2.93443100	2.03108100
H	0.23148200	-3.30854500	3.03730500
H	1.11535700	-3.69562300	1.57207900
P	-2.14272800	-0.43922500	0.47180800
C	-3.23674000	-1.27387300	-0.77978800
C	-2.70514200	-1.55152700	-2.04781200
C	-4.56141500	-1.65263200	-0.50904400
C	-3.47032200	-2.20379700	-3.01798800
H	-1.68486300	-1.24373200	-2.26653800
C	-5.33006700	-2.29618800	-1.47934100
H	-5.00113900	-1.43142300	0.46006500
C	-4.78509600	-2.57639200	-2.73546600
H	-3.04156200	-2.41337700	-3.99485600
H	-6.35648500	-2.57713200	-1.25648200
H	-5.38558800	-3.07720500	-3.49056200
C	-3.34847300	0.65916400	1.35719900
C	-4.00298700	0.32485200	2.55365800
C	-3.59101200	1.92570000	0.79704800
C	-4.87865500	1.22634200	3.16600900
H	-3.83586900	-0.64163000	3.01911100
C	-4.47483400	2.81997500	1.39943500
H	-3.06999700	2.20960800	-0.11470600
C	-5.12049200	2.47343100	2.58950300
H	-5.37312900	0.94962400	4.09397200
H	-4.65151800	3.79239700	0.94661300
H	-5.80173500	3.17324700	3.06644100
C	3.21738700	0.30961000	1.31933900
C	4.25760800	0.69724600	0.45482900
C	3.21386600	0.83175300	2.62357900
C	5.26360900	1.56225400	0.88310400
H	4.28482300	0.31020400	-0.56067000
C	4.21930500	1.70281500	3.05133900
H	2.42310700	0.56409600	3.31810000
C	5.24896700	2.07085400	2.18507400
H	6.06191600	1.83876700	0.19873200
H	4.19640100	2.09023700	4.06703100
H	6.03201100	2.74642800	2.51884200
C	2.72735300	-2.04101100	-0.26340300
C	3.81587900	-2.74132200	0.28356700
C	2.29797500	-2.37167400	-1.55655400
C	4.45341100	-3.74657300	-0.44359800
H	4.17550600	-2.49174000	1.27855700
C	2.93510300	-3.37875100	-2.28711500
H	1.45769700	-1.82898800	-1.98372000
C	4.01305500	-4.06807100	-1.73108500
H	5.29529900	-4.27855700	-0.00757400
H	2.58997200	-3.62157900	-3.28894500
H	4.51135300	-4.85085100	-2.29716400
Pd	-0.06475200	0.28262800	-0.19284100
C	0.71730500	3.67292200	-3.59085600
C	0.71415900	2.32993800	-2.86863600
C	1.02982800	3.44839500	-0.81560900
C	1.02746900	4.78226600	-1.55303400
H	-0.31803100	4.03973600	-3.69312500
H	1.73038000	1.90662000	-2.84982000

H	0.58015500	3.53587800	0.17710400
H	1.69424000	5.49917300	-1.06309700
H	2.05848400	3.07253300	-0.71099000
H	0.03858000	1.61886900	-3.35305400
H	1.15679400	3.57812100	-4.58930100
H	0.00630000	5.19916700	-1.56563700
O	0.23947800	2.49030500	-1.52992500
O	1.50533200	4.62347900	-2.88482000

1,4-Dioxane (sol)

SCF energy: -307.653142

SCF energy in solution: -307.5562929

Free energy in solution: -307.4613749

C	-1.17113700	0.73768100	0.19446400
C	-1.17113700	-0.73768300	-0.19446300
C	1.17116700	-0.73769000	-0.19451400
C	1.17116600	0.73769100	0.19451500
H	-1.22429900	0.82888100	1.29226800
H	-1.22429900	-0.82888200	-1.29226800
H	2.02551500	-1.26318900	0.24455800
H	2.02551400	1.26319100	-0.24455700
H	1.22417000	-0.82867600	-1.29233500
H	-2.02554300	-1.26310400	0.24468300
H	-2.02554400	1.26310200	-0.24468200
H	1.22416800	0.82867700	1.29233600
O	-0.00000100	-1.38301700	0.29335700
O	-0.00000300	1.38301700	-0.29335800

$HP(O)(OEt)_2$

SCF energy: -726.114359

SCF energy in solution: -726.00935865

Free energy in solution: -725.88994465

P	-0.00635600	0.93276900	0.25016800
H	-0.20488100	1.07383800	1.64097200
C	2.38211200	-0.20955100	0.11223600
H	2.63364600	0.56409100	-0.61871700
H	2.72216900	0.12641200	1.10063600
C	-1.97067800	-0.85813000	0.27367300
H	-1.35035000	-1.70096600	-0.04746700
H	-1.94630700	-0.81352700	1.37156900
O	0.46225800	2.15239300	-0.43926300
O	-1.41273300	0.35887300	-0.27100700
O	0.94252700	-0.37414400	0.14077500
C	2.99962400	-1.54802300	-0.24759100
H	2.73192900	-2.31225500	0.48927300
H	4.09143900	-1.45929400	-0.27335700
H	2.65493000	-1.87953300	-1.23216600
C	-3.39611100	-0.98737800	-0.23087800
H	-3.84556200	-1.91033100	0.15231900
H	-3.41440800	-1.01915100	-1.32459000
H	-4.00336600	-0.13930600	0.10033000

***N*-benzoylglutarimide**

SCF energy: -744.339710

SCF energy in solution: -744.08336615

Free energy in solution: -743.91335315

O	0.27721800	2.29165300	0.40160900
C	0.29774000	1.10469500	0.19392900
C	1.52309400	0.28962700	0.05048900
C	1.49218900	-1.09150000	-0.18837300
C	2.75951100	0.94753200	0.16204400
C	2.68212700	-1.80589100	-0.31366700
H	0.54090500	-1.60487200	-0.27582100
C	3.94522700	0.23191600	0.03607000
H	2.76429200	2.01645400	0.34690000
C	3.90800800	-1.14608800	-0.20181700
H	2.65354200	-2.87587400	-0.49847600
H	4.89915500	0.74421500	0.12279300
H	4.83495500	-1.70471100	-0.29994300
C	-2.98517200	-0.63117800	1.16321000
C	-2.99044100	-0.18706600	-1.30395200
C	-3.29916200	-1.21876600	-0.21543300
H	-3.09826900	-1.36112400	1.96923600
H	-3.67822400	0.66688700	-1.21831900
H	-2.70016800	-2.12389900	-0.37978800
N	-1.00105500	0.38842300	0.06857600
C	-1.58088700	0.37030100	-1.21203800
C	-1.57668900	-0.07246400	1.26548600
O	-0.96255000	0.79635200	-2.16834300
O	-0.95572200	-0.00145300	2.30846800
H	-3.10947900	-0.58960400	-2.31341100
H	-4.34984500	-1.52238100	-0.26770700
H	-3.67431500	0.19682500	1.38493200

Diethyl phenylphosphonate

SCF energy: -957.179719

SCF energy in solution: -956.94842

Free energy in solution: -956.753665

C	1.19735200	-0.15889800	0.12575200
C	1.61825600	-0.14832900	-1.21277600
C	2.14487800	-0.24575000	1.15442500
C	2.97639100	-0.23142300	-1.51565700
H	0.88469400	-0.07657300	-2.01027800
C	3.50389700	-0.32743900	0.84630300
H	1.80611400	-0.24816800	2.18587800
C	3.91885300	-0.32136200	-0.48669200
H	3.30147200	-0.22570000	-2.55254800
H	4.23687500	-0.39564700	1.64552500
H	4.97713500	-0.38548700	-0.72602800
P	-0.54802800	-0.04776400	0.56801500
C	-1.12244000	2.50734500	0.13769300
H	-1.48628000	2.53563500	1.16949800
H	-0.07769200	2.84419200	0.13119600
C	-2.57590400	-1.62928600	-0.04660500
H	-2.82170400	-1.67145600	1.01975100
H	-3.15217500	-0.81871300	-0.50658700
O	-0.80804900	0.08254500	2.02618300
O	-1.16455400	-1.33184600	-0.18982200
O	-1.17813100	1.14479800	-0.34442200
C	-1.97370900	3.36444300	-0.78169500
H	-1.60436500	3.31603700	-1.81121800
H	-1.94561900	4.40911700	-0.45194400
H	-3.01471700	3.02566200	-0.77172700
C	-2.84329600	-2.95655800	-0.73185500
H	-3.90570900	-3.21211500	-0.64858100
H	-2.25636400	-3.75586900	-0.26856500
H	-2.58103000	-2.90489400	-1.79346600

Diethyl benzoylphosphonate

SCF energy: -1070.494475

SCF energy in solution: -1070.2397732400

Free energy in solution: -1070.0384302400

O	0.09728400	-1.89400200	1.06326600
C	0.42516700	-0.94408200	0.37022800
C	1.84127500	-0.56651200	0.13251800
C	2.21494900	0.36642500	-0.84859600
C	2.82910900	-1.18406800	0.91993600
C	3.56145600	0.67986400	-1.03031500
H	1.46083300	0.81718300	-1.48557800
C	4.16916100	-0.86083900	0.73998800
H	2.51972900	-1.90829900	1.66663400
C	4.53657600	0.07302500	-0.23584800
H	3.84965900	1.39496600	-1.79550900
H	4.92980800	-1.33356200	1.35512100
H	5.58447200	0.32402500	-0.37788000
P	-0.96056200	0.05425300	-0.42268500
C	-2.87909200	-1.78360600	-0.36291300
H	-2.82285000	-1.73197800	-1.45496900
H	-2.27524500	-2.62575400	-0.01130300
C	-1.81842200	2.48475200	0.22794300
H	-1.89965300	2.71159600	-0.84047400
H	-2.78676900	2.11955200	0.58514900
O	-0.90951800	0.13623900	-1.90903200
O	-0.83704000	1.42823500	0.40767900
O	-2.31200600	-0.56919200	0.19534300
C	-4.31454300	-1.89247900	0.11598500
H	-4.35706900	-1.91760700	1.20948900
H	-4.76559700	-2.81385500	-0.26939500
H	-4.90803200	-1.04265000	-0.23652100
C	-1.35176100	3.69200400	1.01883200
H	-2.07597600	4.50764900	0.91339600
H	-0.37998800	4.04161000	0.65625000
H	-1.25790500	3.44619400	2.08126700

***N*-glutarimide anion**

SCF energy: -399.389134

SCF energy in solution: -399.33380146

Free energy in solution: -399.25762046

C	-1.23495900	1.01638900	0.21147200
C	1.23495300	1.01637500	0.21158700
C	0.00002200	1.71794500	-0.34911400
H	-2.16788300	1.37504900	-0.23789400
H	1.30932800	1.21497900	1.29349100
H	0.00007400	1.63497300	-1.44643700
N	-0.00000300	-1.17474100	-0.08615800
C	1.18615800	-0.52277900	0.01130300
C	-1.18616800	-0.52276800	0.01130000
O	2.28488100	-1.10108500	-0.03289100
O	-2.28488300	-1.10108400	-0.03282800
H	2.16792300	1.37503800	-0.23767300
H	0.00001200	2.79448500	-0.11527300
H	-1.30946900	1.21504300	1.29336100

***N*-glutarimide**

SCF energy: -399.975013

SCF energy in solution: -399.86120383

Free energy in solution: -399.77041383

C	-1.25954500	1.05779300	0.20835100
C	1.25953800	1.05779600	0.20835000
C	-0.00000400	1.72287200	-0.35915200
H	-2.17690500	1.43930300	-0.24770200
H	1.33691800	1.25352600	1.28795000
H	-0.00000400	1.63866200	-1.45336200
N	0.00000300	-1.04902600	-0.03890300
C	1.26180900	-0.45090300	0.02552000
C	-1.26180500	-0.45091300	0.02556600
O	2.26946300	-1.12712900	-0.04574200
O	-2.26945600	-1.12713700	-0.04576100
H	2.17689700	1.43932000	-0.24769000
H	-0.00000500	2.79240500	-0.12459300
H	-1.33693300	1.25354500	1.28794700
H	0.00000500	-2.05931100	-0.15001200

2a

SCF energy: -2638.858177

SCF energy in solution: -2638.01653768

Free energy in solution: -2637.40306168

P	-0.78236200	1.51853100	1.11472900
C	3.05091000	1.20444700	1.91601600
H	2.72252600	0.73310800	2.85012500
H	4.14266800	1.27117200	1.98850800
C	0.05622800	1.93254900	2.75206100
H	-0.69347300	2.34652800	3.43671800
H	0.36971200	0.96997600	3.17251200
C	2.40468200	2.59851400	1.74021300
H	2.05341900	2.72739200	0.70966800
H	3.16979300	3.37101500	1.88843200
C	1.24949000	2.90847800	2.70850100
H	1.65312600	2.96315200	3.73003900
H	0.87488400	3.91147900	2.47417300
P	2.58368100	0.00580300	0.56365800
C	3.62616600	0.50705800	-0.87594400
C	4.64554700	1.46948400	-0.82681200
C	3.34927400	-0.12173300	-2.10379800
C	5.37792600	1.78974400	-1.97372000
H	4.87724700	1.98148900	0.10220200
C	4.09085100	0.18868100	-3.24264700
H	2.54228700	-0.84835600	-2.16079900
C	5.10628000	1.14723500	-3.18166300
H	6.16175000	2.54102500	-1.91893900
H	3.86791900	-0.31096500	-4.18173500
H	5.67776100	1.39556300	-4.07220300
C	3.40648100	-1.53436000	1.17191500
C	4.78992200	-1.74687500	1.06692400
C	2.61617300	-2.50722700	1.80261600
C	5.36982700	-2.90345700	1.58968600
H	5.41530600	-1.01273600	0.56629000
C	3.19887700	-3.66034800	2.33244700
H	1.54041800	-2.36384000	1.85801200
C	4.57612500	-3.86081500	2.22641100
H	6.44186800	-3.05830500	1.49740500
H	2.57406900	-4.40705500	2.81559900
H	5.02913600	-4.76248700	2.63033600
C	-2.54145600	1.30511500	1.65566700
C	-3.59179400	1.66238800	0.79272200
C	-2.86347700	0.71278400	2.88654200
C	-4.92142900	1.46093100	1.16289200
H	-3.36779100	2.11809900	-0.16783200
C	-4.19470000	0.51191600	3.25733300
H	-2.07644600	0.39852600	3.56585000
C	-5.22894900	0.89009900	2.40067900
H	-5.71888200	1.75853900	0.48638100
H	-4.42038100	0.05650900	4.21804200
H	-6.26497800	0.73927200	2.69224000
C	-0.85503400	3.17095800	0.28101000
C	-1.45343600	4.28383500	0.89810400
C	-0.27005400	3.33102000	-0.98317400
C	-1.45854900	5.52798900	0.26845400
H	-1.92668000	4.17648600	1.87078700
C	-0.27757900	4.57922700	-1.61398600
H	0.16916400	2.47135600	-1.47782100
C	-0.86770900	5.67818100	-0.99004400
H	-1.92417900	6.37967100	0.75789600
H	0.17649200	4.68662800	-2.59565200
H	-0.87280400	6.64806300	-1.48090300
O	0.26262500	-2.09700000	-1.04508900
C	-0.98139900	-1.81658600	-0.92694400
C	-1.82012800	-2.42860900	0.14537700
C	-3.16258200	-2.07490300	0.35140900
C	-1.24332300	-3.40101000	0.98043700
C	-3.90714200	-2.67648100	1.36447500
H	-3.62233300	-1.31634900	-0.27483700
C	-1.98922400	-3.99677500	1.99459500
H	-0.21584500	-3.69642100	0.79708300
C	-3.32570200	-3.63850500	2.19352300
H	-4.94328800	-2.38382100	1.51125400
H	-1.53089200	-4.75724200	2.62256100
H	-3.90883200	-4.10829500	2.98139000

C	-2.22942500	-0.06506700	-4.16723900
C	-3.25425000	-2.30560100	-4.01341000
C	-3.55140900	-0.82474300	-4.22056800
H	-2.35443300	1.01838000	-4.24788900
H	-2.71767400	-2.71108800	-4.88280700
H	-4.22470700	-0.45929500	-3.43464200
N	-1.72200000	-1.49309500	-2.17987600
C	-2.39097500	-2.59243200	-2.79118600
C	-1.45344000	-0.31012200	-2.88031900
O	-2.28188600	-3.71700400	-2.35119900
O	-0.63437200	0.50697200	-2.49057800
H	-4.15788800	-2.91250700	-3.89943100
H	-4.05711500	-0.65989700	-5.17822700
H	-1.58444100	-0.36989400	-5.00444200
Pd	0.28037500	-0.23591100	0.00090400

TS1a

SCF energy: -2638.833306

SCF energy in solution: -2637.99245417

Free energy in solution: -2637.38105017

P	1.01280200	1.78765500	0.00264100
C	-2.91427900	2.38163500	1.08158600
H	-3.41635100	3.06015400	0.38170100
H	-3.64340100	2.14423200	1.86315700
C	-0.12384800	3.23730900	-0.39658400
H	0.46939000	3.98884200	-0.93056600
H	-0.86105500	2.85930000	-1.11344400
C	-1.69785200	3.07511800	1.72387600
H	-1.08019600	2.32701400	2.23619000
H	-2.07222900	3.74723300	2.50823500
C	-0.82560900	3.92764600	0.78823800
H	-1.44970500	4.73001400	0.36777200
H	-0.06548800	4.42625700	1.40082600
P	-2.51927300	0.74310400	0.23162200
C	-3.90317700	-0.32629600	0.83200700
C	-3.96335200	-0.60706500	2.20871100
C	-4.84934300	-0.92092800	-0.01518900
C	-4.96204600	-1.42956800	2.72652300
H	-3.21373900	-0.19343100	2.87897900
C	-5.84350900	-1.75457700	0.50428600
H	-4.81867500	-0.73111700	-1.08304100
C	-5.90797700	-2.00643500	1.87472400
H	-4.99447700	-1.62991800	3.79438600
H	-6.57152500	-2.20241900	-0.16744100
H	-6.68427800	-2.65198900	2.27688800
C	-2.92681700	1.00775600	-1.55295700
C	-4.00052200	1.80182400	-1.99121700
C	-2.13145000	0.35997200	-2.51467500
C	-4.26399400	1.95663000	-3.35284400
H	-4.64762800	2.29363400	-1.27001300
C	-2.40139800	0.51073800	-3.87792000
H	-1.29406300	-0.25925100	-2.19809700
C	-3.46335400	1.31200400	-4.29948000
H	-5.09726500	2.57643400	-3.67380400
H	-1.77558200	0.00158600	-4.60586800
H	-3.66970900	1.43287800	-5.35969000
C	2.15824500	1.86935300	-1.44174800
C	3.55373100	1.85300000	-1.30288200
C	1.60970200	1.88485300	-2.73583200
C	4.37895900	1.88139000	-2.42953900
H	4.00278500	1.81723000	-0.31634300
C	2.43554200	1.91372100	-3.85817200
H	0.53247800	1.86015100	-2.87347500
C	3.82436300	1.91633300	-3.70887600
H	5.45834400	1.87165900	-2.30204400
H	1.99303900	1.92722900	-4.85077200
H	4.46816900	1.93735500	-4.58418400
C	1.99539400	2.46546300	1.41402300
C	2.72354600	3.66451400	1.31592100
C	1.96262700	1.79614100	2.64494000
C	3.40243600	4.17494300	2.42226800
H	2.76989400	4.19754900	0.37003500
C	2.64009900	2.30891300	3.75436300
H	1.40122400	0.86907600	2.72293800
C	3.36127100	3.49763600	3.64458100
H	3.96364100	5.10128400	2.33082100
H	2.60654100	1.77560500	4.70072300
H	3.89158100	3.89644500	4.50537600
O	1.13484200	-1.37273000	-1.61272200
C	1.33174100	-1.45568900	-0.40557000
C	2.69389700	-1.51123300	0.23207100
C	2.86237000	-1.60357400	1.61883000
C	3.82127300	-1.45980700	-0.59670700
C	4.14040400	-1.64735400	2.17228500
H	1.98380800	-1.64554900	2.25704500
C	5.10083600	-1.49859100	-0.04082300
H	3.67608600	-1.40975400	-1.66988600
C	5.26516900	-1.59189700	1.34258400
H	4.26178700	-1.72428500	3.25001500
H	5.97134900	-1.46645000	-0.69151900
H	6.26258300	-1.62628900	1.77371400

C	-1.10788300	-4.32656200	1.61257600
C	0.39200500	-5.58626000	0.07083700
C	-0.19340800	-5.54559400	1.48354500
H	-1.41242100	-4.13213300	2.64548300
H	-0.41239200	-5.74107900	-0.66373200
H	0.62109900	-5.47760700	2.21673800
N	0.57187800	-3.09826200	0.23355200
C	1.10666700	-4.28138300	-0.28671100
C	-0.46739300	-3.05688100	1.07300100
O	2.08594800	-4.27313400	-1.01035900
O	-0.96018100	-1.95714500	1.43641500
H	1.11423800	-6.39537000	-0.06471200
H	-0.74643800	-6.46507400	1.70619400
H	-2.03386400	-4.47942500	1.03963700
Pd	-0.17955600	-0.20330900	0.39425500

3a

SCF energy: -2638.857569

SCF energy in solution: -2638.0112782900

Free energy in solution: -2637.3987242900

P	1.77688000	-1.24558500	-0.16525900
C	-0.93438200	-1.17770200	-3.12052200
H	-1.48631000	-2.03702400	-3.51816800
H	-1.23427600	-0.32257700	-3.73695900
C	1.21486200	-2.74837500	-1.12429700
H	1.85854500	-3.58702200	-0.83357900
H	0.21264200	-2.98979900	-0.76078600
C	0.58282500	-1.37164900	-3.28970400
H	1.09574900	-0.47104300	-2.93042900
H	0.78231500	-1.41829800	-4.36921800
C	1.22872300	-2.61770000	-2.66071500
H	0.75147800	-3.51895300	-3.07099800
H	2.27221000	-2.64763000	-2.99705500
P	-1.54448500	-0.72992400	-1.39934300
C	-3.03658300	0.27394700	-1.82150600
C	-2.83917400	1.57409100	-2.31763200
C	-4.34722300	-0.20177300	-1.67467200
C	-3.92688900	2.37005800	-2.67686500
H	-1.83336500	1.97554300	-2.39957400
C	-5.43496800	0.60020100	-2.02817200
H	-4.52385900	-1.19721200	-1.28120600
C	-5.22902000	1.88482400	-2.53271700
H	-3.75623900	3.37393800	-3.05684900
H	-6.44468400	0.21625800	-1.90826100
H	-6.07707100	2.50694800	-2.80649600
C	-2.25151900	-2.26888300	-0.66384900
C	-2.53545900	-3.43893100	-1.38849100
C	-2.54061900	-2.23548700	0.71237500
C	-3.08709000	-4.55177000	-0.75000700
H	-2.33441300	-3.49769300	-2.45346600
C	-3.11000200	-3.34463400	1.34145200
H	-2.34542300	-1.33958000	1.29557700
C	-3.37738400	-4.50690000	0.61582500
H	-3.29656400	-5.45065400	-1.32437100
H	-3.34325100	-3.27799700	2.40012800
H	-3.81423200	-5.37255800	1.10722300
C	2.07901100	-1.95007900	1.50772100
C	3.27927500	-1.74520600	2.20195400
C	1.03834200	-2.65296200	2.13720200
C	3.44604000	-2.25947600	3.48868400
H	4.08441700	-1.17989500	1.74503900
C	1.20946900	-3.16529100	3.42246300
H	0.08246600	-2.78815200	1.63957400
C	2.41513000	-2.97335900	4.10014100
H	4.38200400	-2.09242300	4.01503800
H	0.39389700	-3.70402300	3.89664600
H	2.54560300	-3.36887000	5.10384700
C	3.44809300	-0.94895100	-0.88623000
C	4.41756700	-1.96847400	-0.90244400
C	3.74972100	0.27821500	-1.49112400
C	5.65759000	-1.75810200	-1.50374200
H	4.21054000	-2.92577900	-0.43208200
C	4.99302600	0.48797600	-2.09415300
H	3.01357700	1.07453300	-1.48525400
C	5.94776100	-0.52810600	-2.10168700
H	6.39791300	-2.55366400	-1.50464500
H	5.21137400	1.44867700	-2.55225700
H	6.91538800	-0.36521900	-2.56868700
O	1.80421400	1.23013700	2.17889000
C	1.52374200	1.56908400	1.04877600
C	2.04625800	2.87283300	0.49062100
C	1.69152400	3.34168400	-0.78107600
C	2.93389500	3.62436100	1.27720600
C	2.21883100	4.54035500	-1.26244200
H	0.98758400	2.76959800	-1.37781800
C	3.46166300	4.82007700	0.79572000
H	3.19413600	3.25057800	2.26252700
C	3.10568000	5.28004500	-0.47610600
H	1.93323400	4.90129900	-2.24717400
H	4.15019500	5.39529700	1.40950900
H	3.51643600	6.21393500	-0.85154400

C	-2.72255400	3.34753500	1.38952500
C	-3.90932500	2.02612500	3.13682100
C	-3.20854000	3.35233900	2.84163500
H	-2.10130900	4.21623900	1.15333600
H	-4.86656800	1.98160400	2.59540900
H	-2.34683900	3.47331300	3.51157300
N	-2.11809000	0.93689600	1.71949700
C	-3.09032300	0.80496900	2.69504700
C	-1.91982000	2.08718900	1.10029300
O	-3.33200800	-0.29057300	3.19733000
O	-1.02298200	2.19920700	0.19022100
H	-4.14471700	1.89967100	4.19772700
H	-3.87693900	4.20218600	3.02457100
H	-3.57949200	3.36733700	0.69983300
Pd	0.21808300	0.46675500	-0.07003300

4a

SCF energy: -2638.872920

SCF energy in solution: -2638.0332922700

Free energy in solution: -2637.4188142700

P	1.67997300	-1.21535600	-0.46463500
C	-1.63173300	-1.45006600	-2.73032600
H	-1.95567300	-2.48534500	-2.88733100
H	-2.32606200	-0.82360200	-3.29801900
C	1.09671300	-2.66331100	-1.50007500
H	1.86901500	-3.43990900	-1.44629300
H	0.20621200	-3.07000000	-1.01001500
C	-0.21024100	-1.24023100	-3.28417100
H	0.17027100	-0.27169600	-2.93828500
H	-0.28526900	-1.16379600	-4.37718900
C	0.80647700	-2.35101900	-2.97914600
H	0.45981900	-3.28482600	-3.44480600
H	1.74990300	-2.09606800	-3.47631300
P	-1.87006400	-0.95030200	-0.93143600
C	-3.54335800	-0.16164900	-0.98064500
C	-3.78385400	0.88514100	-1.88769200
C	-4.57036900	-0.54302000	-0.10403700
C	-5.03039100	1.51043700	-1.93571300
H	-2.98902800	1.24222600	-2.53538300
C	-5.81418900	0.09156000	-0.14872500
H	-4.40530400	-1.33796400	0.61516700
C	-6.05134800	1.11392200	-1.06826800
H	-5.19851500	2.31421900	-2.64771400
H	-6.59893000	-0.22133900	0.53507000
H	-7.02157400	1.60214400	-1.10613600
C	-2.18252700	-2.50740800	0.01386900
C	-2.75119300	-3.66282100	-0.54808700
C	-1.85796000	-2.50641200	1.38270000
C	-2.96794800	-4.79968100	0.23171500
H	-3.04080300	-3.68324900	-1.59474900
C	-2.08810000	-3.64372900	2.16206600
H	-1.45138700	-1.60735100	1.84059300
C	-2.63389800	-4.79319900	1.58844700
H	-3.40458600	-5.68701100	-0.21937200
H	-1.83690400	-3.62427500	3.21898300
H	-2.80599900	-5.67848900	2.19510800
C	2.46827400	-2.06761300	0.96747100
C	3.60561600	-1.52456200	1.58449100
C	1.90122700	-3.23448800	1.50326100
C	4.17479800	-2.14648800	2.69495700
H	4.05076000	-0.61323700	1.19854900
C	2.47076800	-3.85277000	2.61756100
H	1.00666000	-3.66436700	1.06445000
C	3.61067500	-3.31307400	3.21419000
H	5.05645800	-1.71271900	3.15889200
H	2.01963400	-4.75689700	3.01772300
H	4.05361400	-3.79510600	4.08155400
C	3.10309000	-0.60338200	-1.46578800
C	4.24029700	-1.40053100	-1.68617200
C	3.02532500	0.65245300	-2.08264300
C	5.27596000	-0.94410500	-2.50036100
H	4.32373600	-2.37354500	-1.21002700
C	4.06356700	1.10788300	-2.89948300
H	2.15381400	1.27654200	-1.91503200
C	5.18935100	0.31200400	-3.10845400
H	6.15208800	-1.56747600	-2.65845200
H	3.99126500	2.08804800	-3.36252400
H	5.99965000	0.66740800	-3.73946600
O	1.58457400	0.73767900	2.39172600
C	1.35149300	1.27614500	1.32811600
C	1.98923300	2.60488000	1.00408700
C	1.67184700	3.33679100	-0.14633800
C	2.95082200	3.10789300	1.89859500
C	2.30514000	4.55618600	-0.39739900
H	0.90688200	2.96896000	-0.82343400
C	3.58690900	4.31878500	1.64121300
H	3.17814000	2.53180300	2.79010400
C	3.26466600	5.04657100	0.49025000
H	2.04270700	5.12456100	-1.28609300
H	4.33112200	4.69981800	2.33623300
H	3.75879100	5.99425500	0.29018100

C	-2.69026800	3.92163200	0.21327600
C	-3.02185600	2.72774000	2.36431500
C	-2.75442000	4.09183200	1.73055100
H	-2.39391200	4.83900800	-0.30418800
H	-4.03596000	2.38573300	2.11001400
H	-1.80013100	4.49120400	2.09889800
N	-1.39171500	1.83773600	0.67921300
C	-2.05022700	1.65381700	1.87679700
C	-1.70870200	2.83004400	-0.21001100
O	-1.88314200	0.63053300	2.54039400
O	-1.22719000	2.85030900	-1.35022700
H	-2.95971600	2.74664600	3.45645300
H	-3.53192600	4.81249300	2.01055800
H	-3.67922700	3.64071800	-0.17745800
Pd	0.00395200	0.32582800	0.10662700

TS2a

SCF energy: -2638.810709

SCF energy in solution: -2637.974284

Free energy in solution: -2637.3616744700

P	-2.09194000	-0.05447000	-0.72852700
C	1.09441600	-0.10558000	-3.13772400
H	1.06553600	0.75615000	-3.81458100
H	1.99250000	-0.67199600	-3.40159900
C	-1.97586600	0.65209300	-2.45321300
H	-2.97235900	1.01075800	-2.73711500
H	-1.32223600	1.52832700	-2.39062100
C	-0.13211300	-1.00790700	-3.36343000
H	-0.19838300	-1.73153100	-2.54253900
H	0.04939100	-1.59568000	-4.27403700
C	-1.48867400	-0.30974100	-3.55397500
H	-1.45550600	0.27148900	-4.48638500
H	-2.24947800	-1.08502300	-3.70811500
P	1.38340000	0.51735900	-1.36535700
C	3.22422000	0.37307800	-1.25836900
C	3.83149800	-0.85843000	-1.55183000
C	4.03499700	1.44527000	-0.85860100
C	5.21663400	-1.00750700	-1.47586300
H	3.22599600	-1.71887300	-1.82001800
C	5.42085800	1.29516000	-0.79020300
H	3.58405800	2.38865400	-0.57925800
C	6.01745000	0.07259900	-1.10231200
H	5.66531300	-1.97083000	-1.70349400
H	6.03398400	2.13862200	-0.48341200
H	7.09709400	-0.04021900	-1.04625300
C	1.07813600	2.33264000	-1.54023200
C	1.65663300	3.06953100	-2.58757400
C	0.23565500	2.99429500	-0.63628400
C	1.38944200	4.43116200	-2.73360400
H	2.33532200	2.58558200	-3.28479000
C	-0.04142500	4.35463900	-0.78972300
H	-0.19648700	2.44430600	0.19153700
C	0.53419800	5.07573000	-1.83656700
H	1.85045300	4.98724400	-3.54577200
H	-0.70447600	4.84792200	-0.08427400
H	0.32272100	6.13569100	-1.95157900
C	-2.96494800	1.25409600	0.23109900
C	-3.12472300	1.03839800	1.61094300
C	-3.47029900	2.43378000	-0.33792600
C	-3.79625100	1.97662800	2.39518200
H	-2.69859400	0.15514500	2.08037200
C	-4.13204200	3.37467200	0.45557100
H	-3.35153000	2.63574900	-1.39681600
C	-4.30123900	3.14610500	1.82173900
H	-3.91375800	1.79268200	3.45967500
H	-4.51638400	4.28411400	0.00092800
H	-4.81901000	3.87785600	2.43644500
C	-3.38944700	-1.35610000	-0.95013100
C	-4.75750100	-1.05132800	-0.86479200
C	-3.01070400	-2.66903700	-1.26831900
C	-5.71863100	-2.03734500	-1.09150900
H	-5.07450600	-0.04460200	-0.61148000
C	-3.97272200	-3.65253600	-1.50313800
H	-1.95750300	-2.92726300	-1.32323800
C	-5.32956500	-3.33929400	-1.41234000
H	-6.77323800	-1.78679400	-1.01299900
H	-3.65971400	-4.66517300	-1.74262100
H	-6.07963200	-4.10672800	-1.58336700
O	-1.11754500	-3.26231100	1.55599800
C	-0.54032100	-2.36826400	1.09395600
C	1.37977300	-2.48134300	0.68064500
C	1.62436500	-3.48423600	-0.26969600
C	2.28735200	-2.28144000	1.72761900
C	2.78538200	-4.25681700	-0.19242500
H	0.90388900	-3.67435400	-1.06086500
C	3.44730700	-3.05629300	1.80076400
H	2.08576000	-1.51570800	2.46829600
C	3.69900500	-4.04137500	0.84273800
H	2.96931200	-5.03241000	-0.93215200
H	4.15449300	-2.89015700	2.60944000
H	4.59945900	-4.64653300	0.90821800

C	1.75660300	2.11775900	3.67456100
C	-0.02518700	0.77836600	4.75739600
C	1.41128200	1.27618300	4.90082000
H	2.81148600	2.40462200	3.63919100
H	-0.72168200	1.62777000	4.83153200
H	2.09501300	0.41812500	4.96657400
N	0.44621200	0.45561300	2.30112800
C	-0.27625100	0.09794800	3.40594500
C	1.43280200	1.40050000	2.35795900
O	-1.16396500	-0.76585300	3.34731300
O	2.07714400	1.72126300	1.35050900
H	-0.30903300	0.06778700	5.53872100
H	1.53942900	1.85284000	5.82497400
H	1.17488400	3.05216100	3.68928400
Pd	-0.00225300	-0.79551100	0.19476200

TS3a

SCF energy: -3364.967965

SCF energy in solution: -3364.0272707900

Free energy in solution: -3363.2719877900

P	-2.42357500	0.68214100	-0.51879700
C	0.33857500	1.98434700	-3.16884400
H	0.50244200	3.00399000	-3.54004000
H	1.05317600	1.34201000	-3.69372700
C	-2.54617000	2.28313500	-1.48563700
H	-3.55426400	2.67961300	-1.31484300
H	-1.85169400	2.98241000	-1.01291100
C	-1.06095800	1.45414400	-3.51649100
H	-1.09064700	0.40367300	-3.21908800
H	-1.12754400	1.44488700	-4.61322300
C	-2.29900000	2.20529700	-3.00585400
H	-2.28742900	3.24007300	-3.37894700
H	-3.17378300	1.72940200	-3.46524000
P	0.88322000	1.84323300	-1.38507900
C	2.71776500	1.76503100	-1.58635400
C	3.35929900	0.52192600	-1.49752000
C	3.47589000	2.90907800	-1.88246400
C	4.73539400	0.42703700	-1.71649800
H	2.78132800	-0.36174400	-1.24838400
C	4.85048600	2.80899200	-2.09835700
H	2.99680500	3.88236200	-1.93829700
C	5.48284400	1.56604900	-2.01794400
H	5.22431900	-0.54038400	-1.63814400
H	5.42690500	3.70203900	-2.32650200
H	6.55462100	1.48892500	-2.18270900
C	0.66114400	3.51433600	-0.61442500
C	0.29533300	4.67815000	-1.30743900
C	0.87527900	3.59909800	0.77450300
C	0.14519300	5.89434500	-0.63371000
H	0.11934000	4.65022700	-2.37832100
C	0.73327800	4.81502200	1.44296800
H	1.15559500	2.70489100	1.32522100
C	0.36492100	5.96662500	0.74179900
H	-0.14083700	6.78409900	-1.18884700
H	0.90682700	4.86193900	2.51496500
H	0.24980900	6.91247500	1.26452700
C	-3.52526600	1.04631400	0.91662200
C	-4.42810000	0.09876400	1.42309200
C	-3.39539100	2.27749000	1.58110000
C	-5.19886100	0.38701200	2.55120000
H	-4.53382700	-0.86661900	0.93962500
C	-4.16824600	2.56283200	2.70613400
H	-2.67874900	3.01580600	1.23272300
C	-5.07513400	1.61941500	3.19352600
H	-5.89666600	-0.35706600	2.92622400
H	-4.05655600	3.52202400	3.20469500
H	-5.67673400	1.84189600	4.07073000
C	-3.36562500	-0.51022700	-1.55591300
C	-4.74654300	-0.35411900	-1.77357600
C	-2.67885900	-1.53893100	-2.21567100
C	-5.42873800	-1.22561300	-2.62152000
H	-5.29321300	0.44144200	-1.27513000
C	-3.36732300	-2.40447200	-3.07007000
H	-1.60336500	-1.63797800	-2.10066800
C	-4.73947100	-2.25520600	-3.26907700
H	-6.49680300	-1.09917300	-2.77838500
H	-2.82028400	-3.18982800	-3.58394200
H	-5.27254000	-2.93250900	-3.93133400
O	-1.01520200	-0.16607900	2.77480900
C	-1.05242500	-0.79318700	1.73247600
C	-1.57974400	-2.19336100	1.69584700
C	-1.28791900	-3.06562400	0.64050600
C	-2.37946400	-2.63012000	2.76910500
C	-1.79526800	-4.36621900	0.66007200
H	-0.63133300	-2.73023700	-0.15810100
C	-2.89626600	-3.92166300	2.77208100
H	-2.58782800	-1.93989400	3.58047600
C	-2.60318200	-4.79234400	1.71538100
H	-1.55418800	-5.04871500	-0.15048200
H	-3.52366200	-4.25480300	3.59503700
H	-3.00266600	-5.80359600	1.72048200

C	2.09538200	-3.03128900	-3.57009700
C	2.92602300	-4.08825900	-1.48557700
C	2.41297000	-4.36607000	-2.89731700
H	1.62049400	-3.15115700	-4.54814100
H	3.92959700	-3.63731800	-1.53669600
H	1.50034600	-4.97622700	-2.84392900
N	1.21263800	-2.23593600	-1.34573000
C	2.03001100	-3.11299500	-0.70542200
C	1.17316500	-2.15996500	-2.70641400
O	2.09445600	-3.15015400	0.53840400
O	0.41245000	-1.36762900	-3.28842100
H	3.02463000	-4.99762400	-0.88451100
H	3.14373100	-4.94163200	-3.47916100
H	3.02641300	-2.46698400	-3.73505100
Pd	-0.25428400	0.19435700	0.14162000
P	2.38649600	-0.68619400	2.25038700
H	1.71950600	-1.88462600	2.49680500
C	1.62959900	0.47248900	4.52618900
H	1.12651200	1.27072600	3.97344000
H	0.89235500	-0.31537900	4.71798300
C	4.54535800	-2.21522500	2.22471100
H	4.66408900	-2.13056500	3.31115900
H	3.93299200	-3.08613900	1.97605100
O	1.66565300	0.26213200	1.33358300
O	3.85332700	-1.03221500	1.73635800
O	2.70079400	-0.06249700	3.70632000
C	2.24742400	0.98012200	5.81573300
H	2.74489400	0.16855700	6.35675800
H	1.46710000	1.39933700	6.46077900
H	2.98613200	1.76137400	5.60960000
C	5.89426800	-2.27133500	1.53361800
H	6.45253000	-3.14765800	1.88205100
H	6.48269100	-1.37367300	1.74819800
H	5.76418000	-2.35264100	0.44988100

5a

SCF energy: -3364.973154

SCF energy in solution: -3364.0329502400

Free energy in solution: -3363.2788272400

P	-2.74550000	-0.05498500	-0.49242600
C	-0.24686500	2.00056700	-2.88350800
H	-0.61831600	2.94944000	-3.28960000
H	0.75881300	1.86690700	-3.29454700
C	-3.19067100	1.21583800	-1.78876900
H	-4.28614200	1.23901500	-1.83771500
H	-2.87160800	2.19197100	-1.41137300
C	-1.11135500	0.81722700	-3.34975800
H	-0.75227700	-0.09827000	-2.86814500
H	-0.91020100	0.67554400	-4.42029600
C	-2.63139600	0.96852600	-3.20065400
H	-2.97340700	1.80552800	-3.82687000
H	-3.10308700	0.06856500	-3.61234300
P	0.05513100	2.14858600	-1.03128800
C	1.80486000	2.73594300	-1.03729400
C	2.80439900	1.77464400	-1.25757500
C	2.16450600	4.08512500	-0.90665500
C	4.14087000	2.16323400	-1.37043600
H	2.55228600	0.71709800	-1.33362800
C	3.50239100	4.46853100	-1.02088300
H	1.40656400	4.84012900	-0.72400500
C	4.49086600	3.51130200	-1.26088200
H	4.89857100	1.39946600	-1.51816200
H	3.76956700	5.51807800	-0.92573400
H	5.53071200	3.81500100	-1.35403700
C	-0.88481200	3.61847800	-0.42004900
C	-1.35433100	4.66453000	-1.23012900
C	-1.11865100	3.68483100	0.96585300
C	-2.04849400	5.74150900	-0.67323800
H	-1.17866900	4.65321100	-2.30151400
C	-1.80251600	4.76679300	1.52258600
H	-0.76419000	2.88277400	1.60902400
C	-2.27386900	5.79532300	0.70357400
H	-2.40740400	6.54043500	-1.31682300
H	-1.97115900	4.79999500	2.59546500
H	-2.81222300	6.63479400	1.13534400
C	-4.02628200	0.25920200	0.79613000
C	-4.56852300	-0.79198900	1.55163100
C	-4.42439800	1.57405300	1.08774700
C	-5.50370800	-0.53684400	2.55405900
H	-4.26507100	-1.81533300	1.35609600
C	-5.35661500	1.82688900	2.09507100
H	-4.00559600	2.41213700	0.54006400
C	-5.90186600	0.77256100	2.82859100
H	-5.91554600	-1.36431900	3.12530300
H	-5.65482000	2.85078200	2.30416500
H	-6.62862600	0.96999600	3.61192500
C	-3.24610900	-1.62643400	-1.30760800
C	-4.60229100	-1.94931000	-1.49646000
C	-2.25913300	-2.46301700	-1.84916000
C	-4.96066800	-3.10109400	-2.19537100
H	-5.37927000	-1.30848900	-1.09017600

C	-2.62675300	-3.61193000	-2.55524000
H	-1.20574800	-2.21944300	-1.75250600
C	-3.97223800	-3.93668100	-2.72394100
H	-6.01152100	-3.34476900	-2.32829600
H	-1.84909500	-4.24489600	-2.97263400
H	-4.25415600	-4.83391000	-3.26889300
O	-1.68968100	-0.96700900	2.71325500
C	-1.08695900	-1.29173800	1.71338900
C	-0.55097200	-2.68279500	1.53711900
C	0.31738700	-3.01801500	0.49051500
C	-0.92141700	-3.65979400	2.48007700
C	0.82176700	-4.31761600	0.39842100
H	0.61316600	-2.27940400	-0.25030500
C	-0.42567700	-4.95559200	2.37507500
H	-1.59095200	-3.37773600	3.28684500
C	0.45158000	-5.28514100	1.33393200
H	1.50521700	-4.56495300	-0.40852300
H	-0.71705300	-5.70971600	3.10182700
H	0.84249800	-6.29659500	1.25488600
C	2.76579700	-2.69997100	-3.74988800
C	4.93094900	-2.34663600	-2.58386500
C	4.08375900	-3.36357500	-3.34818000
H	2.05909800	-3.40183000	-4.20288000
H	5.28871900	-1.56684000	-3.27366200
H	3.87688100	-4.22975900	-2.70376600
N	2.78525200	-1.57000600	-1.49989000
C	4.14335600	-1.64425000	-1.46827900
C	2.06844900	-2.03766400	-2.55238700
O	4.79386300	-1.12154700	-0.54241500
O	0.82588000	-1.92956600	-2.59278000
H	5.82234600	-2.79175600	-2.13093800
H	4.61949100	-3.74522700	-4.22630600
H	2.95864500	-1.91761800	-4.50013700
Pd	-0.60473600	0.16086900	0.37089300
P	2.59487100	0.01072500	1.85362600
H	3.14008300	-0.71864800	0.78779900
C	2.34123500	-2.08860000	3.50501800
H	1.28251400	-1.94858500	3.73958600
H	2.41821000	-2.73402200	2.62251100
C	4.92981200	1.20203900	2.17270300
H	5.16010500	0.54811400	3.01999200
H	5.30692900	0.74062900	1.25458600
O	1.14281200	0.38516600	1.68585100
O	3.48111600	1.32265000	2.06495200
O	2.92056000	-0.79320900	3.21337200
C	3.09605400	-2.67977300	4.68130800
H	4.15284800	-2.82310100	4.43406600
H	2.66530800	-3.65205700	4.94513300
H	3.02854200	-2.02144800	5.55341300
C	5.49121300	2.59441800	2.38648100
H	6.58297700	2.54258600	2.46988800
H	5.09311800	3.03503700	3.30633000
H	5.23400500	3.24616400	1.54672200

6a

SCF energy: -2965.445163

SCF energy in solution: -2964.6234604600

Free energy in solution: -2963.9726314600

P	2.40584900	-0.98704300	0.03839600
C	-0.23665300	-3.26460200	-1.93746600
H	-0.05083100	-4.15471400	-1.32554000
H	-0.97776400	-3.55023400	-2.69024200
C	2.42361900	-2.80983100	-0.36898000
H	3.35544200	-3.20455800	0.05270100
H	1.60847500	-3.27419700	0.19712900
C	1.07029300	-2.80002000	-2.61622100
H	1.05320500	-1.71505400	-2.77900500
H	1.12938800	-3.24978200	-3.61430700
C	2.34667400	-3.19468800	-1.85618900
H	2.45326100	-4.28700500	-1.90214000
H	3.21559700	-2.78311900	-2.38223500
P	-1.03568700	-1.97029500	-0.83284100
C	-2.38046900	-1.32601900	-1.91936000
C	-2.01630100	-0.62075400	-3.08086000
C	-3.74077200	-1.50672100	-1.63625400
C	-2.99058100	-0.12897900	-3.94922100
H	-0.96666100	-0.46148600	-3.31716600
C	-4.71457000	-1.01064500	-2.50706900
H	-4.04523900	-2.03864000	-0.74125000
C	-4.34465700	-0.32465100	-3.66436400
H	-2.69300300	0.40190000	-4.84943700
H	-5.76530800	-1.17096100	-2.28113500
H	-5.10439000	0.05287900	-4.34284300
C	-1.87088100	-2.94287500	0.47956000
C	-2.44733000	-4.20166200	0.23473700
C	-1.92058000	-2.41112800	1.77866300
C	-3.05345500	-4.91344500	1.27004200
H	-2.43153400	-4.62807500	-0.76439900
C	-2.53094800	-3.12519300	2.81211100
H	-1.48732100	-1.43442300	1.97538300
C	-3.09472600	-4.37692300	2.55989600

H	-3.49409000	-5.88595600	1.06969200
H	-2.56232500	-2.70394900	3.81302800
H	-3.56570500	-4.93434500	3.36455600
C	3.01623500	-0.97553100	1.77049100
C	3.98207700	-0.05672800	2.20597700
C	2.45635300	-1.86918900	2.70003700
C	4.39776900	-0.04976700	3.53801200
H	4.41588000	0.65262400	1.50909500
C	2.87402300	-1.85765900	4.03034400
H	1.69039100	-2.57736700	2.39619400
C	3.84795500	-0.94965000	4.45176300
H	5.15127200	0.66327800	3.85991800
H	2.43916700	-2.55971000	4.73607500
H	4.17434300	-0.94282400	5.48770800
C	3.76470900	-0.32505700	-0.99948200
C	5.07911600	-0.80137000	-0.83818900
C	3.49564100	0.59946600	-2.01822600
C	6.09854800	-0.35036100	-1.67485600
H	5.31197000	-1.51472600	-0.05276700
C	4.51973100	1.04829900	-2.85592700
H	2.48701000	0.97425000	-2.15497500
C	5.82060200	0.57558200	-2.68491100
H	7.11022600	-0.72125100	-1.53805600
H	4.29809200	1.76875500	-3.63796900
H	6.61757500	0.92571300	-3.33453600
O	1.49787900	1.87497600	1.73336200
C	1.14118000	1.72888300	0.58380100
C	1.08479900	2.89507000	-0.36718000
C	0.50138300	2.79600700	-1.63950400
C	1.62654800	4.12402800	0.04908600
C	0.45333600	3.90756500	-2.48123700
H	0.08043000	1.84682000	-1.96325400
C	1.58635900	5.22997700	-0.79653000
H	2.07744500	4.18814100	1.03438500
C	0.99774200	5.12427300	-2.06125600
H	-0.00355600	3.82570300	-3.46353700
H	2.01376600	6.17496700	-0.47327700
H	0.96649700	5.98822500	-2.71916900
Pd	0.31117800	-0.03342100	-0.02906000
P	-2.62131000	2.01361500	0.67332900
H	-2.45553800	3.03922600	-0.27181600
C	-1.49547200	3.38330700	2.68878400
H	-0.72873700	2.62246600	2.85054900
H	-1.11088500	4.12590700	1.97966500
C	-5.27459200	2.29566700	0.69733700
H	-5.29383000	2.61271900	1.74316800
H	-5.18401300	3.18310600	0.05906600
O	-1.60923600	0.92227700	0.51205400
O	-4.09568700	1.45472200	0.49948200
O	-2.66795900	2.73746300	2.09299100
C	-1.93774800	4.03102000	3.98490500
H	-2.70571400	4.78957100	3.80520400
H	-1.07803300	4.51451000	4.46089500
H	-2.33793600	3.28239300	4.67526500
C	-6.49283400	1.47400000	0.32854900
H	-7.39579900	2.07968100	0.45978700
H	-6.57201000	0.59085200	0.96946800
H	-6.43889600	1.14824100	-0.71438400

TS4a

SCF energy: -3364.961896

SCF energy in solution: -3364.0153595200

Free energy in solution: -3363.2660685200

P	-2.75404000	-0.16319200	-0.43487900
C	-0.48999200	1.92995800	-3.03750800
H	-1.00180200	2.82479200	-3.41097100
H	0.48325900	1.90296000	-3.53725900
C	-3.30297200	1.01226800	-1.78318300
H	-4.39939700	0.99207000	-1.79218000
H	-3.00989100	2.02091200	-1.47342300
C	-1.26922200	0.65797700	-3.41584600
H	-0.82701300	-0.20608800	-2.90797000
H	-1.10523300	0.47871800	-4.48683800
C	-2.78892400	0.70783300	-3.20108000
H	-3.21451900	1.47655700	-3.86257700
H	-3.21280900	-0.24705500	-3.53307400
P	-0.07040300	2.11759800	-1.20960700
C	1.67926700	2.69243700	-1.32038500
C	2.65910600	1.72300900	-1.58896600
C	2.06096000	4.03423500	-1.18952000
C	3.99506500	2.09634500	-1.74013700
H	2.38299100	0.67276300	-1.65856400
C	3.39922100	4.40326000	-1.34397300
H	1.31942100	4.79523500	-0.96879500
C	4.36784400	3.43755100	-1.62308900
H	4.74519300	1.33238300	-1.92477400
H	3.68246600	5.44821300	-1.24582900
H	5.40881000	3.72769300	-1.74083400
C	-0.97382700	3.60066800	-0.57934200
C	-1.50533800	4.62051200	-1.38432200
C	-1.11463700	3.70154200	0.81751200

C	-2.17361400	5.70531200	-0.81109300
H	-1.39694300	4.58440300	-2.46415700
C	-1.77398200	4.79109000	1.38851000
H	-0.70365500	2.92373200	1.45664900
C	-2.31039000	5.79230000	0.57559800
H	-2.58168500	6.48416500	-1.45007300
H	-1.87124000	4.85159900	2.46894900
H	-2.82958500	6.63738300	1.01983700
C	-4.02442000	0.14235700	0.86627400
C	-4.48659200	-0.89797900	1.68696900
C	-4.48729300	1.44612000	1.10602400
C	-5.40810500	-0.64508500	2.70252500
H	-4.12885200	-1.91120700	1.53408100
C	-5.40599200	1.69740000	2.12615700
H	-4.12850100	2.27777800	0.50790600
C	-5.87214000	0.65249400	2.92467100
H	-5.75700900	-1.46415600	3.32551700
H	-5.75448800	2.71273900	2.29536100
H	-6.58762200	0.84862100	3.71865400
C	-3.18289800	-1.79977100	-1.15974300
C	-4.51899100	-2.21724500	-1.29719400
C	-2.15932000	-2.59831400	-1.68949800
C	-4.81874500	-3.42067000	-1.93454100
H	-5.32536100	-1.60939700	-0.89764800
C	-2.46638400	-3.79714000	-2.33817000
H	-1.12201000	-2.28646900	-1.62830700
C	-3.79192000	-4.21392600	-2.45526100
H	-5.85445200	-3.73718900	-2.02682900
H	-1.65836200	-4.39260000	-2.75264900
H	-4.02887500	-5.15014800	-2.95411000
O	-1.56587300	-0.67551600	2.83100900
C	-0.97968400	-1.09576800	1.85831900
C	-0.42525600	-2.49101800	1.81917000
C	0.42402100	-2.92295600	0.79334600
C	-0.77489000	-3.37538800	2.85512700
C	0.92255300	-4.22693200	0.80738300
H	0.71897700	-2.24104100	0.00037800
C	-0.28439200	-4.67820700	2.85793000
H	-1.42553400	-3.01702700	3.64683300
C	0.56719600	-5.10569300	1.83250400
H	1.59072700	-4.55197900	0.01465100
H	-0.55981700	-5.36101100	3.65770700
H	0.95245200	-6.12241500	1.83629600
C	2.94209500	-3.12567400	-3.68187800
C	4.83919800	-2.67219700	-2.13458700
C	4.13846500	-3.75119300	-2.96082100
H	2.33391400	-3.86457300	-4.21066200
H	5.37144500	-1.97304200	-2.79681700
H	3.78858100	-4.55338400	-2.29675200
N	2.56031900	-1.74947800	-1.59986600
C	3.84689200	-1.85441000	-1.31824700
C	2.02655000	-2.37121000	-2.71238400
O	4.36275000	-1.23545200	-0.31499700
O	0.81999200	-2.30562500	-2.94994200
H	5.58866600	-3.08130800	-1.45042500
H	4.83383500	-4.21063900	-3.67260900
H	3.29715200	-2.40568900	-4.43501500
Pd	-0.60552200	0.20351400	0.33604600
P	2.68365100	0.25396000	1.60086900
H	3.56488100	-0.61953200	0.41167000
C	3.00790900	-1.85545000	3.23406300
H	1.99588800	-2.24651800	3.38534700
H	3.41265800	-2.31241500	2.32038600
C	4.71472000	1.83562500	2.26883700
H	4.89957800	1.28476500	3.19855800
H	5.33221500	1.38521000	1.47786800
O	1.19049400	0.56788500	1.42147900
O	3.32625500	1.73222900	1.92216300
O	2.94368700	-0.42855700	3.08813500
C	3.89221200	-2.17804900	4.42843000
H	4.91283600	-1.81469000	4.26690400
H	3.92997700	-3.26165400	4.59142700
H	3.49836400	-1.70505000	5.33407800
C	5.05040300	3.30873400	2.43371900
H	6.10671300	3.42994100	2.70207600
H	4.43714800	3.75371400	3.22413800
H	4.85915900	3.85090000	1.50246900

7a

SCF energy: -3364.977863

SCF energy in solution: -3364.0336812000

Free energy in solution: -3363.2790442000

P	2.94741300	0.09007800	0.56129900
C	1.20341900	3.19439900	2.32744400
H	2.00525800	3.84313400	1.95587300
H	0.54581300	3.82280600	2.93723300
C	3.71367800	1.55846800	1.44290400
H	4.79988200	1.41368100	1.41561200
H	3.49966600	2.44147600	0.83024100
C	1.79506100	2.04602000	3.17316000
H	1.22213500	1.12145200	3.03018200

H	1.69106000	2.29232500	4.23662800	H	5.13214900	-2.96902600	3.83254400
C	3.28695800	1.78848000	2.90434700	H	0.81691800	-3.09357000	3.68053200
H	3.85907500	2.65548100	3.26444300	H	2.98370500	-3.89489700	4.67554000
H	3.61156700	0.93419600	3.50868700	O	1.86781600	-0.24147500	-2.89036200
P	0.21115400	2.59661700	0.85392100	C	1.37702700	-0.75751300	-1.91169700
C	-1.47479500	2.45055300	1.58809900	C	1.02492700	-2.20988900	-1.85598700
C	-1.95077500	1.18456900	1.96288700	C	0.31152600	-2.75976500	-0.78355500
C	-2.27391800	3.58139900	1.82383000	C	1.43565100	-3.03557200	-2.91957300
C	-3.20176400	1.05867000	2.57408200	C	0.01696700	-4.12465400	-0.76992500
H	-1.37156300	0.28302600	1.77759500	H	-0.03630800	-2.13784400	0.03535300
C	-3.51954300	3.45037000	2.43582000	C	1.14293300	-4.39539200	-2.89882300
H	-1.92970600	4.56493300	1.51701100	H	1.98424500	-2.58922200	-3.74295000
C	-3.98500200	2.18730400	2.81424500	C	0.43411500	-4.94229500	-1.82131800
H	-3.56199200	0.06925000	2.83551400	H	-0.53651800	-4.53643800	0.06826100
H	-4.12956100	4.33299600	2.61074900	H	1.46565700	-5.03274400	-3.71807400
H	-4.95877200	2.08538900	3.28635900	H	0.20811400	-6.00560800	-1.80603900
C	0.14064100	4.08866200	-0.23185300	C	-3.06561400	-3.73711200	2.76959300
C	0.40476300	5.38748500	0.23644300	C	-5.12166000	-3.49562300	1.38953900
C	-0.17368300	3.91061400	-1.59099600	C	-4.16659000	-4.50140400	2.03313900
C	0.35812800	6.48037900	-0.63156200	H	-2.27143000	-4.39371700	3.13887500
H	0.64450200	5.56008400	1.28118600	H	-5.68284300	-2.96136300	2.17177000
C	-0.22144200	5.00691700	-2.45357800	H	-3.71679600	-5.12986800	1.25167400
H	-0.39128000	2.91592700	-1.96693200	N	-3.09057700	-2.10398200	0.85579900
C	0.04641000	6.29218700	-1.97905200	C	-4.37463600	-2.44743100	0.55390800
H	0.56515300	7.47769000	-0.25207000	C	-2.41386300	-2.66092900	1.88807500
H	-0.46525700	4.85091400	-3.50095100	O	-4.97780500	-1.91132100	-0.39168500
H	0.01281400	7.14288600	-2.65461000	O	-1.24910200	-2.30848000	2.16865200
C	4.27696800	-0.36179400	-0.63082600	H	-5.86341500	-3.97110000	0.74098300
C	4.63013900	-1.69950900	-0.86513800	H	-4.70048800	-5.17719600	2.71276500
C	4.88971700	0.64542500	-1.39367600	H	-3.48831700	-3.23249900	3.65210700
C	5.59160400	-2.01783300	-1.82582500	Pd	0.91334800	0.56766500	-0.43824300
H	4.15939000	-2.49508600	-0.29675400	P	-2.34083000	0.17748600	-1.56667500
C	5.85047000	0.32380300	-2.35169000	H	-2.59404200	-0.70409100	-0.48875400
H	4.60973700	1.68597200	-1.25502900	C	-2.61707900	-2.06701900	-3.00178400
C	6.20572500	-1.00884700	-2.56901400	H	-1.75874600	-2.27960700	-3.64620800
H	5.85799000	-3.05816000	-1.99207000	H	-2.42241300	-2.48720600	-2.01079500
H	6.31496100	1.11526900	-2.93339600	C	-4.80191100	1.16286900	-1.70389000
H	6.95265800	-1.25914900	-3.31738000	H	-5.00638000	0.99900500	-2.76665900
C	2.97798700	-1.22471400	1.84308200	H	-5.07012000	0.25729200	-1.15135500
C	4.19228500	-1.67215900	2.39782800	O	-0.93890800	0.76645600	-1.58223100
C	1.77273400	-1.74473800	2.32991900	O	-3.36724900	1.40479800	-1.56670800
C	4.18946900	-2.62727500	3.41306900	O	-2.72285500	-0.61756300	-2.91027400
H	5.13908800	-1.28516800	2.03066500	C	-3.91219200	-2.61605600	-3.57051600
C	1.77317900	-2.70512500	3.34548200	H	-4.72912600	-2.44414300	-2.86441600
H	0.81798900	-1.42250900	1.93060900	H	-3.81210400	-3.69569800	-3.73600600
C	2.97922400	-3.14653800	3.88716900	H	-4.14709100	-2.14159600	-4.52939900

C	-5.52437700	2.38796700	-1.17725400
H	-6.60622500	2.25532300	-1.29428700
H	-5.22343000	3.28641700	-1.72663900
H	-5.30394900	2.53973200	-0.11613000

TS5a

SCF energy: -3364.972319

SCF energy in solution: -3364.024467

Free energy in solution: -3363.2729002600

P	2.98063200	0.27862000	0.52397400
C	1.19241000	3.48772700	1.93382500
H	1.96117000	4.06085600	1.40262300
H	0.57934600	4.21200100	2.47975400
C	3.75093000	1.84313400	1.22082800
H	4.83757800	1.70250700	1.19461100
H	3.52337500	2.64403600	0.50825900
C	1.84368500	2.47961100	2.90617100
H	1.31540100	1.51916600	2.87696000
H	1.73516400	2.84346800	3.93462100
C	3.34086500	2.24868000	2.64834100
H	3.88532400	3.17464200	2.88241900
H	3.70496100	1.49176900	3.35202500
P	0.10778200	2.65790200	0.65305800
C	-1.47968800	2.51306200	1.58251000
C	-1.86574300	1.26201600	2.08377100
C	-2.28221800	3.63474500	1.84711600
C	-3.02727400	1.14165700	2.85199500
H	-1.28392900	0.36959200	1.86992600
C	-3.44253900	3.50916900	2.60953200
H	-2.00889000	4.60673800	1.44548100
C	-3.81568400	2.26092000	3.11752300
H	-3.31457100	0.16479300	3.22950200
H	-4.05792200	4.38398500	2.80345300
H	-4.72089700	2.16386500	3.71142900
C	-0.18206600	3.99901200	-0.58229900
C	0.10402700	5.35044000	-0.32189100
C	-0.69556700	3.64434200	-1.84266200
C	-0.11850900	6.32500700	-1.29709000
H	0.49935500	5.65742200	0.64145700
C	-0.91871900	4.62394200	-2.81140000
H	-0.92406000	2.60482800	-2.05716900
C	-0.62999200	5.96358400	-2.54431900
H	0.10843000	7.36552200	-1.07905600
H	-1.31564100	4.33334100	-3.78032100
H	-0.80089800	6.72222500	-3.30369700
C	4.30817300	-0.28878900	-0.62228600
C	4.69366800	-1.63597500	-0.69195400
C	4.88643500	0.62937800	-1.51356300
C	5.65339700	-2.04914400	-1.61794600
H	4.24823500	-2.36519600	-0.02295300
C	5.84579600	0.21372700	-2.43601200
H	4.57850500	1.67115200	-1.50482500
C	6.23380700	-1.12654700	-2.48925400
H	5.94445400	-3.09543700	-1.65661200
H	6.28284100	0.93680900	-3.11919600
H	6.97938400	-1.45026500	-3.21038400
C	3.05070900	-0.89063000	1.94224600
C	4.27059900	-1.20302100	2.57060600
C	1.86520400	-1.44286300	2.44402400
C	4.29591400	-2.05403300	3.67455300
H	5.20274000	-0.79194200	2.19189500
C	1.89402700	-2.29771200	3.54919300
H	0.90937800	-1.22178400	1.98275200
C	3.10644400	-2.60360200	4.16557600
H	5.24398600	-2.29073500	4.15036700
H	0.95755000	-2.71575900	3.90538000
H	3.13136800	-3.26918400	5.02455100
O	1.91964100	-0.30353900	-2.86575700
C	1.43838600	-0.80710900	-1.87570100
C	1.14520100	-2.27211800	-1.78788500
C	0.45716800	-2.82625200	-0.70226400
C	1.58413500	-3.10265400	-2.83478900
C	0.21113900	-4.20021200	-0.66222000
H	0.09514900	-2.19218000	0.10081600
C	1.34115400	-4.47190500	-2.78766200
H	2.11343600	-2.65216400	-3.66838900
C	0.65402600	-5.02320100	-1.69938600
H	-0.32697300	-4.62124500	0.18215300
H	1.68452500	-5.11251900	-3.59590600
H	0.46440100	-6.09312200	-1.66378800
C	-2.87413900	-3.56453000	2.89397700
C	-4.97662200	-3.70971200	1.56722600
C	-3.89736900	-4.52327800	2.28293800
H	-2.00897300	-4.08442900	3.31652800
H	-5.57211500	-3.14876600	2.30335700
H	-3.39715700	-5.18492900	1.56267700
N	-3.12105000	-2.19662000	0.81496200
C	-4.38303100	-2.69386200	0.58924000
C	-2.34908200	-2.54325000	1.88058400
O	-5.04658600	-2.31722200	-0.37920200
O	-1.22921900	-2.03810200	2.06482300

H	-5.67759800	-4.33436900	1.00622900
H	-4.33694500	-5.16829300	3.05280200
H	-3.33624300	-3.00208400	3.71946500
Pd	0.90085600	0.54971700	-0.45828300
P	-2.37617900	-0.17601300	-1.37213400
H	-2.69032600	-1.23924100	-0.18415400
C	-2.56727300	-2.21010300	-3.09997100
H	-1.72828000	-2.26104400	-3.80330000
H	-2.27057700	-2.74089700	-2.18717100
C	-4.80300000	0.93163200	-1.49242400
H	-5.01625100	0.81977600	-2.56122000
H	-5.12238200	0.01434200	-0.98703000
O	-0.97464200	0.45361600	-1.49610100
O	-3.37452700	1.11134500	-1.33588700
O	-2.81394100	-0.81880600	-2.81383400
C	-3.82750500	-2.82614900	-3.68540300
H	-4.63201900	-2.80565500	-2.94464200
H	-3.63856200	-3.86682800	-3.97640300
H	-4.14703700	-2.27251600	-4.57497600
C	-5.49318000	2.15612800	-0.91682500
H	-6.57844700	2.07125500	-1.04873500
H	-5.15242600	3.06627000	-1.42222500
H	-5.27686800	2.25604300	0.15170500

8a

SCF energy: -2964.999337

SCF energy in solution: -2964.1695163100

Free energy in solution: -2963.5283613100

P	-2.13533800	-1.34536400	-0.31141600
C	1.08082600	-3.61140200	-0.08442200
H	0.82205200	-3.98023000	-1.08402200
H	1.96261500	-4.17396000	0.23958200
C	-1.91056900	-3.12632000	-0.86397700
H	-2.87298800	-3.46581400	-1.26325300
H	-1.21491800	-3.09591300	-1.71043200
C	-0.09365200	-3.83847100	0.89250800
H	-0.20815800	-2.98047800	1.56658800
H	0.13597600	-4.69101200	1.54274500
C	-1.43177200	-4.13437100	0.19640400
H	-1.35569900	-5.10894700	-0.30655600
H	-2.20888500	-4.24530100	0.96119100
P	1.56341100	-1.80786300	-0.24484800
C	2.62366900	-1.61634400	1.25518500
C	2.13175200	-0.89164200	2.34879200
C	3.88874900	-2.21571500	1.35197500
C	2.87736100	-0.78420700	3.52483400
H	1.17205000	-0.38923200	2.26739400
C	4.63598800	-2.10490700	2.52430800
H	4.29961600	-2.75770600	0.50432300
C	4.12953500	-1.39242900	3.61536800
H	2.48542000	-0.21234300	4.36172000
H	5.61647400	-2.57012400	2.58482800
H	4.71424400	-1.30488900	4.52732400
C	2.74088700	-1.82190200	-1.66546300
C	3.26664300	-3.00870500	-2.20599300
C	3.11317900	-0.58985600	-2.23341300
C	4.14757200	-2.96612300	-3.28861300
H	3.00053000	-3.97531600	-1.79014200
C	3.99718400	-0.55689800	-3.31297400
H	2.71093600	0.33200400	-1.82178600
C	4.51501000	-1.73960400	-3.84419600
H	4.54537400	-3.89279500	-3.69474000
H	4.27675100	0.40245000	-3.74002000
H	5.20023600	-1.70746900	-4.68750500
C	-3.48169900	-0.79216200	-1.44367300
C	-4.58156100	-0.05306400	-0.98354100
C	-3.35843400	-1.03768400	-2.82071900
C	-5.54846300	0.40748400	-1.87923400
H	-4.68833500	0.16523700	0.07411700
C	-4.32653700	-0.57793000	-3.71249300
H	-2.49616800	-1.57358700	-3.20748700
C	-5.42622600	0.14366300	-3.24397800
H	-6.39677500	0.97510900	-1.50613500
H	-4.21498900	-0.77585200	-4.77498500
H	-6.17872700	0.50434200	-3.93988000
C	-2.96624000	-1.53149600	1.32410600
C	-4.17451800	-2.23930200	1.45448900
C	-2.36229300	-1.00956700	2.47556800
C	-4.76025100	-2.41552900	2.70758100
H	-4.66648800	-2.64440400	0.57432200
C	-2.94921400	-1.18625300	3.73119600
H	-1.42992500	-0.46158200	2.38105600
C	-4.14807600	-1.88894000	3.84877100
H	-5.69532600	-2.96245500	2.79343300
H	-2.46926700	-0.77220500	4.61367500
H	-4.60685800	-2.02591700	4.82421600
O	-1.53420600	1.73431300	-2.07061600
C	-1.37864900	1.56165400	-0.88193000
C	-1.93480900	2.52375400	0.12766000
C	-1.57086800	2.47792200	1.47808600
C	-2.84940200	3.49670700	-0.31032800

C	-2.10934600	3.39344800	2.38306500
H	-0.84107000	1.74380000	1.80327900
C	-3.39621600	4.40121000	0.59558200
H	-3.11396500	3.52231800	-1.36267700
C	-3.02602100	4.35115400	1.94422800
H	-1.80827700	3.36462400	3.42677300
H	-4.10731500	5.14910600	0.25415100
H	-3.44888100	5.06162600	2.65002800
Pd	-0.22175000	-0.03890300	-0.38576300
P	1.98653300	2.37934700	0.47103900
C	1.20079700	4.64301800	-0.70145700
H	0.49669100	4.23165000	-1.43798900
H	0.64312800	4.79553500	0.23675300
C	4.56227500	2.60268600	1.10387000
H	4.74074000	3.54370000	0.56695500
H	4.20991500	2.86359600	2.11543600
O	1.34797200	1.34030800	-0.54314800
O	3.57599500	1.83733200	0.41569900
O	2.27776200	3.73218900	-0.50063400
C	1.76669300	5.96705200	-1.19569600
H	2.45016500	6.39518800	-0.45420300
H	0.95998500	6.68624400	-1.38351400
H	2.32357200	5.81983400	-2.12728400
C	5.84134800	1.78258200	1.18990600
H	6.62883600	2.35058100	1.70069200
H	6.19611200	1.52345600	0.18652800
H	5.66492800	0.85265000	1.74027500

TS6a

SCF energy: -2964.957636

SCF energy in solution: -2964.127094

Free energy in solution: -2963.487047

P	-1.63665900	-1.61886300	-0.44875100
C	1.86093900	-2.90700700	-1.21588300
H	1.42301900	-2.84911700	-2.21842400
H	2.84445900	-3.37652300	-1.32537000
C	-1.26411900	-3.12291100	-1.50979300
H	-2.21160400	-3.59092700	-1.79871000
H	-0.81723200	-2.72972300	-2.43084900
C	0.95627400	-3.72741200	-0.26379700
H	0.72663200	-3.15593100	0.64358400
H	1.50949600	-4.60662300	0.08475500
C	-0.35908400	-4.20636300	-0.89286500
H	-0.13938200	-4.93580800	-1.68538400
H	-0.92512100	-4.74648400	-0.12570200
P	2.10211300	-1.16365800	-0.60603600
C	3.03063500	-1.44818100	0.96133800
C	2.47605900	-1.06285000	2.18859300
C	4.28529000	-2.08349600	0.93627000
C	3.16969800	-1.31766700	3.37677700
H	1.52511200	-0.53567500	2.20681400
C	4.96849400	-2.33640800	2.12351700
H	4.73677200	-2.36793800	-0.01081100
C	4.40925900	-1.95448200	3.34777000
H	2.73754600	-1.00291400	4.32276700
H	5.93894100	-2.82521500	2.09482800
H	4.94634800	-2.14772700	4.27288500
C	3.40289200	-0.48243000	-1.72019100
C	3.70838000	-1.04684700	-2.96764600
C	4.08231700	0.68043900	-1.31769000
C	4.67752600	-0.46654300	-3.79043800
H	3.19943200	-1.94274300	-3.30938800
C	5.05066400	1.25443100	-2.13908000
H	3.84681800	1.14117000	-0.36197200
C	5.35170100	0.68262800	-3.37802900
H	4.90518600	-0.91828100	-4.75243600
H	5.56523900	2.15397700	-1.81295700
H	6.10510400	1.13293500	-4.01859400
C	-3.28870400	-1.09810600	-1.09820200
C	-4.11663800	-0.31929000	-0.27286700
C	-3.73910100	-1.42613300	-2.38540700
C	-5.37067000	0.09744400	-0.71616700
H	-3.78159400	-0.04457200	0.72323600
C	-4.99737600	-1.00954300	-2.82677200
H	-3.11661200	-2.00804300	-3.05776400
C	-5.81799900	-0.25095700	-1.99281700
H	-5.99963600	0.69443300	-0.06135500
H	-5.33299400	-1.28108600	-3.82439000
H	-6.79795400	0.07036200	-2.33541400
C	-2.10479200	-2.35159300	1.17994000
C	-2.99255700	-3.44116600	1.24517100
C	-1.59404600	-1.80670900	2.36677800
C	-3.34512200	-3.99186600	2.47549800
H	-3.42222500	-3.85277000	0.33533000
C	-1.95809400	-2.36257700	3.59881500
H	-0.94587100	-0.93239500	2.32595000
C	-2.82333800	-3.45397500	3.65667600
H	-4.02995000	-4.83507400	2.51423100
H	-1.56301200	-1.93069300	4.51466100
H	-3.10052600	-3.88217700	4.61661600
O	1.42691200	2.54542100	-1.95123300

C	0.77775300	1.72807800	-1.44933000
C	-1.21606200	1.70418800	-1.52323800
C	-1.83813300	2.63412700	-0.68116400
C	-1.65955400	1.53131000	-2.84250400
C	-2.93713200	3.35428000	-1.15814800
H	-1.47435500	2.79915200	0.32894900
C	-2.75887900	2.25573400	-3.30621300
H	-1.14516600	0.84319400	-3.50773900
C	-3.39977300	3.16652000	-2.46258300
H	-3.42604800	4.07238900	-0.50413700
H	-3.10779500	2.11398300	-4.32602700
H	-4.25091900	3.73654300	-2.82653600
Pd	0.08133400	0.17501900	-0.63468200
P	0.41388300	2.06572100	2.52124600
C	-1.83914200	3.20732500	3.42615300
H	-2.63012300	2.47571400	3.19725100
H	-1.38074700	2.89900300	4.38002400
C	1.88736200	4.12321600	1.66313700
H	1.11360300	4.88508700	1.50027900
H	2.16453900	4.16419300	2.72857200
O	-0.06609500	0.80546300	1.74601400
O	1.36423900	2.83655400	1.33767000
O	-0.86718400	3.21494300	2.39028000
C	-2.44125900	4.59996800	3.56544900
H	-1.66559100	5.32818900	3.82570200
H	-3.21139900	4.61521100	4.34675500
H	-2.90076600	4.91782200	2.62262200
C	3.10712900	4.40577700	0.79698400
H	3.50585800	5.40571300	1.00869800
H	2.84629900	4.35439200	-0.26521200
H	3.89701500	3.67135800	0.99307900

9a

SCF energy: -2965.031330

SCF energy in solution: -2964.1994459000

Free energy in solution: -2963.5534579000

P	-1.89975900	-1.33778900	0.60389800
C	1.29195100	-1.66807300	2.74179200
H	1.11321800	-2.74496000	2.66093400
H	2.17352400	-1.55384100	3.37870200
C	-1.57580000	-2.49304500	2.03676000
H	-2.46869500	-3.11125900	2.18540700
H	-0.77122400	-3.16538400	1.71733700
C	0.06551300	-0.96215900	3.36828300
H	-0.13247600	-0.01851400	2.84481400
H	0.29011400	-0.69159600	4.40759900
C	-1.21233300	-1.82148300	3.37167900
H	-1.09451800	-2.62407400	4.11321700
H	-2.05560000	-1.21007000	3.71630500
P	1.73767500	-1.04645100	1.01886500
C	3.28060100	-0.09161500	1.38095400
C	3.38446900	0.67397100	2.55291100
C	4.34763100	-0.08451800	0.47045700
C	4.54007100	1.40860300	2.82385700
H	2.56400000	0.70802800	3.26485600
C	5.50333300	0.64751300	0.74624300
H	4.26688600	-0.63162700	-0.46145200
C	5.60669700	1.39185000	1.92350300
H	4.60532200	1.99036700	3.73977300
H	6.32493400	0.63521000	0.03490200
H	6.51000800	1.95763600	2.13597400
C	2.35722600	-2.55412500	0.15955500
C	3.04743500	-3.57110400	0.84158800
C	2.13122200	-2.68831000	-1.21899900
C	3.48356200	-4.70841100	0.16278700
H	3.25773500	-3.47498800	1.90332200
C	2.57519100	-3.82723000	-1.89611200
H	1.64421400	-1.88503500	-1.76195200
C	3.24393900	-4.83979500	-1.20787800
H	4.01493300	-5.48848000	0.70192300
H	2.39758000	-3.91744100	-2.96424600
H	3.58480500	-5.72618600	-1.73660400
C	-2.21774900	-2.50738400	-0.78992900
C	-2.29336300	-1.97627100	-2.09094300
C	-2.36627000	-3.89304900	-0.61396400
C	-2.51879700	-2.81681800	-3.18168800
H	-2.18602400	-0.90582300	-2.24398300
C	-2.58429300	-4.72927500	-1.71144900
H	-2.31288400	-4.33670100	0.37412800
C	-2.66168300	-4.19361100	-2.99730900
H	-2.57681300	-2.39085000	-4.17979500
H	-2.69342000	-5.79954800	-1.55680900
H	-2.83108700	-4.84562800	-3.85021300
C	-3.56451600	-0.68098100	1.05771300
C	-4.75020900	-1.34134600	0.70002300
C	-3.64379400	0.48623600	1.83319800
C	-5.98679900	-0.84620600	1.11546300
H	-4.70830500	-2.23839900	0.08963700
C	-4.88207700	0.97569900	2.25352400
H	-2.73902000	1.02896300	2.09025800
C	-6.05545000	0.31073000	1.89506400

H	-6.89772000	-1.36362800	0.82600500
H	-4.92666400	1.88499800	2.84648000
H	-7.02012300	0.69638000	2.21399200
O	-2.20794600	1.19696000	-1.85295800
C	-1.54560600	1.47265200	-0.86410200
C	-1.82230200	2.75695000	-0.12049400
C	-0.99123900	3.20982300	0.91250500
C	-2.96290100	3.50190700	-0.46231000
C	-1.29608200	4.38772900	1.59687300
H	-0.09208200	2.64993300	1.15235100
C	-3.26912800	4.67409000	0.22375600
H	-3.59444600	3.13992000	-1.26737600
C	-2.43659700	5.11875200	1.25682200
H	-0.63927000	4.73886100	2.38861700
H	-4.15496900	5.24455200	-0.04433400
H	-2.67438600	6.03584600	1.79024200
Pd	-0.12886100	0.19546200	-0.08746900
P	1.40422500	1.39470600	-1.37914700
C	0.44284300	1.91043000	-3.83021700
H	1.27809700	1.29572900	-4.18273300
H	-0.45768900	1.28562300	-3.77906400
C	3.10215800	3.40776400	-0.94117400
H	3.96993700	2.78934700	-1.19654400
H	2.74187000	3.89530800	-1.85355900
O	2.42289700	0.48904800	-2.03184800
O	2.05877200	2.55901900	-0.41819000
O	0.74262200	2.40906300	-2.51601800
C	0.21131500	3.10265100	-4.74485200
H	-0.62000200	3.71460500	-4.37941200
H	-0.02983600	2.76021500	-5.75842400
H	1.10650600	3.73197900	-4.79561600
C	3.45221000	4.43302600	0.12378300
H	4.24163500	5.10189200	-0.24023200
H	3.80877100	3.93739000	1.03234300
H	2.57557200	5.03882600	0.37740300

TS7a

SCF energy: -2964.994199

SCF energy in solution: -2964.1676930000

Free energy in solution: -2963.5232020000

P	-2.11236300	0.98543900	-0.44391100
C	0.98964300	2.08437300	-2.77520000
H	0.81138600	3.16041900	-2.66782500
H	1.82982000	1.97757600	-3.46836100
C	-1.93635600	2.44320800	-1.60337000
H	-2.87315200	3.01322500	-1.59847500
H	-1.16380600	3.08934600	-1.16720700
C	-0.26437900	1.38902400	-3.35168600
H	-0.31434800	0.35498000	-2.98821700
H	-0.16021200	1.32649200	-4.44306400
C	-1.59633500	2.10813800	-3.06798400
H	-1.59512300	3.05978700	-3.61889300
H	-2.41140100	1.51202100	-3.49723600
P	1.55165700	1.41082900	-1.09790500
C	3.26709100	0.83360100	-1.49205400
C	3.46868900	-0.02995500	-2.58286300
C	4.36918200	1.16425200	-0.68902500
C	4.73842900	-0.52711800	-2.87742700
H	2.62872600	-0.32011000	-3.21027200
C	5.63949200	0.66269400	-0.98231300
H	4.23976000	1.82333600	0.16361500
C	5.83108800	-0.18000900	-2.07862500
H	4.87371900	-1.18607400	-3.73136500
H	6.48227900	0.93910400	-0.35374900
H	6.82119400	-0.56442600	-2.30832600
C	1.84215600	2.91924700	-0.07576400
C	2.37950600	4.10534500	-0.60625700
C	1.51849500	2.86665400	1.29017300
C	2.57112700	5.22200800	0.20674200
H	2.66045300	4.15802800	-1.65493100
C	1.71940200	3.98723700	2.10239700
H	1.12762900	1.94688100	1.71993400
C	2.23771600	5.16488300	1.56339300
H	2.98425300	6.13420300	-0.21632700
H	1.46473300	3.93341200	3.15732800
H	2.38689400	6.03598300	2.19631100
C	-2.74033000	1.76858800	1.10734600
C	-2.85881900	0.94409100	2.24159800
C	-3.07889900	3.12645800	1.22095900
C	-3.32482300	1.46667100	3.44760900
H	-2.56751100	-0.10085200	2.18294200
C	-3.53640500	3.64641800	2.43479700
H	-2.98743700	3.79459100	0.37144300
C	-3.66535900	2.81766600	3.54922200
H	-3.40974200	0.81593400	4.31389200
H	-3.79155000	4.70085900	2.50442900
H	-4.02217000	3.22307400	4.49254300
C	-3.60380100	0.14526300	-1.14362700
C	-4.91252900	0.58261100	-0.88347700
C	-3.41366400	-0.94830600	-2.00188200
C	-6.00260300	-0.05535100	-1.47611600

H	-5.08104800	1.41824800	-0.21027700
C	-4.50534800	-1.58200700	-2.59990000
H	-2.40822600	-1.31564700	-2.18538900
C	-5.80162000	-1.13693500	-2.33785700
H	-7.01061600	0.29104500	-1.26256400
H	-4.33962400	-2.43115200	-3.25757400
H	-6.65284500	-1.63413300	-2.79568500
O	-1.62008400	-2.02075900	1.63841800
C	-0.71197400	-1.96267500	0.80075300
C	-0.64602300	-2.94008100	-0.33921600
C	0.46084900	-3.04758600	-1.20089600
C	-1.77907200	-3.74077500	-0.57635800
C	0.41815200	-3.92077300	-2.29101900
H	1.36385900	-2.48336500	-0.99745500
C	-1.81111600	-4.61453600	-1.65840900
H	-2.62139900	-3.65393100	0.10166800
C	-0.71423100	-4.70233400	-2.52435100
H	1.28100000	-4.00250200	-2.94703100
H	-2.68954000	-5.23183500	-1.82943600
H	-0.73938200	-5.38783500	-3.36766700
Pd	-0.04546900	-0.13837900	-0.12760300
P	1.06857500	-1.48631300	1.81083200
C	0.20779700	-2.82208100	3.98092400
H	0.25091100	-1.83010400	4.44160100
H	-0.82978300	-3.03447100	3.70421900
C	3.67997500	-2.07828900	1.67143200
H	4.10125100	-1.08960300	1.88183900
H	3.49806500	-2.59539200	2.61790100
O	1.12184900	-0.22865400	2.62935200
O	2.41634700	-1.89289900	0.98110500
O	1.00079600	-2.81643200	2.77450700
C	0.76685700	-3.88873200	4.90822400
H	0.74924900	-4.87175300	4.42578500
H	0.16355200	-3.94217300	5.82217800
H	1.80045000	-3.66044700	5.18989700
C	4.59517500	-2.88884000	0.77144400
H	5.56587700	-3.03292200	1.26108300
H	4.76196300	-2.37281300	-0.17901000
H	4.16136900	-3.87325500	0.56717200

10a

SCF energy: -2965.017365

SCF energy in solution: -2964.1608224300

Free energy in solution: -2963.5258394300

P	-3.32935700	-3.43704700	3.62537600
C	0.96410400	-2.11414900	1.59159700
H	0.24893500	-2.55516900	0.88699500
H	1.51637600	-2.93771400	2.06199500
C	-2.06540100	-2.48284500	2.61692200
H	-1.78940300	-3.05441900	1.72184700
H	-2.55190500	-1.55938100	2.27686600
C	0.22344800	-1.29930000	2.66530700
H	-0.26958000	-0.43457200	2.20023900
H	0.95764900	-0.89597000	3.37344400
C	-0.82264100	-2.11939400	3.44521100
H	-0.35193600	-3.03174600	3.83585200
H	-1.13855900	-1.53696700	4.32024800
P	2.13230300	-1.07366600	0.57260100
C	3.40666500	-0.57239500	1.80209600
C	4.29775000	-1.51115700	2.34604500
C	3.46075600	0.75726000	2.24308200
C	5.21845100	-1.12769700	3.32053600
H	4.28069700	-2.54105200	1.99927400
C	4.38119100	1.13752100	3.22236000
H	2.79640100	1.49872800	1.80948900
C	5.25950200	0.19748500	3.76222900
H	5.90621900	-1.86178100	3.73202700
H	4.41636000	2.17164400	3.55437900
H	5.97923600	0.49591500	4.51994700
C	2.99195700	-2.28596800	-0.51625200
C	2.63817900	-3.64337800	-0.56872500
C	4.02412000	-1.81388700	-1.34867100
C	3.30651900	-4.51608200	-1.43142200
H	1.84511900	-4.03533400	0.05952800
C	4.69062700	-2.69396200	-2.20102100
H	4.28725200	-0.75871400	-1.33386800
C	4.33551200	-4.04470100	-2.24651000
H	3.02161100	-5.56461800	-1.46038800
H	5.48882200	-2.31890000	-2.83628800
H	4.85621800	-4.72503500	-2.91538800
C	-4.65621500	-3.77083500	2.37610600
C	-5.73754200	-4.57279500	2.78629400
C	-4.69106100	-3.22265900	1.08448000
C	-6.80497700	-4.83445400	1.92997000
H	-5.74007500	-4.99795700	3.78761700
C	-5.76769800	-3.47553800	0.22862600
H	-3.88088600	-2.59275100	0.73078400
C	-6.82477000	-4.28359500	0.64534600
H	-7.62567100	-5.46253300	2.26705200
H	-5.77350800	-3.04016700	-0.76752600
H	-7.65990100	-4.48033100	-0.02169300

C	-2.49277600	-5.09347300	3.72109000
C	-2.34528200	-5.95281000	2.61955400
C	-1.96560800	-5.49377900	4.95860100
C	-1.68434900	-7.17403100	2.75211400
H	-2.76174600	-5.66874700	1.65668700
C	-1.29729000	-6.71397700	5.09210000
H	-2.08541900	-4.84655000	5.82421800
C	-1.15683800	-7.55658300	3.98901200
H	-1.58275000	-7.82999400	1.89102100
H	-0.89504300	-7.00769900	6.05829300
H	-0.64424300	-8.50954100	4.09175200
O	-1.50937600	0.53085000	-0.50024100
C	-0.91978500	1.49112700	-1.00702300
C	-1.60574900	2.64057800	-1.61787900
C	-0.87415700	3.73368600	-2.10526200
C	-3.01236500	2.63975800	-1.69966000
C	-1.54708400	4.81731200	-2.66988400
H	0.20714100	3.72061300	-2.04428400
C	-3.67465500	3.72188500	-2.26714500
H	-3.56159600	1.78654000	-1.31399700
C	-2.94109100	4.81193700	-2.75207700
H	-0.98268300	5.66535200	-3.04717600
H	-4.75923900	3.72286400	-2.33231400
H	-3.46085800	5.65792700	-3.19448200
Pd	0.80565400	0.65488300	-0.51178400
P	2.48241600	1.97797000	-1.27273400
C	2.34049400	1.76932100	-3.92250400
H	3.37110200	1.39711700	-3.92936900
H	1.66491800	0.90359200	-3.85767800
C	3.43983700	4.35087500	-0.54744600
H	4.40179000	3.84893600	-0.40066900
H	3.41894600	4.76415300	-1.56279900
O	3.86553300	1.38166700	-1.25794800
O	2.37541800	3.37905000	-0.41884700
O	2.14845400	2.61049300	-2.77374700
C	2.03996100	2.58821400	-5.16719500
H	1.00778600	2.95402500	-5.15149200
H	2.17667700	1.97454100	-6.06514700
H	2.71102300	3.45122800	-5.23236000
C	3.21388200	5.43558900	0.49123800
H	3.99842500	6.19780900	0.41677400
H	3.23564600	5.01425600	1.50186400
H	2.24355500	5.92125600	0.34327500

TS8a

SCF energy: -2964.984280

SCF energy in solution: -2964.1371144900

Free energy in solution: -2963.5034284900

P	5.32439300	0.39181500	-1.60019500
C	1.03235500	-1.51749300	-0.12291000
H	1.49342000	-0.79548200	0.55991200
H	1.43372800	-2.51037700	0.11704600
C	3.49215900	0.23683500	-1.22516000
H	3.32956300	0.26099600	-0.14088700
H	3.00191900	1.12467500	-1.64430000
C	1.36129400	-1.16360900	-1.58278600
H	0.85786100	-0.22778800	-1.86100100
H	0.95314500	-1.94297400	-2.23734000
C	2.87323400	-1.02309300	-1.84971100
H	3.39319100	-1.91852100	-1.48325300
H	3.03284900	-0.99759600	-2.93530300
P	-0.79079100	-1.50133500	0.24549400
C	-1.43416500	-2.85745100	-0.81410500
C	-1.15458500	-4.19522100	-0.49058000
C	-2.14075700	-2.56625000	-1.98866600
C	-1.57038900	-5.22413000	-1.33444200
H	-0.62317100	-4.43507300	0.42637200
C	-2.55171900	-3.60085700	-2.83215900
H	-2.40033900	-1.54071300	-2.23070100
C	-2.26765300	-4.92774200	-2.50849900
H	-1.35476700	-6.25652900	-1.07255200
H	-3.10556300	-3.36609600	-3.73712600
H	-2.59485400	-5.73075200	-3.16360900
C	-0.94205800	-2.11718400	1.97038600
C	0.17561600	-2.35075600	2.78691800
C	-2.23440200	-2.32185300	2.48960500
C	0.00680800	-2.78862100	4.10273000
H	1.18155500	-2.19765400	2.41017400
C	-2.39027600	-2.76385400	3.80352300
H	-3.10948500	-2.12272000	1.87123800
C	-1.27504000	-2.99723100	4.61248900
H	0.87974500	-2.96767800	4.72486900
H	-3.39134100	-2.92174500	4.19580400
H	-1.40439600	-3.33872000	5.63619400
C	5.77575500	1.93617900	-0.68198600
C	7.13139800	2.31369800	-0.69312800
C	4.85590900	2.78214900	-0.04207900
C	7.55718600	3.48430900	-0.06896700
H	7.86004700	1.68107900	-1.19544600
C	5.28203800	3.96343900	0.57349500
H	3.79948000	2.53436600	-0.01463800
C	6.63093600	4.31648400	0.56624100

H	8.61066800	3.75193200	-0.08463700
H	4.55242800	4.60458100	1.06168600
H	6.95950100	5.23432400	1.04664700
C	5.99949800	-0.92295400	-0.47350400
C	6.03213900	-0.80712400	0.92627400
C	6.48290200	-2.10319600	-1.05939600
C	6.52747600	-1.84540900	1.71543600
H	5.67978100	0.10574600	1.39942000
C	6.97263600	-3.14742300	-0.27020200
H	6.48105600	-2.20089800	-2.14248100
C	6.99650300	-3.01954300	1.11893600
H	6.55077200	-1.73805800	2.79714200
H	7.34252000	-4.05442100	-0.74154200
H	7.38438100	-3.82669300	1.73497700
O	0.86343200	2.38811100	0.27756300
C	-0.19284000	1.87978400	0.20619200
C	-1.72596900	2.88513000	0.11453600
C	-2.00653100	3.51520700	-1.10798000
C	-2.13473600	3.48127000	1.31846900
C	-2.70653300	4.72119200	-1.12515200
H	-1.68058700	3.06277400	-2.04077500
C	-2.83210600	4.68884200	1.29666800
H	-1.90146000	3.00539300	2.26761200
C	-3.11844600	5.30653400	0.07545900
H	-2.93051700	5.20451600	-2.07228500
H	-3.14877300	5.14983800	2.22850800
H	-3.65872700	6.24931500	0.05981000
Pd	-1.67445900	0.65663900	0.07469600
P	-3.96931700	0.04539100	-0.13867100
C	-5.46016100	1.39710000	1.62421400
H	-5.91384100	0.43643300	1.89167700
H	-4.63640300	1.58830900	2.32920800
C	-5.56080300	-0.18976400	-2.27466700
H	-5.87850500	-1.16416500	-1.88616400
H	-6.26200000	0.57039500	-1.91177700
O	-4.49430300	-1.22252000	0.49585300
O	-4.24314600	0.11243300	-1.77263600
O	-4.94945800	1.33158900	0.28797800
C	-6.47676100	2.52606200	1.68953300
H	-6.01052800	3.48013400	1.42149700
H	-6.88896600	2.61035900	2.70230700
H	-7.30215100	2.34059300	0.99393000
C	-5.50324000	-0.19507700	-3.79317500
H	-6.49393900	-0.41271700	-4.20975900
H	-4.80391600	-0.95746900	-4.15422500
H	-5.17474100	0.77846400	-4.17281600

11a

SCF energy: -2965.005092

SCF energy in solution: -2964.1569805700

Free energy in solution: -2963.5240005700

P	5.33906600	0.49382800	-1.62475100
C	1.07116100	-1.45694000	-0.12628900
H	1.54422900	-0.76196900	0.57751300
H	1.49424700	-2.45171900	0.06166500
C	3.51017900	0.35109100	-1.22085500
H	3.36751300	0.33838500	-0.13307300
H	3.02526400	1.25822900	-1.60514000
C	1.36440200	-1.03529100	-1.57605700
H	0.85093600	-0.09043700	-1.80434700
H	0.94070300	-1.78532200	-2.25411100
C	2.86904300	-0.88268400	-1.87571100
H	3.39559800	-1.79184400	-1.55564400
H	3.00270400	-0.81599600	-2.96283200
P	-0.75087900	-1.48405300	0.27902100
C	-1.35120100	-2.86209100	-0.78095000
C	-1.16806100	-4.19967900	-0.39822300
C	-1.92443700	-2.57723800	-2.02822300
C	-1.54997100	-5.23438400	-1.25246900
H	-0.73803800	-4.43509900	0.57102800
C	-2.29854100	-3.61609100	-2.88270400
H	-2.10819000	-1.54804400	-2.31866000
C	-2.11311400	-4.94452100	-2.49723200
H	-1.41045300	-6.26680500	-0.94316200
H	-2.74578900	-3.38453200	-3.84575700
H	-2.41205900	-5.75179000	-3.16054700
C	-0.83146100	-2.12523900	2.00171200
C	0.31428500	-2.35031700	2.78122600
C	-2.10204300	-2.34943300	2.56563400
C	0.19498000	-2.79409400	4.10075500
H	1.30603700	-2.18866800	2.37207000
C	-2.20988200	-2.79883400	3.88169900
H	-2.99461700	-2.16507500	1.97064800
C	-1.06587700	-3.02011100	4.65299700
H	1.09056100	-2.96538600	4.69218200
H	-3.19518600	-2.97253100	4.30607700
H	-1.15674900	-3.36632900	5.67920000
C	5.82203600	2.03252300	-0.71348500
C	7.16258800	2.44415800	-0.82897200
C	4.94254900	2.83794400	0.02711000
C	7.61396800	3.60740800	-0.20856100

H	7.85845000	1.84525200	-1.41250600
C	5.39188800	4.01204400	0.63917200
H	3.89830900	2.56202600	0.13536400
C	6.72721600	4.39814600	0.52755100
H	8.65554900	3.90228300	-0.30671000
H	4.69301100	4.62217100	1.20573600
H	7.07463700	5.31063000	1.00469300
C	6.01874800	-0.83089600	-0.51283600
C	6.09263400	-0.71279500	0.88506900
C	6.46510600	-2.02053100	-1.10928900
C	6.59104200	-1.75828500	1.66272800
H	5.77070600	0.20722900	1.36592400
C	6.95734500	-3.07189600	-0.33131300
H	6.43311000	-2.12005800	-2.19172700
C	7.02195700	-2.94184300	1.05635700
H	6.64686400	-1.64893700	2.74301400
H	7.29789700	-3.98617000	-0.81053100
H	7.41236600	-3.75456000	1.66333500
O	0.91914700	2.34689000	0.79137200
C	-0.00551300	1.70929400	0.57319600
C	-2.51304000	2.69809500	0.15022900
C	-2.76956800	3.34085900	-1.06826500
C	-2.75152800	3.39492600	1.34334900
C	-3.26885700	4.64716800	-1.09178200
H	-2.60624500	2.81858900	-2.00728200
C	-3.25900500	4.69950400	1.31880200
H	-2.55055800	2.92553400	2.30411800
C	-3.51902400	5.32940100	0.10069200
H	-3.46858300	5.12807300	-2.04689200
H	-3.44379000	5.22238600	2.25477600
H	-3.90995500	6.34351700	0.08055100
Pd	-1.70626400	0.78020400	0.18540800
P	-3.88911400	0.01059800	-0.21428500
C	-5.63998900	1.14999300	1.43781700
H	-5.97792900	0.15287300	1.74110500
H	-4.85681700	1.47574500	2.13598300
C	-5.20596800	-0.45021200	-2.48825300
H	-5.36057400	-1.49697600	-2.20302800
H	-6.05639700	0.13737500	-2.12714500
O	-4.20746400	-1.32640800	0.40800400
O	-3.99976500	0.03544600	-1.85531800
O	-5.09846200	1.08407500	0.10902900
C	-6.78426000	2.14975800	1.42780800
H	-6.42414100	3.14098200	1.13445800
H	-7.23211900	2.22096500	2.42608100
H	-7.56133800	1.83936200	0.72119200
C	-5.04110800	-0.30437100	-3.99112700
H	-5.94103100	-0.66182400	-4.50522800
H	-4.18583300	-0.88765400	-4.34995900
H	-4.87999500	0.74390900	-4.26348900

12a

SCF energy: -2965.003400

SCF energy in solution: -2964.1567048400

Free energy in solution: -2963.5232038400

P	-4.18866800	0.19706100	0.08531300
C	-0.78617000	-2.11881200	-0.34340600
H	-1.25540500	-1.64070900	-1.21142100
H	-0.89688700	-3.20469100	-0.46217300
C	-3.92112900	-1.66431700	0.04536200
H	-4.87477000	-2.18673500	0.19184400
H	-3.56982300	-1.91823000	-0.96299200
C	-1.46723600	-1.65931500	0.95687000
H	-1.43722900	-0.56430100	1.01683600
H	-0.89586100	-2.03450000	1.81426400
C	-2.91739200	-2.15747200	1.10417300
H	-2.91341000	-3.25670000	1.08715500
H	-3.28114700	-1.87265700	2.09964400
P	1.03398700	-1.70061400	-0.39087800
C	1.68941000	-2.81466500	0.92036200
C	1.87273400	-4.18321400	0.66926100
C	1.92995500	-2.31595300	2.20825200
C	2.28600600	-5.03818300	1.69106100
H	1.70462400	-4.58070900	-0.32754000
C	2.33681400	-3.17676400	3.22974000
H	1.83198900	-1.25381900	2.40710800
C	2.51619800	-4.53685700	2.97412100
H	2.43193300	-6.09485700	1.48302100
H	2.52480400	-2.77893700	4.22352000
H	2.84065200	-5.20328400	3.76893100
C	1.63978100	-2.42649900	-1.96930000
C	0.78491300	-2.99724800	-2.92500200
C	3.02059400	-2.35608900	-2.23507000
C	1.29928500	-3.49363900	-4.12579000
H	-0.28319700	-3.06499100	-2.74510800
C	3.52490100	-2.86048400	-3.43363200
H	3.68578900	-1.90418100	-1.50119900
C	2.66894800	-3.42764300	-4.38166800
H	0.62627300	-3.93367900	-4.85699500
H	4.59285200	-2.80569000	-3.62754400
H	3.06761600	-3.81521400	-5.31552600

C	-5.46826000	0.43459100	-1.23229000
C	-5.81558700	1.76207500	-1.54272700
C	-6.07199700	-0.59738600	-1.96807200
C	-6.74954400	2.04765500	-2.53701800
H	-5.34480300	2.57894900	-1.00037700
C	-6.99909900	-0.31171900	-2.97460900
H	-5.82558400	-1.63485800	-1.76480200
C	-7.34381500	1.00938400	-3.25928700
H	-7.00596800	3.08093600	-2.75583400
H	-7.45288600	-1.12615600	-3.53383000
H	-8.06506300	1.23012400	-4.04163000
C	-5.19489500	0.34936600	1.63791800
C	-6.51618600	-0.11240300	1.75790700
C	-4.58922000	0.94806000	2.75350700
C	-7.20749300	0.01456500	2.96260700
H	-7.01126400	-0.56149600	0.90083800
C	-5.27792100	1.06958700	3.96339600
H	-3.57388700	1.32891100	2.67062700
C	-6.58849600	0.60331200	4.06921100
H	-8.23113400	-0.34359600	3.03865400
H	-4.79291200	1.53507300	4.81746600
H	-7.12925100	0.70285100	5.00674500
O	-1.13708700	1.48632400	-2.04358200
C	-0.25184900	1.14446400	-1.40776300
C	1.74228300	2.77880700	-0.47133800
C	1.54441100	3.54804400	0.68335100
C	2.09096600	3.43070500	-1.66256000
C	1.70210600	4.93728000	0.64879100
H	1.29072300	3.06553000	1.62354400
C	2.25684700	4.82058300	-1.69451300
H	2.24063100	2.86129900	-2.57739100
C	2.06191300	5.57822600	-0.53867100
H	1.54952700	5.51745400	1.55635100
H	2.53128900	5.30794100	-2.62769900
H	2.18660700	6.65785900	-0.56323200
Pd	1.41829200	0.72673500	-0.42094400
P	3.55054100	0.56156800	0.54239300
C	5.34405900	1.96696700	-0.83921000
H	5.98232700	1.07913300	-0.90993000
H	4.70069600	1.99920800	-1.72918900
C	4.37122500	0.65900200	3.07983900
H	4.84686000	-0.32257600	2.97259200
H	5.10665500	1.43016000	2.82844700
O	4.29898600	-0.70017200	0.18803500
O	3.26519600	0.74857400	2.15316400
O	4.52981100	1.87367100	0.34001200
C	6.16576000	3.24139800	-0.74046100
H	5.50943500	4.11562100	-0.68366700
H	6.81105200	3.34389200	-1.62100300
H	6.79937100	3.22400100	0.15277000
C	3.82798500	0.86104500	4.48401300
H	4.64337100	0.80746000	5.21496800
H	3.09052900	0.09040200	4.73467800
H	3.34544700	1.83983100	4.57491200

TS9a

SCF energy: -2964.990588

SCF energy in solution: -2964.163816

Free energy in solution: -2963.5223010600

P	-1.90494600	-1.27526500	-0.94834800
C	1.51110300	-2.14567000	-2.04491200
H	0.92306300	-1.70573500	-2.85739900
H	2.39488200	-2.60399200	-2.50203400
C	-1.58696200	-2.53132200	-2.32042700
H	-2.54097200	-2.96527500	-2.64115900
H	-1.21329400	-1.95312300	-3.17370200
C	0.68895300	-3.20275100	-1.26759000
H	0.41111500	-2.81928300	-0.27870700
H	1.32028400	-4.07630300	-1.07251500
C	-0.59841600	-3.65841900	-1.97218300
H	-0.35020900	-4.19382900	-2.89943200
H	-1.10114300	-4.38421500	-1.32153100
P	2.04355200	-0.74605100	-0.93095000
C	3.11500000	-1.66652300	0.25742800
C	4.36907000	-2.14724900	-0.15123300
C	2.65582300	-1.97065100	1.54522800
C	5.14443200	-2.92327300	0.71032900
H	4.74866300	-1.90694500	-1.14044300
C	3.43113800	-2.75377800	2.40303200
H	1.70851200	-1.57223700	1.89101500
C	4.67504100	-3.23126400	1.98915600
H	6.11636600	-3.28339200	0.38322300
H	3.06551600	-2.97867700	3.40164400
H	5.28015800	-3.83408300	2.66126900
C	3.24131400	0.22169000	-1.94342900
C	3.42505300	-0.00262700	-3.31664900
C	3.95785100	1.25781000	-1.31592000
C	4.31285400	0.78850600	-4.05106600
H	2.88313200	-0.79212200	-3.82768200
C	4.84651600	2.03800300	-2.05522200
H	3.80054800	1.44656600	-0.25623600

C	5.02683900	1.80807400	-3.42195900
H	4.44492100	0.60260700	-5.11380700
H	5.39789400	2.83283700	-1.55967500
H	5.71800700	2.42211300	-3.99341000
C	-3.41035100	-0.44870500	-1.63002800
C	-4.50561400	-0.12733800	-0.81283800
C	-3.43680400	-0.03421000	-2.97326300
C	-5.60014000	0.56831000	-1.32802500
H	-4.50436200	-0.41729500	0.23220100
C	-4.53299100	0.65940100	-3.48766900
H	-2.60010500	-0.25019400	-3.63167700
C	-5.62090300	0.96105600	-2.66693400
H	-6.43692900	0.80613400	-0.67666500
H	-4.53387700	0.96393900	-4.53111000
H	-6.47435100	1.50227300	-3.06633600
C	-2.56491200	-2.35711400	0.39873300
C	-3.64244400	-3.24010400	0.20933000
C	-1.93346700	-2.32248200	1.65138700
C	-4.07308800	-4.06806400	1.24562500
H	-4.15631900	-3.27339600	-0.74785100
C	-2.36593300	-3.15224800	2.69002400
H	-1.10486200	-1.63862000	1.81783600
C	-3.43413400	-4.02610200	2.48862000
H	-4.90822400	-4.74494000	1.08466800
H	-1.86785100	-3.10973200	3.65498400
H	-3.77173000	-4.67112400	3.29559800
O	0.22193400	2.22278300	-3.02377200
C	0.02433300	1.45427400	-2.19576900
C	-1.46275800	1.86639800	0.41387100
C	-2.24879500	1.46067000	1.50401700
C	-1.79486000	3.07583900	-0.21613600
C	-3.34100300	2.22174800	1.93208000
H	-1.99933400	0.55713300	2.04953300
C	-2.88558100	3.84101000	0.21429300
H	-1.20936800	3.44831800	-1.05118000
C	-3.66645300	3.41698100	1.28920000
H	-3.92978600	1.88006300	2.78122800
H	-3.11954300	4.77169800	-0.29857200
H	-4.51222700	4.01191400	1.62489300
Pd	0.09646300	0.66117000	-0.26032200
P	1.16889400	1.36295500	1.66719900
C	1.18355400	4.02116400	1.74705200
H	2.27506200	4.02918100	1.84807800
H	0.93807400	4.07495200	0.67740700
C	1.09293700	0.56573700	4.21418000
H	2.18799500	0.53047600	4.19066000
H	0.78592800	1.55100000	4.57980100
O	2.67631100	1.35031000	1.57704700
O	0.58650200	0.38879100	2.87206000
O	0.66572900	2.80168100	2.29933700
C	0.54382100	5.18097300	2.49209100
H	-0.54344300	5.16139700	2.36673900
H	0.92495500	6.13407100	2.10650800
H	0.77127000	5.12484700	3.56204700
C	0.52407800	-0.54135300	5.08560100
H	0.87512300	-0.42745700	6.11797700
H	0.83916800	-1.52673200	4.72368300
H	-0.57089500	-0.50812700	5.08892700

13a

SCF energy: -2851.685156

SCF energy in solution: -2850.8797931400

Free energy in solution: -2850.2412871400

P	-1.82832600	-1.45501200	-0.13498600
C	1.51657600	-3.09250400	-0.34694200
H	0.98977500	-3.35655800	-1.26808700
H	2.46083700	-3.64659000	-0.35773500
C	-1.54280600	-3.27754500	-0.50379700
H	-2.52727900	-3.74835700	-0.60640000
H	-1.07735600	-3.32777900	-1.49420500
C	0.65797500	-3.46563500	0.88446300
H	0.50016600	-2.58907900	1.52456300
H	1.20013600	-4.18600700	1.50711500
C	-0.71061000	-4.06739100	0.52151900
H	-0.56583200	-5.07725000	0.11255800
H	-1.29552900	-4.18879500	1.44077600
P	1.90805300	-1.26411400	-0.41417500
C	3.23531100	-1.20177700	0.86725400
C	4.49524200	-1.77256900	0.63002700
C	2.96196900	-0.65467100	2.12764200
C	5.45993000	-1.80070100	1.63682900
H	4.72984000	-2.18341600	-0.34829500
C	3.92628700	-0.69203500	3.13732800
H	2.00985100	-0.16723900	2.31114900
C	5.17529800	-1.26428100	2.89505800
H	6.43493500	-2.23779600	1.43738000
H	3.70332900	-0.25917000	4.10909500
H	5.92784100	-1.28526600	3.67900300
C	2.80706900	-1.09600500	-2.02372500
C	2.76631400	-2.09197000	-3.01433900
C	3.52826100	0.08510600	-2.28138900

C	3.42772500	-1.91466500	-4.23221500
H	2.23084500	-3.02093000	-2.85131100
C	4.18954200	0.25195600	-3.49853600
H	3.55290800	0.86905700	-1.52835700
C	4.14184000	-0.74239400	-4.47814200
H	3.38594800	-2.69896100	-4.98376900
H	4.74399300	1.16910700	-3.67998200
H	4.65772000	-0.60544100	-5.42505500
C	-3.24000400	-1.12440300	-1.27719300
C	-4.35256300	-0.37164400	-0.87260500
C	-3.17620500	-1.57051800	-2.60783400
C	-5.38571500	-0.09655800	-1.76923200
H	-4.40663100	0.01737300	0.13841600
C	-4.20977300	-1.29225600	-3.50313000
H	-2.31732500	-2.13540600	-2.95948500
C	-5.32099100	-0.55853900	-3.08448600
H	-6.23769200	0.49054100	-1.43763600
H	-4.14381600	-1.64946600	-4.52746000
H	-6.12624200	-0.34157800	-3.78116700
C	-2.58867300	-1.56583200	1.54307600
C	-3.76611000	-2.29740800	1.77363900
C	-1.93610100	-0.97310600	2.63379600
C	-4.27844600	-2.42795600	3.06428500
H	-4.29305400	-2.75793000	0.94249400
C	-2.44768500	-1.10824400	3.92688900
H	-1.03009900	-0.39704000	2.46563400
C	-3.61901900	-1.83410900	4.14400900
H	-5.19241600	-2.99310000	3.22676300
H	-1.93203600	-0.63969200	4.76074200
H	-4.01959300	-1.93613100	5.14904700
C	-1.56211600	1.61591900	-0.17017400
C	-2.18639200	2.14712400	0.96728600
C	-2.00137600	2.06060500	-1.42869700
C	-3.22261200	3.08131800	0.85209100
H	-1.85326500	1.85638900	1.95886300
C	-3.02820500	3.00254300	-1.54724600
H	-1.54314700	1.67049400	-2.33524500
C	-3.64731100	3.51499300	-0.40490600
H	-3.68902500	3.47828400	1.75179200
H	-3.34690500	3.32963800	-2.53496800
H	-4.44710800	4.24639800	-0.49359100
Pd	-0.03333700	0.22281800	-0.14471100
P	1.32150000	2.06898100	0.34375600
C	1.03888600	3.98796500	-1.47242100
H	2.12500500	4.01226500	-1.62038500
H	0.61091400	3.28057800	-2.19707000
C	1.81790500	3.24277700	2.68304400
H	2.88538800	3.08432200	2.49322900
H	1.54444000	4.23613000	2.31031200
O	2.79260600	1.97877400	0.01083100
O	1.05670200	2.24889100	1.96486300
O	0.74862800	3.54430200	-0.14100100
C	0.42219500	5.36515800	-1.65508700
H	-0.66236400	5.31903300	-1.51470900
H	0.63122000	5.74341000	-2.66301300
H	0.83638900	6.07134000	-0.92739900
C	1.49385200	3.10818200	4.16146500
H	2.04842300	3.85586100	4.74086400
H	1.76818500	2.11375900	4.53136800
H	0.42342600	3.25819600	4.33880100

TS10a

SCF energy: -2851.656285

SCF energy in solution: -2850.8563748300

Free energy in solution: -2850.2178168300

P	1.90737100	-1.46451000	-0.14560900
C	-1.49447600	-3.17750300	-0.17944100
H	-1.02868300	-3.58705600	0.72390100
H	-2.42289000	-3.73643900	-0.33569900
C	1.62642500	-3.31629900	0.04586300
H	2.59739600	-3.81903900	0.12784600
H	1.13463700	-3.44038600	1.01811100
C	-0.55350000	-3.33588100	-1.39719100
H	-0.36783000	-2.36108700	-1.86381500
H	-1.04679100	-3.94379900	-2.16460900
C	0.80051300	-3.98891500	-1.06596400
H	0.63399100	-5.03412700	-0.76828900
H	1.40158500	-4.02363100	-1.98293400
P	-1.91723500	-1.38688900	0.20773300
C	-3.31207300	-1.13029800	-0.98706300
C	-4.64792500	-1.42004200	-0.67079700
C	-3.00800000	-0.68527300	-2.28352000
C	-5.65268100	-1.27806000	-1.63020300
H	-4.90803300	-1.75345800	0.32917300
C	-4.01091800	-0.55886900	-3.24661400
H	-1.98667400	-0.41225100	-2.53014800
C	-5.33693200	-0.85362700	-2.92203700
H	-6.68344200	-1.50031100	-1.36572900
H	-3.75695300	-0.21710500	-4.24695800
H	-6.11955000	-0.74551200	-3.66853200
C	-2.75958700	-1.53261700	1.84855100

C	-3.23234200	-2.75294500	2.36296300
C	-2.92148000	-0.36559600	2.61611200
C	-3.84874300	-2.80780500	3.61497800
H	-3.12991800	-3.67048700	1.79235900
C	-3.54616100	-0.42666700	3.86386000
H	-2.55759700	0.58923500	2.24127600
C	-4.00778000	-1.64361700	4.36862800
H	-4.20579600	-3.76080000	3.99754400
H	-3.66428600	0.48513300	4.44361400
H	-4.48746100	-1.68656100	5.34328200
C	3.24651200	-1.23413600	1.10947300
C	4.52214900	-0.73588200	0.80822600
C	2.93659800	-1.51100400	2.45326800
C	5.46920600	-0.54629100	1.81757700
H	4.78121000	-0.49005600	-0.21610500
C	3.88511900	-1.32915500	3.45880600
H	1.94210800	-1.86049800	2.72093300
C	5.15827100	-0.84815800	3.14344800
H	6.45325200	-0.16100300	1.56248900
H	3.62645500	-1.55677300	4.48976300
H	5.89783100	-0.70350300	3.92653500
C	2.77102900	-1.40696900	-1.78049800
C	3.88416300	-2.20819000	-2.08970000
C	2.25041300	-0.56953000	-2.77835300
C	4.46269100	-2.16480100	-3.35843400
H	4.30918800	-2.86377900	-1.33416500
C	2.82764100	-0.52621000	-4.05020300
H	1.38399000	0.04578200	-2.55013200
C	3.93534300	-1.32260900	-4.34156200
H	5.32407800	-2.78940200	-3.58068800
H	2.41045300	0.12884900	-4.81055600
H	4.38642000	-1.29059500	-5.32983100
C	1.07668800	1.92514000	0.46739100
C	1.97224600	2.41267500	-0.50939900
C	1.44742000	2.02355000	1.82411900
C	3.21297400	2.92557100	-0.14270200
H	1.68436200	2.39923600	-1.55651600
C	2.69762800	2.53477400	2.18741300
H	0.74401100	1.71413800	2.59179600
C	3.58276000	2.98324300	1.20788300
H	3.89473300	3.28780000	-0.90875100
H	2.97235800	2.58803800	3.23776600
H	4.55012100	3.39021500	1.49044000
Pd	-0.00355900	0.07599400	0.11690600
P	-0.95655700	2.32978300	0.21110700
C	-0.29911600	4.86910600	0.82181600
H	-1.00385300	4.75328300	1.65214000
H	0.71389300	4.68323600	1.20170500
C	-2.67560800	2.91227700	-1.80087000
H	-3.54454300	2.28469600	-2.02162400
H	-2.96784800	3.66566600	-1.06536600
O	-1.78643100	2.36510300	1.46720800
O	-1.68888400	2.01508000	-1.22839000
O	-0.60857900	3.91248600	-0.19986600
C	-0.39123900	6.25902300	0.21041100
H	0.30851800	6.36245700	-0.62604100
H	-0.14659700	7.01967700	0.96122500
H	-1.40302100	6.45348400	-0.16135100
C	-2.13210000	3.56062600	-3.06367900
H	-2.90555200	4.18116100	-3.53382200
H	-1.82172900	2.79670900	-3.78571300
H	-1.27113200	4.19183700	-2.82763800

2b

SCF energy: -2638.860127

SCF energy in solution: -2638.01937771

Free energy in solution: -2637.40423771

P	0.63812500	-1.75089000	-0.06989900
C	-3.00552600	-1.63691300	-1.80280400
H	-3.78447800	-2.30114100	-1.40990400
H	-3.43013600	-1.13659700	-2.68015600
C	-0.64841900	-3.11356000	0.03063300
H	-0.20559700	-3.99419800	0.51233900
H	-1.43159100	-2.74595500	0.70285800
C	-1.79070600	-2.46085100	-2.26954700
H	-0.98198100	-1.77631000	-2.54942600
H	-2.08574500	-2.97335300	-3.19567100
C	-1.25582700	-3.54665000	-1.31948300
H	-2.06559400	-4.25829600	-1.10212500
H	-0.49433900	-4.11220800	-1.86984300
P	-2.63368400	-0.25527900	-0.57808300
C	-3.79936700	1.07768600	-1.12479200
C	-3.36946300	2.40986600	-1.02533400
C	-5.08886100	0.81576200	-1.61803200
C	-4.21627100	3.45510200	-1.40559200
H	-2.36846900	2.62572500	-0.66480500
C	-5.92920800	1.86070600	-2.00121400
H	-5.44784400	-0.20617900	-1.70731700
C	-5.49439400	3.18452200	-1.89388800
H	-3.86755000	4.48136500	-1.32586200
H	-6.92353400	1.64157800	-2.38226400

H	-6.14958800	3.99840400	-2.19361600
C	-3.41372600	-0.82549800	1.00975100
C	-4.63231800	-1.52154300	1.06871800
C	-2.76117300	-0.50933600	2.21269900
C	-5.18073400	-1.89986200	2.29432500
H	-5.17083400	-1.76692000	0.15776600
C	-3.31427800	-0.88579100	3.44035400
H	-1.82013300	0.03251200	2.18749700
C	-4.52154600	-1.58353700	3.48492700
H	-6.12487500	-2.43814100	2.31947000
H	-2.79618900	-0.62972100	4.36100200
H	-4.94988300	-1.87783100	4.43960300
C	1.58332000	-1.99982300	1.49910400
C	2.97398900	-1.80237900	1.53576100
C	0.91469100	-2.27875000	2.70198000
C	3.67569500	-1.89102900	2.73918500
H	3.51254200	-1.58783400	0.61734400
C	1.61837300	-2.37270600	3.90379300
H	-0.16333500	-2.40905300	2.71102800
C	3.00106700	-2.17894200	3.92804900
H	4.75304800	-1.74463600	2.74492100
H	1.08274600	-2.59640900	4.82292200
H	3.54855300	-2.25524100	4.86385900
C	1.79318700	-2.41688800	-1.35120900
C	2.37781300	-3.69001400	-1.22668700
C	2.06457200	-1.65651000	-2.49635900
C	3.20726300	-4.19103100	-2.22880800
H	2.19155800	-4.28870100	-0.33869700
C	2.89832700	-2.15880000	-3.50012200
H	1.63160800	-0.66592400	-2.59752100
C	3.46746200	-3.42503300	-3.36980000
H	3.65176000	-5.17712200	-2.12027000
H	3.10637900	-1.54985700	-4.37524500
H	4.11595400	-3.81540600	-4.14994300
O	-0.13176300	2.48355100	-0.43873600
C	1.05701400	2.05121700	-0.21512900
C	2.05874300	1.92277500	-1.31876000
C	3.37141100	1.47138600	-1.10498500
C	1.66627000	2.25216200	-2.62709700
C	4.26464800	1.35080500	-2.16789500
H	3.69456600	1.21450000	-0.09998400
C	2.56040200	2.12581600	-3.68867500
H	0.65812200	2.61882100	-2.78816100
C	3.86521900	1.67472200	-3.46719000
H	5.27737500	1.00218300	-1.98084000
H	2.24095800	2.39476700	-4.69270200
H	4.56455200	1.58593800	-4.29442400
C	3.15084800	3.92059000	2.44424900
C	1.85253100	2.16493300	3.59807000
C	3.25098600	2.74253100	3.40726100
H	4.12619500	4.32551000	2.15724700
H	1.20786500	2.89013600	4.11562500
H	3.91827900	1.97298100	2.99892800
N	1.65520300	2.38889300	1.11274700
C	1.16644700	1.80162200	2.28827000
C	2.43113700	3.58218500	1.14517100
O	0.23081100	1.01786000	2.28693200
O	2.52154500	4.29895600	0.17085900
H	1.84857000	1.25288400	4.20193700
H	3.67510000	3.05892500	4.36649100
H	2.59776100	4.74783400	2.91141400
Pd	-0.32298200	0.35905800	-0.30323500

TS1b

SCF energy: -2638.837879

SCF energy in solution: -2637.99578343

Free energy in solution: -2637.38268143

P	1.37115600	-1.61399000	-0.08586100
C	-2.36247400	-2.85808000	-1.13067000
H	-2.33324900	-3.65351900	-0.37627400
H	-3.30710800	-2.96987200	-1.67387400
C	0.57508800	-3.31562300	-0.13777100
H	1.33066100	-4.03634600	0.19703400
H	-0.21609300	-3.31896800	0.62046200
C	-1.15998100	-2.99575800	-2.09086000
H	-0.82354300	-2.00769300	-2.42895500
H	-1.48357600	-3.52512900	-2.99559400
C	0.02038700	-3.78333500	-1.49541200
H	-0.30074900	-4.82667400	-1.36165900
H	0.83603300	-3.80883700	-2.22743500
P	-2.38358700	-1.20826900	-0.23423800
C	-3.39996200	-0.19201100	-1.40541800
C	-2.74337800	0.69024900	-2.27930800
C	-4.79805500	-0.29983600	-1.47557600
C	-3.47080300	1.43501800	-3.21162900
H	-1.66322600	0.81016300	-2.22629100
C	-5.52232500	0.45143700	-2.40185400
H	-5.32673900	-0.96426500	-0.79769400
C	-4.85987400	1.31849400	-3.27457500
H	-2.94623000	2.11217400	-3.88053100
H	-6.60502800	0.36097300	-2.43993200

H	-5.42545600	1.90345000	-3.99528500
C	-3.51576700	-1.51642500	1.19324400
C	-4.38130500	-2.61999900	1.27990000
C	-3.47494300	-0.60531000	2.26417500
C	-5.18562500	-2.80834800	2.40637800
H	-4.43855600	-3.34009300	0.46914200
C	-4.28507900	-0.79354000	3.38472000
H	-2.81033500	0.25175900	2.20735200
C	-5.13985400	-1.89550500	3.46101300
H	-5.84864600	-3.66835000	2.45667900
H	-4.24254000	-0.08020500	4.20387700
H	-5.76497000	-2.04341100	4.33773500
C	2.36674200	-1.76952200	1.46399900
C	3.68208600	-1.28797900	1.54731700
C	1.77755600	-2.31505300	2.61886000
C	4.39633200	-1.37609100	2.74386600
H	4.15329000	-0.83707200	0.68026000
C	2.49296500	-2.40086000	3.81285600
H	0.75212200	-2.67285700	2.59549400
C	3.80849600	-1.93574900	3.87844000
H	5.41386500	-0.99698000	2.78546500
H	2.02079700	-2.83211000	4.69185300
H	4.36698900	-2.00404500	4.80822800
C	2.61540600	-1.79199500	-1.44030900
C	3.61383800	-2.78166300	-1.38893600
C	2.50748100	-0.99468900	-2.58932200
C	4.48459600	-2.96695200	-2.46177200
H	3.71928400	-3.40385300	-0.50440800
C	3.38177900	-1.18564700	-3.66412500
H	1.76062100	-0.20816200	-2.63208500
C	4.36833400	-2.16921700	-3.60405400
H	5.25352400	-3.73330000	-2.40655000
H	3.29040600	-0.55622300	-4.54536700
H	5.04765300	-2.31422800	-4.44010000
O	0.88702900	1.66950400	-1.84259900
C	1.05001500	1.65867500	-0.62316300
C	2.37094000	1.89984700	0.05443600
C	2.48681200	1.99106400	1.44631600
C	3.51624200	2.02749000	-0.74207800
C	3.72685600	2.23197100	2.03423400
H	1.59918800	1.87695800	2.06211100
C	4.75999400	2.25243600	-0.15106300
H	3.41099400	1.97865200	-1.82019100
C	4.86842400	2.36277800	1.23730500
H	3.80526900	2.30964700	3.11554000
H	5.64206000	2.36151100	-0.77724400
H	5.83560000	2.55188100	1.69645900
C	-0.56443700	5.56342100	0.12013400
C	-2.05373000	3.93263200	1.26974700
C	-1.34145900	5.27893900	1.40575200
H	0.03864100	6.47304000	0.18219800
H	-2.88181700	4.00909600	0.55011200
H	-0.64815200	5.24704000	2.25657200
N	0.00326000	3.12326500	0.11361400
C	-1.12849500	2.83970100	0.75818400
C	0.38521200	4.42039100	-0.24685700
O	-1.47703800	1.64344400	0.95551000
O	1.42167000	4.63278700	-0.84932800
H	-2.49038600	3.58775000	2.21196900
H	-2.06406200	6.07618700	1.61297500
H	-1.26351000	5.69642500	-0.71911600
Pd	-0.21936700	0.10714100	0.02191000

3b

SCF energy: -2638.860572

SCF energy in solution: -2638.01496003

Free energy in solution: -2637.40327003

P	1.68870200	-0.82549200	1.23213400
C	-1.64965000	-0.19817800	3.12784900
H	-1.01314200	0.49209600	3.69373800
H	-2.63786600	-0.17778400	3.59908400
C	1.42137000	-0.76824900	3.08963400
H	2.38993300	-0.97683400	3.55837200
H	1.18161600	0.27362800	3.33250000
C	-1.06139000	-1.63011800	3.14669000
H	-1.08950900	-2.07248700	2.14377600
H	-1.69559000	-2.27466700	3.76619500
C	0.37202500	-1.71840000	3.69523100
H	0.35170800	-1.51485900	4.77547500
H	0.72103800	-2.75106000	3.58337300
P	-1.80860200	0.45896800	1.38389100
C	-3.39795800	-0.33294600	0.87093200
C	-3.35551800	-1.56098300	0.19233700
C	-4.64603800	0.22240700	1.19852300
C	-4.53861400	-2.22627000	-0.13903500
H	-2.40789100	-1.98497100	-0.11955600
C	-5.82536100	-0.44197500	0.85988600
H	-4.69966500	1.17805400	1.71222400
C	-5.77410300	-1.66954200	0.19380300
H	-4.48012100	-3.16948900	-0.67490500
H	-6.78465400	0.00180500	1.11413000

H	-6.69456900	-2.18351500	-0.07124100
C	-2.23674600	2.23823600	1.61871500
C	-2.59720000	2.78860300	2.85972100
C	-2.17469400	3.08335000	0.49515300
C	-2.88857200	4.15004400	2.97668300
H	-2.65951400	2.16228200	3.74409000
C	-2.47349600	4.44113900	0.61640800
H	-1.89061600	2.67170000	-0.46978100
C	-2.82823900	4.97900100	1.85571900
H	-3.16563600	4.55927100	3.94482900
H	-2.42185900	5.08054200	-0.26099100
H	-3.05561400	6.03779200	1.94785000
C	3.44719700	-0.27451400	1.12584700
C	4.35955200	-0.91173500	0.27120100
C	3.87510500	0.84346500	1.86116700
C	5.67245100	-0.44866800	0.16893900
H	4.04344700	-1.76475700	-0.31952100
C	5.18857400	1.30177100	1.75852700
H	3.18386300	1.36756200	2.51585200
C	6.09203600	0.65508800	0.91296800
H	6.36697800	-0.95412200	-0.49667000
H	5.50329300	2.16629800	2.33697100
H	7.11481900	1.01282900	0.83117100
C	1.71524600	-2.61580900	0.82306500
C	2.55747600	-3.51523100	1.50200200
C	0.84304400	-3.09981600	-0.16352100
C	2.51668700	-4.87591300	1.20092900
H	3.25247600	-3.15472700	2.25667900
C	0.80258600	-4.46549300	-0.45818700
H	0.19666700	-2.42310000	-0.71637100
C	1.63643500	-5.35211200	0.22240100
H	3.17111600	-5.56468800	1.72906400
H	0.11133100	-4.80783200	-1.22235600
H	1.60728400	-6.41439600	-0.00684400
O	2.06102000	-0.52629800	-2.15310100
C	1.67113200	0.41785000	-1.50117300
C	2.20022900	1.80774100	-1.75071900
C	1.80590300	2.90652200	-0.97696000
C	3.12496600	1.99350400	-2.79107900
C	2.32659000	4.17421300	-1.23747300
H	1.08549300	2.75966400	-0.17607000
C	3.64216700	3.25938200	-3.05249600
H	3.42160400	1.13101600	-3.37954800
C	3.24432000	4.35230800	-2.27518500
H	2.01391000	5.02236600	-0.63399700
H	4.35635300	3.39751400	-3.86031200
H	3.64901400	5.34043600	-2.47941900
C	-2.61961400	-1.81661500	-4.19343000
C	-2.25750000	0.61219000	-3.74337300
C	-2.21039700	-0.48043100	-4.81627200
H	-2.46422500	-2.66168500	-4.87076100
H	-3.29857200	0.80779100	-3.44531800
H	-1.18854000	-0.55505300	-5.21121600
N	-1.31573200	-1.08682000	-2.16111400
C	-1.48968600	0.17780500	-2.50462100
C	-1.86983000	-2.11870500	-2.88991100
O	-1.01133600	1.11481200	-1.77050900
O	-1.80475800	-3.27915100	-2.48377200
H	-1.84337900	1.56204100	-4.09436800
H	-2.86113600	-0.22300800	-5.66029300
H	-3.69278800	-1.80311200	-3.94908800
Pd	0.16628800	0.25523100	-0.13534100

4b

SCF energy: -2638.876035

SCF energy in solution: -2638.037067

Free energy in solution: -2637.423634

P	-1.78981300	-1.13364500	0.31734000
C	1.66719000	-2.99732400	1.14094700
H	1.95444200	-3.90469800	0.59712000
H	2.45762000	-2.83122600	1.88032400
C	-1.40892600	-2.92879100	-0.05638000
H	-2.33232200	-3.40034600	-0.41313000
H	-0.70943300	-2.93437200	-0.89821500
C	0.34502900	-3.20042000	1.90077500
H	0.06718100	-2.25920300	2.38867000
H	0.54747700	-3.90831400	2.71613100
C	-0.85282800	-3.75923700	1.11679400
H	-0.59009600	-4.74964100	0.71771100
H	-1.66424800	-3.92672500	1.83457700
P	1.77149400	-1.48539000	0.02829900
C	3.54460700	-1.02159000	0.26573800
C	3.92484500	-0.51860000	1.52260800
C	4.51622900	-1.15010500	-0.73564000
C	5.25354300	-0.17495900	1.77384300
H	3.17791700	-0.37246000	2.29901300
C	5.84387600	-0.79515300	-0.48297300
H	4.24256100	-1.52652200	-1.71553600
C	6.21740600	-0.31154600	0.77109600
H	5.53274600	0.20696100	2.75248900
H	6.58570100	-0.90180900	-1.27018400

H	7.25131100	-0.03909800	0.96607900
C	1.71057000	-2.07981700	-1.72105600
C	1.75782000	-3.42749400	-2.11026000
C	1.59467100	-1.09039800	-2.71684100
C	1.68037300	-3.78266100	-3.45940300
H	1.85470200	-4.21571800	-1.37057600
C	1.53115100	-1.45050900	-4.06416500
H	1.57645300	-0.04053600	-2.43105100
C	1.56643000	-2.79569800	-4.43942200
H	1.71482100	-4.83187900	-3.74133300
H	1.45148400	-0.67435300	-4.82071700
H	1.50935300	-3.07334900	-5.48868000
C	-3.05927000	-0.73729800	-0.95789100
C	-4.13425600	0.11516100	-0.66061800
C	-2.91830500	-1.21753200	-2.27016700
C	-5.05653300	0.46105400	-1.64892800
H	-4.25336000	0.50926100	0.34394100
C	-3.84248100	-0.86897500	-3.25583700
H	-2.08295700	-1.85964200	-2.53431000
C	-4.91595600	-0.03157300	-2.94738600
H	-5.88398000	1.12053000	-1.40175700
H	-3.72124400	-1.25309300	-4.26526400
H	-5.63526700	0.23954200	-3.71538100
C	-2.72574600	-1.23039900	1.89910000
C	-3.92216300	-1.96310100	1.99226900
C	-2.20610000	-0.61392500	3.04762600
C	-4.58450900	-2.07963000	3.21345100
H	-4.34368700	-2.43507200	1.10840500
C	-2.87423400	-0.73517000	4.26930700
H	-1.29652600	-0.02464700	2.98448800
C	-4.05912500	-1.46580700	4.35469800
H	-5.50951300	-2.64701900	3.27450300
H	-2.46661000	-0.24714100	5.15013900
H	-4.57744300	-1.55505700	5.30591800
O	-1.68672600	2.14182600	1.72014400
C	-1.23791100	1.86138200	0.62633800
C	-1.55950500	2.72413200	-0.56798500
C	-1.15561200	2.38590900	-1.86454500
C	-2.31034200	3.89445400	-0.36135700
C	-1.49905900	3.20317200	-2.94241200
H	-0.56018300	1.49231400	-2.01753400
C	-2.64689400	4.71182400	-1.43611200
H	-2.61749300	4.13966200	0.65061000
C	-2.24275000	4.36529600	-2.73056000
H	-1.17876000	2.93606600	-3.94588300
H	-3.22402000	5.61818300	-1.27016600
H	-2.50616500	5.00312300	-3.57084100
C	2.79287400	3.20781400	2.33056500
C	3.19656700	3.46748300	-0.10706100
C	2.89171300	4.21859400	1.18888400
H	2.44475800	3.65595200	3.26610200
H	4.19690400	3.01286700	-0.05308900
H	1.94092300	4.75840800	1.08715500
N	1.55418300	1.76653700	0.69742900
C	2.19541700	2.34365100	-0.36915600
C	1.85529500	2.04401900	2.01117100
O	1.99279100	1.95904300	-1.52493300
O	1.40443200	1.34945200	2.92551800
H	3.18979900	4.11822900	-0.98617600
H	3.66395700	4.96860100	1.39703400
H	3.78408400	2.77690700	2.53595000
Pd	0.05395700	0.28076400	0.40232000

TS2b

SCF energy: -2638.807260

SCF energy in solution: -2637.971

Free energy in solution: -2637.36167

P	1.48358400	-1.53221900	-1.04714300
C	-1.62273400	-0.49979600	-3.03458700
H	-1.79237800	-1.58187900	-3.02771000
H	-2.41691100	-0.06417300	-3.64951100
C	0.92642700	-2.32323900	-2.65367600
H	1.67750500	-3.06841800	-2.94011500
H	0.01109400	-2.87821600	-2.41715500
C	-0.22540200	-0.16480000	-3.61068400
H	0.29514400	0.55883700	-2.97264800
H	-0.35327600	0.34720800	-4.57103200
C	0.68804100	-1.37791600	-3.84701400
H	0.27336300	-1.99005700	-4.66042900
H	1.65604600	-1.00768600	-4.20219200
P	-1.84587300	0.13292600	-1.29063800
C	-1.76326100	1.94904600	-1.53561200
C	-0.75724400	2.68526800	-0.89728400
C	-2.63387600	2.60022000	-2.43096100
C	-0.59257600	4.04829500	-1.17151500
H	-0.08205800	2.23254300	-0.17599800
C	-2.48368300	3.96138100	-2.68396600
H	-3.43210800	2.04893400	-2.92202900
C	-1.45573000	4.68281900	-2.06329600
H	0.23207600	4.57393400	-0.69432700
H	-3.16188500	4.45906200	-3.37274600

H	-1.33228700	5.74088500	-2.28065000
C	-3.62495100	-0.21946800	-0.95847800
C	-4.21535100	-1.42401100	-1.37503300
C	-4.40042800	0.68997100	-0.22218000
C	-5.55081400	-1.70254800	-1.08020400
H	-3.64001200	-2.15439700	-1.93715600
C	-5.73401400	0.40754800	0.07564200
H	-3.96393400	1.62653900	0.11057000
C	-6.31473600	-0.78660500	-0.35514600
H	-5.99336700	-2.63514700	-1.42055300
H	-6.31990900	1.12597800	0.64253000
H	-7.35520300	-1.00217200	-0.12755000
C	2.43638100	-2.89142900	-0.24433200
C	3.51447900	-2.57741100	0.59808000
C	2.05442300	-4.23491900	-0.38473900
C	4.20194100	-3.58702100	1.27195800
H	3.81823900	-1.54276600	0.72687600
C	2.74571000	-5.24278300	0.28999400
H	1.21475800	-4.50654100	-1.01840800
C	3.82198700	-4.92174600	1.11855000
H	5.03541600	-3.32748100	1.91881400
H	2.44111600	-6.27867400	0.16645100
H	4.35893000	-5.70647700	1.64424900
C	2.76605400	-0.31998700	-1.54614300
C	3.81781000	-0.69695700	-2.40350300
C	2.68800200	1.00190800	-1.09206500
C	4.75869600	0.24691900	-2.80955300
H	3.90828000	-1.72512800	-2.74594200
C	3.63252700	1.94813200	-1.50517800
H	1.92299400	1.32119700	-0.39109600
C	4.66216200	1.57211700	-2.36627900
H	5.56784700	-0.04990100	-3.47196700
H	3.53553300	2.96790300	-1.14107800
H	5.39648900	2.30475500	-2.69131300
O	0.58820500	-2.34082500	2.84193300
C	0.08303200	-1.73692200	1.99221700
C	-1.71771000	-1.05851500	2.06237300
C	-2.68833600	-2.06938200	1.99327900
C	-1.89922400	0.04457100	2.90848500
C	-3.85757000	-1.95882700	2.74652300
H	-2.53134600	-2.93856400	1.36051800
C	-3.07451800	0.14627600	3.65589900
H	-1.10856500	0.78414000	2.97910000
C	-4.05120400	-0.85009300	3.57506000
H	-4.61324500	-2.73766000	2.68936900
H	-3.22249500	1.00219700	4.30953200
H	-4.95977500	-0.76866300	4.16614800
C	2.82195500	4.49084800	2.75650900
C	2.12572200	2.30882200	3.72767300
C	3.27248700	3.31567300	3.62492900
H	3.63228600	5.19326200	2.54000400
H	1.31322600	2.73042600	4.33973400
H	4.14377500	2.83130900	3.16229300
N	1.62467300	2.80536900	1.31351400
C	1.53724200	1.96335700	2.35321300
C	2.23599500	4.02558900	1.41510000
O	0.95121700	0.85280500	2.24851300
O	2.31414500	4.78850700	0.44226000
H	2.42795100	1.37437700	4.21059900
H	3.58978800	3.65423500	4.61929900
H	2.03985400	5.06143500	3.28087100
Pd	-0.34230700	-0.86290300	0.35240800

TS3b

SCF energy: -3364.965257

SCF energy in solution: -3364.02827

Free energy in solution: -3363.271954

P	-2.31444500	-1.13925900	-0.61104500
C	0.64700000	-3.79440400	-1.17361500
H	0.58160000	-3.81056200	-2.26717700
H	1.41831500	-4.52707600	-0.91306500
C	-2.09359700	-2.42590700	-1.96032800
H	-2.97874300	-2.37392000	-2.60468100
H	-1.24418000	-2.09454900	-2.56691600
C	-0.71473400	-4.17716600	-0.56549100
H	-0.86258200	-3.68758300	0.40463400
H	-0.72326200	-5.25568000	-0.35976300
C	-1.90613300	-3.88126100	-1.49106300
H	-1.79987000	-4.49568000	-2.39668500
H	-2.82514200	-4.21812700	-0.99933500
P	1.32029100	-2.08971200	-0.73177800
C	2.58912500	-2.46934900	0.55282400
C	3.64569500	-1.56331000	0.75344400
C	2.49824100	-3.59509300	1.38373300
C	4.60471900	-1.80713700	1.73619200
H	3.70655500	-0.65670800	0.15727200
C	3.45208400	-3.82655200	2.37918800
H	1.68167100	-4.30208200	1.26852300
C	4.51273600	-2.93829500	2.55241400
H	5.42422900	-1.10514500	1.86867700
H	3.36526800	-4.70607100	3.01211700

H	5.26030300	-3.12205100	3.31967600
C	2.33034500	-1.83025300	-2.26042100
C	3.57713800	-2.44921000	-2.44576300
C	1.76374000	-1.11062300	-3.32220000
C	4.24543600	-2.34338300	-3.66668000
H	4.03222800	-3.01114200	-1.63625800
C	2.43058600	-1.01714400	-4.54649700
H	0.82208600	-0.58735200	-3.18955700
C	3.67248800	-1.62995900	-4.72164700
H	5.21290700	-2.82290700	-3.79283700
H	1.97789700	-0.45143500	-5.35673200
H	4.19328200	-1.55037000	-5.67254600
C	-3.43538300	0.07875100	-1.42164700
C	-4.57599500	0.57904100	-0.77428700
C	-3.10516400	0.56482000	-2.69749600
C	-5.38806200	1.52317500	-1.40456100
H	-4.83642900	0.23289100	0.22075500
C	-3.92332400	1.50562900	-3.32314400
H	-2.18403700	0.26226600	-3.18252000
C	-5.06888600	1.98240000	-2.68324100
H	-6.26918400	1.89959600	-0.89167000
H	-3.65050500	1.87613700	-4.30733700
H	-5.70250800	2.71733100	-3.17283500
C	-3.40180600	-2.01548000	0.59730100
C	-4.65101300	-2.52757100	0.20144700
C	-2.95968700	-2.24373700	1.90793700
C	-5.43666900	-3.25209800	1.09674100
H	-5.01591800	-2.35299300	-0.80711500
C	-3.75036100	-2.96964900	2.80361900
H	-2.01034400	-1.83220000	2.23260100
C	-4.98600200	-3.47536900	2.40120200
H	-6.39952700	-3.64153200	0.77676600
H	-3.39803200	-3.13206000	3.81865500
H	-5.59954400	-4.03860000	3.09946400
P	2.04298300	1.12581000	2.46393300
H	3.40907300	1.14342900	2.21643300
C	0.89756600	0.76502500	4.84178000
H	0.35624200	1.71792700	4.86077900
H	0.26499200	0.02350300	4.34627000
C	2.34359000	3.74989000	2.24177400
H	2.72101800	3.87612100	3.26452800
H	3.18074300	3.55971700	1.56354800
O	1.20904000	0.06268800	1.81776700
O	1.46403400	2.59706300	2.20512300
O	2.11336400	0.94207000	4.06993200
C	1.29318000	0.32555100	6.23935800
H	1.83075400	-0.62759400	6.20684700
H	0.39661800	0.19855200	6.85672400
H	1.93878200	1.07058100	6.71613400
C	1.53805300	4.95804600	1.80223800
H	2.17120400	5.85270900	1.82085400
H	0.68316900	5.11985300	2.46600500
H	1.15865400	4.81391400	0.78654900
Pd	-0.32237200	-0.35410400	0.25340700
C	3.55347100	2.98037100	-2.03488900
C	1.69778100	2.91766300	-3.66743600
C	2.67189600	3.83998000	-2.93833800
H	4.20818300	3.57500800	-1.39046800
H	2.24705800	2.29971200	-4.39451500
H	2.11107500	4.56162700	-2.32769400
N	1.50569500	1.60305900	-1.51596100
C	0.97416100	1.95329600	-2.71576900
C	2.72467100	2.05329600	-1.13337600
O	-0.11462200	1.48326300	-3.10456400
O	3.24086800	1.71681400	-0.04535900
H	0.93483000	3.46249600	-4.23209400
H	3.27425600	4.42326400	-3.64611400
H	4.20902600	2.34535700	-2.65033800
O	-1.70956600	0.56794300	2.51284900
C	-1.42269000	0.93041200	1.39003800
C	-1.71940200	2.31719600	0.91359700
C	-1.46064800	2.72068800	-0.40040600
C	-2.28333200	3.22561600	1.82846400
C	-1.76483600	4.02445700	-0.79706100
H	-1.02482100	2.02599400	-1.10981700
C	-2.57910100	4.52466200	1.42940000
H	-2.47961900	2.89154600	2.84231700
C	-2.31938700	4.92594300	0.11268000
H	-1.57120300	4.32641500	-1.82255700
H	-3.01461500	5.22547600	2.13739400
H	-2.55503800	5.94031900	-0.20064500

5b

SCF energy: -3364.971897

SCF energy in solution: -3364.02906933

Free energy in solution: -3363.27249433

P	-2.28706700	-1.28685600	-0.56103000
C	0.59593400	-4.01629200	0.31428700
H	1.08430600	-4.81270600	-0.25791000
H	0.93715400	-4.12306000	1.35094600
C	-1.86879900	-2.71850500	-1.68624000

H	-2.66812100	-2.78741000	-2.43356200
H	-0.96991500	-2.42198100	-2.23079500
C	-0.93295500	-4.20804600	0.31614400
H	-1.37176100	-3.51914000	1.04665100
H	-1.12157600	-5.21558000	0.71144900
C	-1.70050600	-4.10294700	-1.01575700
H	-1.23917500	-4.76942500	-1.75739800
H	-2.70343200	-4.50365600	-0.82796800
P	1.19126700	-2.33508400	-0.22535000
C	2.91966700	-2.22644500	0.41278600
C	3.58619500	-1.00001500	0.24839200
C	3.60157700	-3.29716700	1.00792800
C	4.90930300	-0.85757900	0.66669800
H	3.07602300	-0.14436900	-0.18761000
C	4.92432200	-3.14624600	1.43315500
H	3.11762000	-4.26017600	1.13853200
C	5.58194500	-1.92786800	1.26222200
H	5.40604800	0.09948800	0.53086300
H	5.43949600	-3.98612400	1.89245800
H	6.61149300	-1.81280900	1.59110200
C	1.49337800	-2.47321800	-2.04623600
C	1.80951100	-3.68464200	-2.68444900
C	1.43399300	-1.29669700	-2.80994800
C	2.03971000	-3.71928200	-4.06004700
H	1.88701800	-4.60903900	-2.12011400
C	1.66145100	-1.33618300	-4.18898400
H	1.22715600	-0.33419600	-2.34514300
C	1.96007100	-2.54615800	-4.81552100
H	2.28111900	-4.66441500	-4.54025300
H	1.58185500	-0.40895200	-4.74758500
H	2.13141700	-2.57899900	-5.88858200
C	-2.93416900	-0.02132800	-1.72806400
C	-4.24259800	0.48119300	-1.65213100
C	-2.05768900	0.49511200	-2.69679500
C	-4.67142300	1.45996400	-2.55085800
H	-4.92868400	0.11743600	-0.89475900
C	-2.49100500	1.47267200	-3.59219000
H	-1.01994000	0.18389600	-2.75474100
C	-3.80078900	1.95163500	-3.52511400
H	-5.68740500	1.84028700	-2.48181100
H	-1.77569100	1.86269000	-4.30905100
H	-4.13868800	2.71682400	-4.21942300
C	-3.75460200	-1.94566100	0.34455100
C	-4.83441700	-2.49481700	-0.37263000
C	-3.78387900	-1.98375300	1.74606500
C	-5.91826700	-3.06012900	0.29753200
H	-4.83645300	-2.47312900	-1.45888300
C	-4.87229900	-2.55308100	2.41397000
H	-2.96964000	-1.55339800	2.31794300
C	-5.93848000	-3.09140700	1.69478300
H	-6.74544300	-3.47674900	-0.27099600
H	-4.88217200	-2.56951900	3.50043100
H	-6.78317300	-3.53297300	2.21690600
P	1.95521400	1.03949100	2.68095900
H	3.18954000	1.22656200	2.07536100
C	1.48475500	0.29741900	5.19001800
H	0.72341300	1.07821100	5.29789900
H	0.99412500	-0.61772100	4.84539600
C	1.97603400	3.68412900	2.75121400
H	2.58594600	3.69490200	3.66304900
H	2.62322700	3.68468300	1.86981300
O	1.07372300	-0.05039800	2.14020300
O	1.20253800	2.44742500	2.72477900
O	2.44460200	0.71374800	4.18277600
C	2.23972200	0.07587000	6.48714400
H	3.00426600	-0.69760300	6.36250400
H	1.54430800	-0.24553800	7.27055200
H	2.73003700	0.99772500	6.81619900
C	0.99670100	4.84121600	2.73483000
H	1.54888300	5.78793900	2.75885500
H	0.33197300	4.80532200	3.60398400
H	0.38559900	4.81407900	1.82843400
Pd	-0.44920500	-0.61552400	0.68488100
C	3.36269800	3.82164500	-1.66973000
C	2.21000800	3.53619600	-3.84597600
C	2.63830700	4.55865300	-2.79505500
H	3.58955100	4.47208600	-0.81899200
H	3.09786600	3.13976900	-4.36210300
H	1.75106100	5.06555300	-2.38957500
N	1.66407900	1.97792100	-1.93103400
C	1.46383700	2.34188800	-3.23076700
C	2.55718500	2.62145400	-1.14721500
O	0.69124300	1.70620900	-3.96886600
O	2.78288800	2.25475100	0.02926900
H	1.56610600	3.96593500	-4.61940200
H	3.27427400	5.33840600	-3.23282800
H	4.32744000	3.43914100	-2.03707600
O	-2.03246600	0.43266400	2.75678900
C	-1.60898400	0.74227100	1.66058400
C	-1.80110700	2.11066900	1.09237400
C	-1.09004400	2.55090300	-0.03137000
C	-2.72319400	2.96749900	1.72077000

C	-1.30553000	3.83966100	-0.52258100
H	-0.35142800	1.91540100	-0.51506300
C	-2.94108900	4.24636900	1.21918100
H	-3.25547300	2.60988200	2.59670600
C	-2.23180000	4.68354600	0.09364700
H	-0.75027000	4.17378200	-1.39393500
H	-3.66045700	4.90415300	1.70042800
H	-2.40424900	5.68208200	-0.30083000

6b

SCF energy: -3364.971374

SCF energy in solution: -3364.03162096

Free energy in solution: -3363.27774196

P	2.87577300	-0.53967500	0.52969900
C	0.81481600	-4.00362900	0.51586500
H	0.73698100	-4.40403000	1.53239900
H	0.33570900	-4.73722100	-0.13848700
C	2.92470700	-1.92440500	1.78628800
H	3.69385500	-1.66529400	2.52345100
H	1.96568700	-1.91315800	2.31417800
C	2.29604700	-3.86226600	0.12269900
H	2.38367000	-3.24595800	-0.78055800
H	2.66855600	-4.85754000	-0.15425600
C	3.22449000	-3.32581500	1.22277900
H	3.20210900	-4.02386800	2.07169200
H	4.25285300	-3.34042200	0.84402500
P	-0.21783300	-2.43223100	0.39749700
C	-1.74029000	-2.99655400	-0.47374900
C	-2.99747500	-2.50240600	-0.09547200
C	-1.64861100	-3.83756000	-1.59654300
C	-4.14395700	-2.86423700	-0.80677200
H	-3.11075100	-1.81352700	0.73510700
C	-2.79724300	-4.21038900	-2.29496700
H	-0.68377900	-4.20204500	-1.94079000
C	-4.04833800	-3.72918100	-1.89741100
H	-5.08912000	-2.43581000	-0.48995000
H	-2.71199800	-4.87426700	-3.15188600
H	-4.94165100	-4.02217900	-2.44357900
C	-0.77561200	-2.10800100	2.12644200
C	-1.07646300	-3.14009000	3.03295300
C	-0.92340700	-0.77624900	2.54390400
C	-1.47864000	-2.84638000	4.33497200
H	-1.01608200	-4.17972300	2.72376900
C	-1.32988100	-0.48524400	3.84943700
H	-0.76526800	0.04545100	1.85138200
C	-1.59728800	-1.51638100	4.74901800
H	-1.70788300	-3.65547800	5.02343700
H	-1.44621300	0.55349700	4.14460400
H	-1.91223600	-1.28934800	5.76421800
C	3.20057800	0.94574800	1.56652000
C	4.04104900	1.97497400	1.11538700
C	2.54138300	1.09586900	2.79786200
C	4.23197000	3.12064500	1.88826800
H	4.54900200	1.88448400	0.16059300
C	2.73655500	2.24265800	3.56774000
H	1.86023000	0.32994700	3.15691000
C	3.58375200	3.25642800	3.11673900
H	4.88513200	3.90908900	1.52475100
H	2.22014200	2.34404100	4.51827500
H	3.73222900	4.15017900	3.71649400
C	4.43713300	-0.81375200	-0.40793300
C	5.67993900	-0.79019700	0.25094500
C	4.39368100	-1.13224600	-1.77267100
C	6.85306300	-1.07910200	-0.44412000
H	5.73341800	-0.53551400	1.30598300
C	5.57284400	-1.42115200	-2.46548000
H	3.44590000	-1.12433700	-2.29949800
C	6.80053300	-1.39675300	-1.80482300
H	7.80744500	-1.05503000	0.07500000
H	5.52633000	-1.65726900	-3.52492100
H	7.71611500	-1.61968100	-2.34610500
P	-2.14559000	0.60421700	-1.80451200
H	-2.85397800	0.58521500	-0.56974800
C	-2.83625600	-0.38701200	-4.18005700
H	-2.32502700	0.43632600	-4.69274000
H	-2.13543700	-1.21959000	-4.07251700
C	-2.76054200	3.19217200	-1.82697400
H	-3.78882600	2.88344100	-2.05052200
H	-2.65576500	3.34395000	-0.74910100
O	-0.85124700	-0.18348800	-1.90267100
O	-1.84265200	2.13388700	-2.21612600
O	-3.23205600	0.05097400	-2.85582700
C	-4.09224500	-0.80603100	-4.92096600
H	-4.59395300	-1.61990800	-4.38864500
H	-3.83267700	-1.15299800	-5.92776500
H	-4.79044600	0.03226100	-5.01151600
C	-2.38695100	4.43783900	-2.60865500
H	-3.05108100	5.26381300	-2.32862200
H	-2.48196000	4.26599800	-3.68588400
H	-1.35562700	4.73077100	-2.39059600
Pd	0.90752400	-0.44890600	-0.67454200

C	-5.76588100	1.22442300	2.55094800
C	-3.80663300	2.72588300	2.81096600
C	-5.32527800	2.68513100	2.64081200
H	-6.82435700	1.11597800	2.29558900
H	-3.53593600	2.32123300	3.79879900
H	-5.60499500	3.21218900	1.71786200
N	-3.69305500	0.82557400	1.16726600
C	-3.08730700	1.88464200	1.74696100
C	-4.95717300	0.42440300	1.51643500
O	-1.91397300	2.20742200	1.44684300
O	-5.47206300	-0.59050400	1.03594200
H	-3.40015600	3.74122300	2.76599400
H	-5.83081500	3.20327800	3.46557000
H	-5.62721100	0.73339900	3.52650900
O	2.19043000	0.82596100	-2.82454500
C	1.67168300	1.10565500	-1.76368300
C	1.48697400	2.51745900	-1.30956300
C	0.67677000	2.83321600	-0.21327300
C	2.13956800	3.54426400	-2.01494800
C	0.51138300	4.16235500	0.17636000
H	0.13942000	2.05886900	0.32295600
C	1.98989400	4.86799400	-1.61214100
H	2.75365800	3.28333100	-2.87147200
C	1.17471000	5.17835900	-0.51547400
H	-0.14680300	4.38235500	1.01091800
H	2.50067900	5.66092600	-2.15282600
H	1.05511100	6.21440500	-0.20736600

TS4b

SCF energy: -3364.964885

SCF energy in solution: -3364.01857467

Free energy in solution: -3363.26669767

P	-2.77257900	0.44905000	0.15172700
C	-0.94595100	3.87008800	-0.99371900
H	-0.88804800	4.81830900	-0.44681100
H	-0.49959700	4.04955000	-1.97788200
C	-3.06913900	2.11887200	0.94287300
H	-3.92788600	2.01434600	1.61639500
H	-2.20132900	2.32243500	1.57449700
C	-2.41259400	3.47006400	-1.23784800
H	-2.43264600	2.56286300	-1.85262300
H	-2.85569200	4.25906300	-1.86084700
C	-3.33655400	3.29310700	-0.02189300
H	-3.32927100	4.21501800	0.57678100
H	-4.35728100	3.18948300	-0.40791700
P	0.14107700	2.56917800	-0.20862500
C	1.84999300	3.04820800	-0.71939900
C	2.89575600	2.20690600	-0.30403700
C	2.16020600	4.18848600	-1.47389600
C	4.21690700	2.49363300	-0.64449300
H	2.67901100	1.31881300	0.28247100
C	3.48577300	4.47585100	-1.81133900
H	1.38280000	4.87176400	-1.80039300
C	4.51532600	3.62907300	-1.40163100
H	5.00164500	1.81003600	-0.33457300
H	3.70827100	5.36501000	-2.39591500
H	5.54413100	3.84964800	-1.67377900
C	0.20393800	2.97044400	1.59894700
C	0.11140200	4.27598200	2.10824800
C	0.41766600	1.90937400	2.49333800
C	0.20796900	4.51030600	3.48046100
H	-0.02531400	5.12201000	1.44070400
C	0.52541500	2.14705900	3.86664200
H	0.51485700	0.88823700	2.13542500
C	0.41293600	3.44616200	4.36320400
H	0.13012900	5.52640300	3.85896100
H	0.69988800	1.30260500	4.52670000
H	0.49005200	3.63320200	5.43121400
C	-3.17193000	-0.70830900	1.52748800
C	-3.95254700	-1.85430100	1.31262400
C	-2.62700800	-0.48474600	2.80240500
C	-4.19863700	-2.74654600	2.35696800
H	-4.37149800	-2.05271800	0.33131300
C	-2.87701300	-1.37855600	3.84338100
H	-1.99075700	0.37507400	2.98896400
C	-3.66522800	-2.50975800	3.62458200
H	-4.80479800	-3.62986100	2.17506000
H	-2.44337100	-1.19375000	4.82202100
H	-3.85547100	-3.20734200	4.43575500
C	-4.20673800	0.31220900	-1.00066100
C	-5.52104500	0.44603900	-0.51671800
C	-4.00199600	0.14412300	-2.37753300
C	-6.60484200	0.41299100	-1.39254000
H	-5.70083000	0.56488700	0.54834000
C	-5.09212000	0.11056700	-3.25231200
H	-2.99723300	0.00738000	-2.76181600
C	-6.39119600	0.24633200	-2.76420300
H	-7.61499800	0.51542100	-1.00500300
H	-4.91928900	-0.02971100	-4.31578500
H	-7.23672400	0.21844600	-3.44644500
P	2.47248500	-0.91472600	-1.82667200

H	3.62390600	-0.83169200	-0.60185400
C	2.56648800	-0.38895700	-4.45604700
H	1.97418700	-1.29456500	-4.63526400
H	1.87574000	0.45820000	-4.38967500
C	3.01988600	-3.48436500	-2.15589300
H	3.53309900	-3.42074700	-3.12450500
H	3.76997500	-3.30467500	-1.37259000
O	1.17011900	-0.09596000	-1.80269700
O	1.99694000	-2.47526700	-2.09861000
O	3.27272500	-0.51729700	-3.20501600
C	3.59364200	-0.17897000	-5.55614300
H	4.18591200	0.72157000	-5.36281600
H	3.09348400	-0.06497800	-6.52522000
H	4.27788300	-1.03191400	-5.61745900
C	2.37119700	-4.84608300	-1.97399900
H	3.12852500	-5.63632100	-2.04279900
H	1.61760200	-5.01838500	-2.74936600
H	1.87898100	-4.91318400	-0.99931000
Pd	-0.65523700	0.21976200	-0.76258500
C	5.32124800	-1.20565000	2.44568600
C	3.55625600	-1.21641300	4.19758100
C	4.82882800	-1.91129000	3.70986800
H	6.12415600	-1.75058300	1.94052100
H	3.79940000	-0.20359800	4.55416300
H	4.60902600	-2.96268300	3.48110700
N	2.91000100	-0.93880200	1.77019500
C	2.51379600	-1.06908400	3.08352000
C	4.19124700	-0.99335400	1.44719600
O	1.31774700	-1.03444600	3.38817300
O	4.57315200	-0.84457600	0.22796900
H	3.08156400	-1.74037400	5.03198400
H	5.60345600	-1.90974400	4.48544600
H	5.72624100	-0.21406300	2.69773700
O	-1.59245400	-1.82748800	-2.46520900
C	-1.15115900	-1.67128900	-1.34633500
C	-0.89016000	-2.82114400	-0.42394100
C	-0.23891100	-2.65574200	0.80422300
C	-1.33594900	-4.09722500	-0.81089500
C	-0.03460000	-3.75462900	1.63944200
H	0.12695700	-1.68239500	1.11563000
C	-1.13734000	-5.18971300	0.02735300
H	-1.83128500	-4.20745800	-1.77054600
C	-0.48594500	-5.01896700	1.25552600
H	0.46915800	-3.60518700	2.58931400
H	-1.48648000	-6.17484000	-0.27234100
H	-0.33356000	-5.87344500	1.91077900

7b

SCF energy: -2965.004062

SCF energy in solution: -2964.17393501

Free energy in solution: -2963.53252801

P	2.11399200	-1.32187100	0.31126900
C	-1.02425300	-3.40447100	1.42926900
H	-0.68421800	-3.24103200	2.45838900
H	-1.91036900	-4.04407700	1.50391100
C	2.00573600	-2.63853300	1.64488100
H	3.00845700	-2.75751500	2.07044200
H	1.37804500	-2.21333400	2.43636300
C	0.08644900	-4.07685100	0.58865700
H	0.13654200	-3.63144800	-0.41252200
H	-0.16519800	-5.13315100	0.43042400
C	1.48032800	-4.02498200	1.23217400
H	1.47304000	-4.64433400	2.14038200
H	2.19823900	-4.49061500	0.54764600
P	-1.55537600	-1.72995100	0.78083700
C	-2.87254800	-2.16783200	-0.43287900
C	-3.82445100	-1.19709700	-0.79249200
C	-2.93534300	-3.43230100	-1.04137800
C	-4.82141000	-1.49953900	-1.72010400
H	-3.78024900	-0.20338600	-0.36164000
C	-3.92826300	-3.72451300	-1.97954000
H	-2.21605700	-4.20529000	-0.79130400
C	-4.87725200	-2.76051600	-2.31812700
H	-5.55432300	-0.74028200	-1.97893100
H	-3.95972800	-4.70968800	-2.43784800
H	-5.65378200	-2.98883200	-3.04341100
C	-2.49118300	-1.07582500	2.22617800
C	-3.69447500	-1.65813900	2.65801900
C	-1.95555100	-0.00398300	2.95445300
C	-4.33922700	-1.18286300	3.79926900
H	-4.13559200	-2.47533400	2.09392600
C	-2.60147600	0.46987900	4.09870700
H	-1.04355300	0.47412200	2.60888000
C	-3.79224900	-0.11947300	4.52303100
H	-5.27164000	-1.63908300	4.12139800
H	-2.18186700	1.31007800	4.64513300
H	-4.29983700	0.25357900	5.40861600
C	3.55149500	-0.33121900	0.91203100
C	4.47238200	0.21976600	0.00773200
C	3.69965500	-0.05438800	2.28081400
C	5.52461900	1.01377300	0.46558000

H	4.36818600	0.03158100	-1.05626600
C	4.75305500	0.73934500	2.73553800
H	2.99196700	-0.45293800	3.00248500
C	5.67010100	1.27398600	1.82902200
H	6.22962700	1.43136700	-0.24799700
H	4.85489400	0.93990000	3.79876600
H	6.48979100	1.89318500	2.18287300
C	2.77799200	-2.21760500	-1.15272800
C	3.95631900	-2.98031000	-1.06818900
C	2.08622500	-2.16048800	-2.37133200
C	4.42463800	-3.68103500	-2.17858200
H	4.51627500	-3.01899100	-0.13724100
C	2.56052100	-2.86224900	-3.48311800
H	1.19410300	-1.54789000	-2.45487100
C	3.72490000	-3.62397800	-3.38796100
H	5.33585700	-4.26825200	-2.10182800
H	2.02058500	-2.80268500	-4.42390800
H	4.09286200	-4.16796100	-4.25383700
P	-2.07253100	2.34752200	-0.07319400
C	-3.84930000	2.23917000	-2.12873800
H	-3.16111900	2.89782600	-2.66981600
H	-3.63680800	1.21015600	-2.44132900
C	-1.51178100	4.85594300	-0.76565800
H	-2.58148000	5.09780000	-0.67617300
H	-1.04345300	5.06853400	0.20751700
O	-1.48354500	1.00806900	-0.68951900
O	-1.33889400	3.48092900	-1.10487400
O	-3.62943900	2.36876100	-0.71467400
C	-5.29668500	2.60766400	-2.42117300
H	-5.98509600	1.95428500	-1.87228100
H	-5.50903600	2.51176300	-3.49332000
H	-5.50244900	3.64009200	-2.11813900
C	-0.87442700	5.70944000	-1.85291700
H	-0.98187100	6.77570500	-1.61775300
H	-1.34958700	5.51809600	-2.82119000
H	0.19131200	5.47731500	-1.94281400
Pd	0.17007800	-0.13783900	-0.11322300
O	1.59433500	1.06203700	-2.23061500
C	1.31723300	1.25612100	-1.06515100
C	1.74195300	2.51165900	-0.35827800
C	1.44972100	2.73352600	0.99101500
C	2.46314800	3.47789300	-1.07726600
C	1.86681100	3.90747300	1.61889900
H	0.88640400	1.98262200	1.53846900
C	2.88201100	4.64856300	-0.45106600
H	2.67654900	3.29134500	-2.12502200
C	2.58341400	4.86572800	0.89887400
H	1.63042700	4.07632800	2.66612500
H	3.43864200	5.39530600	-1.01175000
H	2.90801000	5.78144500	1.38669000

TS5b

SCF energy: -3364.968844

SCF energy in solution: -3364.02656241

Free energy in solution: -3363.27607041

P	2.89060900	-0.53779600	0.52038000
C	0.85661700	-4.00944200	0.68317200
H	0.83701400	-4.28628600	1.74310700
H	0.35133600	-4.81700300	0.14607600
C	2.98843900	-1.91277300	1.78698400
H	3.76993500	-1.63734100	2.50489800
H	2.04084100	-1.90822000	2.33612100
C	2.31419700	-3.89425200	0.19930600
H	2.35716700	-3.31237300	-0.72990100
H	2.67255800	-4.89985000	-0.05748400
C	3.29269300	-3.31646200	1.23303800
H	3.33108300	-3.99813600	2.09470300
H	4.29920100	-3.31659900	0.79969100
P	-0.19425700	-2.46092200	0.45557600
C	-1.66595500	-3.08798500	-0.45682700
C	-2.94096300	-2.57542500	-0.17751200
C	-1.51582200	-3.99224400	-1.52174200
C	-4.04764300	-2.97436800	-0.92899900
H	-3.08985000	-1.84626800	0.61169700
C	-2.62504500	-4.40113000	-2.26267400
H	-0.53516600	-4.37784000	-1.78927700
C	-3.89385400	-3.89687600	-1.96471100
H	-5.01056500	-2.53121000	-0.69885300
H	-2.49457300	-5.10995300	-3.07666200
H	-4.75557100	-4.21500200	-2.54605700
C	-0.82997400	-2.10735100	2.15182300
C	-1.21802300	-3.12654700	3.03998900
C	-0.93470800	-0.77187100	2.56835500
C	-1.67063400	-2.81613300	4.32139200
H	-1.18085500	-4.16744100	2.72987700
C	-1.39009900	-0.46237600	3.85355700
H	-0.69246100	0.03902400	1.88812600
C	-1.75032600	-1.48221500	4.73366200
H	-1.96704900	-3.61464500	4.99651100
H	-1.46731500	0.58055200	4.14667300
H	-2.10260800	-1.24307000	5.73373400

C	3.24070600	0.95192000	1.54511100
C	4.06120700	1.98525500	1.06767900
C	2.61978400	1.10038300	2.79631900
C	4.27054000	3.13245700	1.83365500
H	4.53886600	1.89713200	0.09715400
C	2.83268200	2.24851800	3.55938300
H	1.95574000	0.32996300	3.17735700
C	3.66056100	3.26606800	3.08174300
H	4.90786600	3.92395100	1.44928300
H	2.34624100	2.34777900	4.52589000
H	3.82340900	4.16088800	3.67616600
C	4.42542300	-0.80629100	-0.46119300
C	5.68845500	-0.77647100	0.15768400
C	4.34031100	-1.12381900	-1.82436800
C	6.84047900	-1.05834000	-0.57455400
H	5.77428400	-0.52249300	1.21083000
C	5.49851300	-1.40557800	-2.55459500
H	3.37618900	-1.11999400	-2.32106300
C	6.74644300	-1.37495800	-1.93331400
H	7.81079100	-1.02943400	-0.08605600
H	5.41958600	-1.64056100	-3.61237300
H	7.64557700	-1.59213800	-2.50376300
P	-2.18712000	0.63788200	-1.64322900
H	-2.95635800	0.75655200	-0.26706300
C	-2.85732300	-0.35607300	-4.03359100
H	-2.30784000	0.45653100	-4.52404900
H	-2.18387100	-1.21183000	-3.92712800
C	-2.66501500	3.23219500	-1.96117200
H	-3.69581600	2.95352900	-2.21608200
H	-2.62118900	3.47670900	-0.89362900
O	-0.90917700	-0.20891100	-1.75331100
O	-1.78068000	2.12090200	-2.21823100
O	-3.27058900	0.07329200	-2.71677400
C	-4.10608800	-0.72694600	-4.81394700
H	-4.64688200	-1.53199900	-4.30648200
H	-3.83419800	-1.06784900	-5.81994700
H	-4.77705500	0.13324400	-4.90801400
C	-2.20331000	4.40564900	-2.80799400
H	-2.84699800	5.27513400	-2.62916300
H	-2.24665100	4.15444600	-3.87295600
H	-1.17328900	4.67616100	-2.55666600
Pd	0.88596800	-0.45348000	-0.62473900
C	-5.82648000	1.14503500	2.29629100
C	-3.93179400	2.63305600	2.91612100
C	-5.43290500	2.58500200	2.62778600
H	-6.86608400	1.05380800	1.96813300
H	-3.71668700	2.09849100	3.85414600
H	-5.66459500	3.23646800	1.77414200
N	-3.66627800	1.01040700	1.02537100
C	-3.10464700	1.96994500	1.81012900
C	-4.94522100	0.53415600	1.20090600
O	-1.91834500	2.31034500	1.66113700
O	-5.38558700	-0.38600700	0.51191400
H	-3.55486800	3.65266500	3.04296900
H	-6.00885300	2.96438900	3.48055500
H	-5.72169100	0.51438500	3.19219200
O	2.09879800	0.83758900	-2.80149000
C	1.60320400	1.11201400	-1.72842700
C	1.43834800	2.52376300	-1.26323600
C	0.65774600	2.84185100	-0.14678200
C	2.08304200	3.54823200	-1.97809800
C	0.51356700	4.16993600	0.25391400
H	0.12979100	2.06654200	0.39686100
C	1.95506300	4.87162600	-1.56550400
H	2.67348100	3.28599800	-2.85067000
C	1.16923300	5.18377500	-0.44852500
H	-0.12067300	4.39398600	1.10584000
H	2.46000100	5.66261000	-2.11456000
H	1.06572900	6.21922500	-0.13270400

8b

SCF energy: -2965.022837

SCF energy in solution: -2964.20207298

Free energy in solution: -2963.55437098

P	1.84682400	-1.44747700	0.67625800
C	-1.42712200	-2.08734200	2.32304600
H	-0.78505500	-1.58835900	3.05611100
H	-2.33449200	-2.37719500	2.86172900
C	1.65193800	-2.41934300	2.27614000
H	2.64537600	-2.77539300	2.57121700
H	1.35625000	-1.68704100	3.03648100
C	-0.72438700	-3.31398500	1.69510600
H	-0.62946500	-3.18372500	0.60934500
H	-1.35005300	-4.20372000	1.82677900
C	0.67093300	-3.60491000	2.26803400
H	0.57844700	-3.95958900	3.30422700
H	1.11249400	-4.42972200	1.69696400
P	-1.85562800	-0.80856800	1.02697300
C	-3.25154100	-1.66343200	0.17294500
C	-3.21779600	-1.83408100	-1.21955200
C	-4.32011700	-2.21994200	0.90011900

C	-4.23360500	-2.54651400	-1.86523500
H	-2.41895800	-1.39693400	-1.81241900
C	-5.33392400	-2.92305400	0.25075800
H	-4.37167900	-2.10007200	1.97902800
C	-5.29041700	-3.09054500	-1.13618900
H	-4.19156800	-2.66823200	-2.94415400
H	-6.15443500	-3.34237100	0.82737300
H	-6.07815700	-3.64252400	-1.64242800
C	-2.59850800	0.51846000	2.07245000
C	-3.94447400	0.90207400	2.01629400
C	-1.74067400	1.20191900	2.95191200
C	-4.42360600	1.93091700	2.83062200
H	-4.62080000	0.40251200	1.33172500
C	-2.22040500	2.22539700	3.76876500
H	-0.68544500	0.94002800	2.99145300
C	-3.56683700	2.59267300	3.71069900
H	-5.47071500	2.21633300	2.77228200
H	-1.54215200	2.73881100	4.44545600
H	-3.94288200	3.39239800	4.34300700
C	3.50723000	-0.69349000	0.97964200
C	4.50606000	-0.70246200	-0.00557900
C	3.76580800	-0.04181700	2.19708900
C	5.73760200	-0.08910600	0.23055800
H	4.32077300	-1.18037100	-0.96132700
C	4.99836700	0.56786600	2.43112800
H	3.00465600	-0.00216900	2.97195900
C	5.98946500	0.54409800	1.44825100
H	6.49996100	-0.10633800	-0.54369400
H	5.18133000	1.06415200	3.38052000
H	6.94914300	1.02065600	1.62904300
C	2.16375500	-2.74894400	-0.58716900
C	3.06408100	-3.80098100	-0.34350800
C	1.48698600	-2.69783500	-1.81573100
C	3.27227500	-4.78970800	-1.30399300
H	3.61379600	-3.84383400	0.59320100
C	1.70101500	-3.68988600	-2.77665600
H	0.80825900	-1.87761300	-2.03226800
C	2.58793800	-4.73582000	-2.52215500
H	3.96929100	-5.59924000	-1.10377300
H	1.17564700	-3.63341300	-3.72567400
H	2.75266400	-5.50578800	-3.27136500
P	-1.17730300	1.07918800	-1.86331700
C	-3.73540300	1.72006100	-2.19846100
H	-3.36177000	2.35161200	-3.01333400
H	-4.04842600	0.76555900	-2.63554200
C	-0.89681600	3.76401900	-1.71011500
H	-1.96930800	3.99437300	-1.68800200
H	-0.56216600	3.64285600	-0.67253500
O	-1.30073600	0.14177700	-3.03528800
O	-0.68398000	2.55258100	-2.44693800
O	-2.67783800	1.47416100	-1.24693200
C	-4.88900300	2.39798800	-1.47779300
H	-5.26759400	1.76551800	-0.66854300
H	-5.71039300	2.58986300	-2.17860900
H	-4.57314100	3.35255300	-1.04342900
C	-0.12023600	4.87736200	-2.39477100
H	-0.29097300	5.82995500	-1.87886400
H	-0.44088900	4.98321700	-3.43654500
H	0.95244600	4.66226200	-2.38411500
Pd	0.11262100	0.04454600	-0.19880000
O	2.22216500	0.53387400	-2.12832100
C	1.68194200	1.00556100	-1.14727900
C	2.20712700	2.28306500	-0.53321900
C	1.66701800	2.81514100	0.64316000
C	3.28096800	2.93991900	-1.15450100
C	2.18705900	3.98737600	1.19418200
H	0.83039400	2.30349800	1.11476300
C	3.79765600	4.11273700	-0.60908900
H	3.68956000	2.51159400	-2.06424600
C	3.25195500	4.63830300	0.56733400
H	1.75963300	4.39555000	2.10662800
H	4.62527600	4.62041400	-1.09813500
H	3.65541400	5.55409100	0.99217900

TS6b

SCF energy: -2964.964239

SCF energy in solution: -2964.13425628

Free energy in solution: -2963.49535828

P	0.43941900	2.20765400	-0.49832700
C	0.34986300	-1.04504000	-2.79179100
H	1.13561200	-1.08689800	-3.55626300
H	-0.26771600	-1.93828200	-2.92357300
C	1.12844600	2.08193400	-2.22711300
H	1.45855500	3.08110000	-2.53789400
H	2.02345300	1.45304000	-2.16555400
C	-0.54759200	0.19165100	-2.98032300
H	-1.21300500	0.26794200	-2.11413500
H	-1.19784300	-0.01929600	-3.84045600
C	0.14853100	1.52848800	-3.27874600
H	0.70600300	1.44688100	-4.22322200
H	-0.63254400	2.27902000	-3.44991500

P	1.15866300	-1.26514300	-1.10313700
C	0.95236600	-3.07024500	-0.78997400
C	2.03122800	-3.92256400	-0.51329100
C	-0.35403600	-3.59055500	-0.76652800
C	1.80986000	-5.27543600	-0.24467800
H	3.04645800	-3.53984900	-0.50973200
C	-0.56731700	-4.94258800	-0.50032400
H	-1.20607700	-2.93564500	-0.91837900
C	0.51292800	-5.79004800	-0.24343000
H	2.65621300	-5.92538600	-0.03760100
H	-1.58448300	-5.32404200	-0.48382300
H	0.34420200	-6.84356200	-0.03597500
C	2.96629700	-1.06640500	-1.43335100
C	3.60566900	-1.70568200	-2.51022700
C	3.73211100	-0.25010200	-0.58744500
C	4.97029000	-1.52630600	-2.73583200
H	3.04063100	-2.35976900	-3.16871300
C	5.09971700	-0.06974100	-0.81275100
H	3.24719100	0.25010700	0.24658600
C	5.72024200	-0.70615800	-1.88795200
H	5.44925400	-2.02893000	-3.57187700
H	5.67561400	0.56820200	-0.14761000
H	6.78328900	-0.56718800	-2.06553500
C	1.62318800	3.34057200	0.34963800
C	1.21126900	4.00275500	1.51980700
C	2.94596000	3.50878400	-0.08856500
C	2.09701000	4.81484200	2.22594100
H	0.19234500	3.88720200	1.87831800
C	3.83242400	4.32192600	0.62320000
H	3.29839500	3.00778100	-0.98436900
C	3.41179100	4.97685200	1.78039200
H	1.75897200	5.32087800	3.12608700
H	4.85160300	4.44474500	0.26593800
H	4.10144500	5.61000400	2.33184800
C	-1.08459500	3.21188800	-0.68855000
C	-1.02091200	4.57055900	-1.04638000
C	-2.33190100	2.59566700	-0.51136500
C	-2.19398000	5.30173200	-1.22361700
H	-0.05864500	5.05988100	-1.17252100
C	-3.50305200	3.33722100	-0.69263400
H	-2.39467900	1.54152000	-0.25072100
C	-3.43714700	4.68464600	-1.04570600
H	-2.13920000	6.35250600	-1.49638600
H	-4.45933700	2.84395100	-0.54840800
H	-4.35012900	5.25909300	-1.18127100
P	-3.09757900	-1.29341000	0.54565200
C	-4.07170600	-1.88058100	-1.92386500
H	-4.51290000	-0.87610300	-1.89503000
H	-3.13215600	-1.80969800	-2.49032400
C	-5.49076600	-0.29732500	1.16885100
H	-6.12902200	-0.92597500	0.52959300
H	-5.31404200	-0.86314200	2.09747300
O	-1.91653200	-0.61236900	-0.21439800
O	-4.25732100	-0.02616900	0.51077300
O	-3.80691600	-2.33552600	-0.59476800
C	-5.01964000	-2.86481900	-2.59541300
H	-4.58179200	-3.86915600	-2.61771300
H	-5.23233000	-2.55734700	-3.62718900
H	-5.96715500	-2.92243500	-2.04870600
C	-6.19490300	1.01463200	1.48727100
H	-7.14528000	0.82856600	2.00271500
H	-6.40948500	1.57296900	0.56859500
H	-5.56706300	1.64142100	2.12980300
Pd	0.27298600	0.14103200	0.69148300
O	-0.31331600	1.25711200	3.44287900
C	-0.03780500	0.68863100	2.46659500
C	0.62603300	-1.16005000	2.44316100
C	1.93943300	-1.25252700	2.92929700
C	-0.30758400	-2.16054400	2.74155400
C	2.32926900	-2.36791000	3.67250700
H	2.65198400	-0.45535600	2.73652700
C	0.09144600	-3.27201700	3.48774500
H	-1.33125700	-2.07834700	2.38532500
C	1.40528700	-3.37913000	3.94952900
H	3.34900800	-2.44158500	4.04221700
H	-0.63004800	-4.05458800	3.70754500
H	1.70742000	-4.24464000	4.53358300

9b

SCF energy: -2965.012568

SCF energy in solution: -2964.158859

Free energy in solution: -2963.52249838

P	5.02836600	0.81275300	-1.42640000
C	0.99947900	-1.84799000	-0.32198300
H	1.43074800	-1.23178200	0.47587700
H	1.45980600	-2.83966700	-0.22664600
C	3.25854500	0.31433200	-1.04959100
H	3.15039500	0.10039000	0.02091700
H	2.62458500	1.18177500	-1.27101300
C	1.30207000	-1.22484600	-1.69650600
H	0.70313000	-0.31391200	-1.82636500

H	0.98517900	-1.91391400	-2.48842500
C	2.78946800	-0.87457700	-1.90271800
H	3.41058500	-1.75577100	-1.69269400
H	2.94329000	-0.63495700	-2.96309400
P	-0.81335400	-1.93306600	0.11758200
C	-1.51255500	-3.30008300	-0.90205700
C	-2.89798500	-3.53790700	-0.84487100
C	-0.71278800	-4.12260100	-1.71233100
C	-3.45973000	-4.57659200	-1.58803800
H	-3.52985600	-2.91714400	-0.21414000
C	-1.28409000	-5.15698700	-2.45714400
H	0.36001700	-3.97130500	-1.76865600
C	-2.65909200	-5.38530200	-2.39762900
H	-4.53115400	-4.74960300	-1.53334000
H	-0.65094000	-5.78278000	-3.08079200
H	-3.10356000	-6.18963500	-2.97808700
C	-0.75303000	-2.62019900	1.82457000
C	-0.43700300	-3.96560600	2.06759600
C	-0.98660200	-1.76565000	2.91128200
C	-0.34408700	-4.44219500	3.37504700
H	-0.27619200	-4.64540900	1.23531600
C	-0.89003400	-2.24393100	4.21937000
H	-1.26247600	-0.73021600	2.72989800
C	-0.56781200	-3.58153800	4.45273800
H	-0.10212400	-5.48683000	3.55235000
H	-1.07947600	-1.57356400	5.05334000
H	-0.49939500	-3.95581300	5.47078500
C	5.32857300	2.13502000	-0.16364200
C	6.65567700	2.55671900	0.04102300
C	4.30711300	2.80426600	0.52901700
C	6.95299800	3.59565900	0.92040700
H	7.46492300	2.05997400	-0.48942500
C	4.60509500	3.85267400	1.40513700
H	3.26896100	2.51647400	0.39540900
C	5.92614000	4.25005200	1.60699700
H	7.98679200	3.89798100	1.06753900
H	3.79776700	4.35411400	1.93319900
H	6.15581100	5.06346300	2.29016300
C	5.94956300	-0.61849500	-0.68259300
C	5.98958500	-0.88355000	0.69683900
C	6.61917500	-1.49260800	-1.55244900
C	6.67480500	-1.99404000	1.18926700
H	5.49242200	-0.20943200	1.38942300
C	7.30266700	-2.60858400	-1.06158200
H	6.60829200	-1.29301400	-2.62132100
C	7.33157800	-2.86053800	0.31022400
H	6.69862400	-2.18374400	2.25948600
H	7.81639900	-3.27468900	-1.75006800
H	7.86699200	-3.72450100	0.69539500
P	-3.81883900	-0.03221000	0.28313200
C	-5.86156500	1.12420900	1.54181400
H	-6.59223200	0.91457100	0.75036100
H	-5.82904600	0.25970400	2.21073600
C	-4.46771300	0.85858800	-2.18157600
H	-4.99196100	1.75759200	-1.83062500
H	-3.41347700	1.12391600	-2.34092800
O	-4.15532500	-1.26943800	1.06706400
O	-4.56395300	-0.16951300	-1.18784200
O	-4.55542500	1.30111900	0.94222300
C	-6.21750200	2.39651800	2.29165300
H	-5.47645800	2.60612300	3.07009500
H	-7.19908600	2.28875200	2.76786400
H	-6.25981800	3.25708200	1.61457400
C	-5.08851200	0.33612200	-3.46709900
H	-5.04292200	1.10399500	-4.24829500
H	-6.13702900	0.06402500	-3.30762400
H	-4.55344000	-0.55200400	-3.81856500
Pd	-1.60890000	0.37717600	-0.01336600
O	-0.03412700	2.02072200	-0.33606700
C	-1.23120200	2.31458200	-0.23481700
C	-1.73471100	3.69345200	-0.32602800
C	-3.08591700	3.97630000	-0.07862600
C	-0.84559300	4.73207500	-0.66777200
C	-3.54287600	5.29103400	-0.17163600
H	-3.75192800	3.16599700	0.19983200
C	-1.31138000	6.03782100	-0.76559700
H	0.19696900	4.49449000	-0.85465900
C	-2.66110600	6.31751000	-0.51674800
H	-4.58748300	5.51541700	0.02562600
H	-0.62940600	6.83999700	-1.03370400
H	-3.02266800	7.33980000	-0.59228400

TS7b

SCF energy: -2964.977916

SCF energy in solution: -2964.14035212

Free energy in solution: -2963.50242612

P	-3.00659900	-1.10984100	-0.54046300
C	0.71773400	-2.15842900	-1.60686600
H	0.10049300	-1.59752500	-2.31757700
H	1.23658200	-2.95113700	-2.16061700
C	-2.49564500	-2.57730400	-1.61605900

H	-3.37572400	-3.18753500	-1.85376800
H	-2.13587000	-2.15899100	-2.56490200
C	-0.14600600	-2.77024200	-0.48654500
H	-0.42553100	-1.99666900	0.23759500
H	0.46104900	-3.49495900	0.06707900
C	-1.41727300	-3.47870200	-0.98616800
H	-1.14306700	-4.25189500	-1.71867400
H	-1.86032100	-4.00708500	-0.13404900
P	1.95812500	-0.94400200	-0.93504800
C	3.03270000	-1.98188300	0.14437100
C	2.64222000	-2.24594000	1.46789900
C	4.19992600	-2.57761200	-0.36155800
C	3.40969800	-3.10170000	2.26126000
H	1.75568600	-1.77767700	1.88847900
C	4.96475500	-3.42430800	0.44180400
H	4.51616500	-2.38170800	-1.38109700
C	4.57029800	-3.68958300	1.75446000
H	3.09765300	-3.30072700	3.28296900
H	5.86781800	-3.87579000	0.03943100
H	5.16645200	-4.34937400	2.37951900
C	3.04607500	-0.48045500	-2.34388800
C	4.05180100	0.47453100	-2.10826800
C	2.88772000	-0.99260900	-3.63880300
C	4.88424900	0.89604100	-3.14319100
H	4.18027300	0.88765200	-1.11065500
C	3.71821800	-0.56043400	-4.67703700
H	2.11684400	-1.72590200	-3.85145400
C	4.71745100	0.38085800	-4.43221900
H	5.65939600	1.63130600	-2.94498300
H	3.58034200	-0.96309100	-5.67684000
H	5.36193900	0.71501900	-5.24063000
C	-4.64023500	-0.66704200	-1.28816700
C	-5.60821000	-0.01939900	-0.49815800
C	-4.90765600	-0.83020000	-2.65763100
C	-6.80524800	0.43006600	-1.05392600
H	-5.42913700	0.12059500	0.56477300
C	-6.10545200	-0.37576400	-3.21507400
H	-4.18174100	-1.31501400	-3.30369200
C	-7.06007600	0.25376100	-2.41640100
H	-7.54157600	0.91829400	-0.42034800
H	-6.29059100	-0.51812000	-4.27688000
H	-7.99253900	0.60519800	-2.84994400
C	-3.49818500	-1.95515700	1.03164000
C	-4.58101600	-2.84862100	1.12007400
C	-2.72119400	-1.71118500	2.17647200
C	-4.87943400	-3.48424100	2.32463500
H	-5.20023800	-3.03747400	0.24666800
C	-3.02215300	-2.35424100	3.38171200
H	-1.87073700	-1.03263000	2.14259800
C	-4.09830900	-3.23781600	3.45865300
H	-5.72087100	-4.17069700	2.38035300
H	-2.40848500	-2.15415500	4.25574600
H	-4.33280100	-3.73338700	4.39756000
P	1.03221600	0.91708200	2.07391400
C	3.04856300	0.64582600	3.82055500
H	2.71765800	1.45528000	4.48494800
H	2.55291500	-0.27497100	4.14766100
C	1.14769600	3.51764100	2.76270400
H	2.15826100	3.44448800	3.18586700
H	1.24902500	3.78565900	1.70278200
O	0.32576300	-0.27040600	2.69328800
O	0.47902800	2.25922600	2.89347300
O	2.65240300	0.94340500	2.46858300
C	4.56119300	0.50092300	3.85560000
H	4.88278700	-0.32183300	3.20891200
H	4.89991000	0.29334400	4.87792700
H	5.04746400	1.42045100	3.51154300
C	0.33219300	4.56966900	3.49852500
H	0.83125500	5.54482700	3.44458600
H	0.21564100	4.29694000	4.55275200
H	-0.66406400	4.66287700	3.05514500
Pd	0.79672100	1.00479200	-0.28888900
O	-0.36409300	1.57592500	-3.06719000
C	0.01784800	1.53402900	-1.96083800
C	-0.42562900	2.82667900	-0.72500400
C	0.25753700	4.04149500	-0.90375000
C	-1.73940000	2.82628900	-0.23064700
C	-0.36443300	5.24553900	-0.57355600
H	1.26506100	4.04352200	-1.31221100
C	-2.35430900	4.03410300	0.10130600
H	-2.27092500	1.88627400	-0.11337400
C	-1.66881900	5.24049400	-0.06920700
H	0.16368600	6.18531000	-0.71212100
H	-3.36901200	4.03393900	0.49010300
H	-2.15439900	6.17948300	0.18316600

10b

SCF energy: -2964.999502

SCF energy in solution: -2964.16588812

Free energy in solution: -2963.52390412

P	2.86890200	-1.22103300	-0.29120500

C	-0.56197300	-2.79486200	0.00463800
H	0.16135700	-2.73553800	0.82569000
H	-1.04678800	-3.77751900	0.05541600
C	2.58326900	-3.06622500	-0.51784600
H	3.49967800	-3.56707000	-0.85386500
H	2.35334100	-3.46429000	0.47954500
C	0.14133500	-2.61580500	-1.35467400
H	0.34712200	-1.55367100	-1.52629600
H	-0.54559700	-2.92202300	-2.15148000
C	1.45281500	-3.40698000	-1.51098000
H	1.24683900	-4.48466200	-1.44153500
H	1.81993300	-3.23037300	-2.52919700
P	-1.80927800	-1.44222000	0.31514700
C	-3.09285400	-1.78615500	-0.96618000
C	-2.90578700	-1.31701900	-2.27753500
C	-4.21751100	-2.57373900	-0.67350800
C	-3.82479500	-1.64877200	-3.27520800
H	-2.06640500	-0.66958200	-2.51617100
C	-5.13701400	-2.89210600	-1.67479500
H	-4.38091900	-2.93979200	0.33499600
C	-4.94084500	-2.43409300	-2.97867800
H	-3.66847300	-1.28079200	-4.28579000
H	-6.00519900	-3.49963700	-1.43289800
H	-5.65629800	-2.68397500	-3.75778000
C	-2.63219600	-1.87408000	1.90375200
C	-3.47221500	-0.90264300	2.47820000
C	-2.43625300	-3.08633500	2.58087400
C	-4.10797100	-1.14549700	3.69494400
H	-3.62190500	0.04590600	1.96799500
C	-3.06590500	-3.32236700	3.80637100
H	-1.79270900	-3.85318700	2.16160300
C	-3.90321600	-2.35561700	4.36368100
H	-4.75601700	-0.38669900	4.12495400
H	-2.90127600	-4.26457600	4.32215300
H	-4.39162800	-2.54165900	5.31627800
C	4.41626700	-1.17701800	0.72285200
C	4.84013400	0.09051900	1.16499300
C	5.15069600	-2.30174000	1.13047500
C	5.97376600	0.22950000	1.96367100
H	4.27030900	0.97447800	0.88721300
C	6.28038600	-2.16336400	1.94232300
H	4.84907000	-3.29768000	0.82150700
C	6.69853100	-0.89904200	2.35652200
H	6.28492900	1.21867400	2.28930200
H	6.83376700	-3.04796200	2.24791700
H	7.57743600	-0.79287400	2.98693600
C	3.47008200	-0.73581000	-1.97681600
C	4.72250700	-1.12056900	-2.48389600
C	2.62284100	0.04464800	-2.78167100
C	5.11647600	-0.73999400	-3.76645600
H	5.39766600	-1.70848000	-1.86726100
C	3.01791000	0.42003900	-4.06930600
H	1.65024300	0.36646500	-2.41477400
C	4.26318800	0.03009700	-4.56261100
H	6.09056100	-1.04094300	-4.14440700
H	2.34916800	1.02341800	-4.67713000
H	4.57280900	0.32809800	-5.56114800
P	-1.45155100	1.81571800	-1.09100700
C	-3.93962300	2.06068100	-2.04230400
H	-3.77934400	3.12543000	-2.25231100
H	-3.65550800	1.49609100	-2.93655300
C	-1.93609900	4.30957400	-0.19646500
H	-3.00428200	4.37252900	-0.44183200
H	-1.84441000	3.89192600	0.81226300
O	-0.91487600	1.27057900	-2.39005400
O	-1.28629100	3.45211300	-1.14831300
O	-3.09755600	1.65543800	-0.94171300
C	-5.38461300	1.79143500	-1.65872400
H	-5.53980700	0.72528000	-1.46526400
H	-6.05379400	2.09725000	-2.47176500
H	-5.65857400	2.35140700	-0.75781800
C	-1.28020800	5.67867700	-0.26586400
H	-1.78485000	6.37274200	0.41692400
H	-1.34246000	6.08416500	-1.28135500
H	-0.22629300	5.61210600	0.01902200
Pd	-0.58228500	0.66194500	0.73817900
O	0.97893600	-0.52885400	3.17204900
C	0.39480000	-0.15067400	2.26576900
C	0.51513600	2.36951500	1.20340500
C	0.25478300	3.09362100	2.37657900
C	1.60140700	2.75976900	0.40622500
C	1.05227100	4.18632500	2.73967400
H	-0.57489100	2.81314100	3.02237500
C	2.40223700	3.84749500	0.77187900
H	1.82394900	2.22894000	-0.51512000
C	2.13076300	4.56537000	1.93938100
H	0.82890600	4.73505100	3.65213700
H	3.23454600	4.13755700	0.13419400
H	2.75295500	5.41111000	2.22118600

TS8b

SCF energy: -2964.989202

SCF energy in solution: -2964.169532

Free energy in solution: -2963.52572

P	2.02719600	-1.27578600	0.70100300
C	-1.27709100	-2.31027900	1.89996600
H	-0.66581200	-1.91068600	2.71614400
H	-2.14224400	-2.80173900	2.35783900
C	1.82699200	-2.62234100	2.01046900
H	2.81302900	-3.04010700	2.24416400
H	1.49251900	-2.10781700	2.91892300
C	-0.47701100	-3.31657400	1.03728700
H	-0.26493900	-2.89378400	0.04840700
H	-1.09687700	-4.19940500	0.84713600
C	0.85716600	-3.76267200	1.65512300
H	0.67163000	-4.34987400	2.56556100
H	1.34803300	-4.43923400	0.94557200
P	-1.86326600	-0.85233000	0.89522100
C	-3.01228000	-1.71430500	-0.26951500
C	-2.62651400	-1.97495600	-1.59235800
C	-4.24940700	-2.19573300	0.19045200
C	-3.46203900	-2.71624700	-2.43281400
H	-1.70184700	-1.56698600	-1.98929300
C	-5.08202900	-2.92965600	-0.65473600
H	-4.57030200	-1.99120300	1.20815400
C	-4.68749000	-3.19534200	-1.96844000
H	-3.15310100	-2.90534400	-3.45735300
H	-6.03871500	-3.29152200	-0.28689300
H	-5.33662900	-3.76641000	-2.62711200
C	-2.99500300	0.05151600	2.04052000
C	-3.65537800	1.19671300	1.55946600
C	-3.18312700	-0.32417100	3.37971400
C	-4.49076800	1.93393200	2.39732300
H	-3.50415500	1.50577300	0.52997200
C	-4.01572400	0.42312400	4.21781700
H	-2.68451300	-1.19799100	3.78584500
C	-4.67300600	1.55135200	3.72897200
H	-4.99613700	2.81482100	2.01015000
H	-4.14804800	0.11839900	5.25264400
H	-5.31982500	2.13188300	4.38128300
C	3.55649700	-0.46639800	1.35024200
C	4.66170000	-0.18473600	0.53354900
C	3.59084700	-0.04433200	2.69094300
C	5.77601800	0.48012500	1.04880600
H	4.65342600	-0.47885600	-0.51016600
C	4.70718600	0.61479600	3.20575500
H	2.74062400	-0.22380500	3.34385300
C	5.80646200	0.87709600	2.38583200
H	6.62091200	0.68962100	0.39813900
H	4.71490100	0.92593600	4.24725800
H	6.67585200	1.39276500	2.78479800
C	2.60205900	-2.25573300	-0.75583600
C	3.67628900	-3.15962200	-0.67312100
C	1.91345800	-2.13008400	-1.97262900
C	4.05128400	-3.92020400	-1.77997700
H	4.23084300	-3.26163400	0.25609300
C	2.29291000	-2.89321500	-3.08133800
H	1.08579900	-1.43115300	-2.06978700
C	3.35826400	-3.78828000	-2.98729500
H	4.88447600	-4.61396200	-1.70155900
H	1.75274700	-2.77750500	-4.01692900
H	3.65241100	-4.38033700	-3.85009100
P	-0.89003300	1.18139900	-1.82871900
C	-3.38899000	1.34114000	-2.73393500
H	-3.13022300	2.23967600	-3.30718300
H	-3.20248800	0.47008000	-3.36978400
C	-0.93061200	3.85151300	-1.56491300
H	-2.02086400	3.98461700	-1.55499000
H	-0.60052400	3.68529000	-0.53185900
O	-0.55659700	0.23569400	-2.95477300
O	-0.60344800	2.71144800	-2.37074200
O	-2.53712700	1.26034200	-1.56752500
C	-4.83585600	1.38430600	-2.27263400
H	-5.08736900	0.48513400	-1.70115300
H	-5.50350800	1.44008200	-3.14062900
H	-5.02247900	2.26137100	-1.64262800
C	-0.23433000	5.06636900	-2.15600100
H	-0.49281000	5.96516800	-1.58324900
H	-0.53961600	5.21834900	-3.19674100
H	0.85125700	4.93272500	-2.12816100
Pd	0.05661000	0.58552200	0.20598900
O	-0.26158400	2.26543500	2.89243600
C	0.01085600	1.45931000	2.12231800
C	1.62748900	1.79935400	-0.47101500
C	2.09209100	2.88493400	0.28876100
C	2.29728400	1.51096400	-1.67148500
C	3.19512100	3.64143800	-0.12525300
H	1.60766700	3.16578100	1.21809400
C	3.40217200	2.26322300	-2.08294500
H	1.94141700	0.71844400	-2.32037300
C	3.85875700	3.33302900	-1.31220600
H	3.53008900	4.47398000	0.48990800
H	3.89362600	2.01504900	-3.02131800
H	4.71385900	3.92167500	-1.63516200

11b

SCF energy: -2964.999270

SCF energy in solution: -2964.164909

Free energy in solution: -2963.527334

P	-3.15535400	1.02308800	0.02072600
C	0.24128300	2.72700000	0.56767700
H	-0.43039800	2.42405500	1.37896000
H	0.63631000	3.72124500	0.81131000
C	-2.94000200	2.88787400	0.19329600
H	-3.89312200	3.40073200	0.01356400
H	-2.67766300	3.07197600	1.24338800
C	-0.51098500	2.76447300	-0.77560900
H	-0.66419900	1.74195900	-1.13871400
H	0.12280500	3.25645000	-1.52162000
C	-1.86798300	3.48915600	-0.73638800
H	-1.71666600	4.54071100	-0.45313900
H	-2.26222000	3.50094700	-1.75949300
P	1.62744200	1.47833000	0.52974000
C	2.75527900	2.19885200	-0.74023200
C	2.57634200	1.87593600	-2.09537700
C	3.73838400	3.13505300	-0.38048200
C	3.36535900	2.49323800	-3.06906200
H	1.85227000	1.12086700	-2.39052900
C	4.52859600	3.74027400	-1.35907300
H	3.89350700	3.39152800	0.66300400
C	4.34132800	3.42327900	-2.70599800
H	3.21893600	2.23416300	-4.11428100
H	5.28918300	4.45953800	-1.06663200
H	4.95660600	3.89553900	-3.46742000
C	2.54228400	1.68938600	2.11202200
C	3.61085000	0.80782300	2.36042300
C	2.19800700	2.63215100	3.09143800
C	4.32156600	0.87889200	3.55738500
H	3.88145500	0.06750500	1.61147200
C	2.90701200	2.69304200	4.29492300
H	1.37821000	3.32453100	2.92724800
C	3.96893700	1.81975900	4.52937000
H	5.14670600	0.19441600	3.73461700
H	2.62747400	3.42678800	5.04618800
H	4.51866600	1.86915800	5.46531100
C	-4.78448600	0.75411100	0.85454100
C	-5.47083400	-0.44856800	0.60275800
C	-5.31680900	1.63193200	1.81213500
C	-6.65635100	-0.75109000	1.26930900
H	-5.07578700	-1.15011000	-0.12772100
C	-6.50206100	1.32459400	2.48637700
H	-4.81292500	2.56575400	2.04164400
C	-7.17782400	0.13541100	2.21589200
H	-7.17253100	-1.68269300	1.05211400
H	-6.89671700	2.02130200	3.22180800
H	-8.10017900	-0.10216900	2.73909400
C	-3.60070400	0.86573100	-1.77137300
C	-4.77789200	1.40087800	-2.32242700
C	-2.70127700	0.19759500	-2.61831400
C	-5.04531500	1.27437000	-3.68526400
H	-5.49371500	1.90706900	-1.67969600
C	-2.96804800	0.07477600	-3.98515900
H	-1.78357600	-0.22798100	-2.21889000
C	-4.13930600	0.61175900	-4.51950400
H	-5.96110500	1.69094800	-4.09745300
H	-2.25816200	-0.44439100	-4.62315700
H	-4.35007000	0.51316600	-5.58132100
P	1.74002400	-1.57449400	-1.30986500
C	4.24388400	-1.27584700	-2.20594700
H	4.29958900	-2.32197900	-2.53188600
H	3.85376700	-0.68400500	-3.04041400
C	2.61755600	-4.04532800	-0.68892700
H	3.68519500	-3.89720800	-0.89701800
H	2.43638300	-3.77920400	0.35856200
O	1.14023100	-0.97366800	-2.55458800
O	1.84871800	-3.19731000	-1.55665100
O	3.33706300	-1.16923100	-1.08713800
C	5.60498500	-0.76774300	-1.76255800
H	5.54115100	0.28039100	-1.45322900
H	6.32324000	-0.84252300	-2.58761800
H	5.98510300	-1.35709100	-0.92077000
C	2.20675900	-5.48526100	-0.94845900
H	2.80750500	-6.16497300	-0.33228000
H	2.35902200	-5.74530700	-2.00140600
H	1.15103600	-5.63103200	-0.70244500
Pd	0.67408600	-0.79917400	0.61397400
O	-1.05689300	-0.19281900	3.14581000
C	-0.43321300	-0.34951800	2.20133000
C	-0.16449200	-2.69388600	0.80934500
C	0.17721700	-3.51830000	1.89201900
C	-1.15667500	-3.13342300	-0.07833400
C	-0.44805100	-4.75760900	2.07630000
H	0.93575300	-3.20191900	2.60518600
C	-1.78613900	-4.36847100	0.10932700
H	-1.43689300	-2.52310900	-0.93242900

C	-1.43358900	-5.18594900	1.18576800
H	-0.16530200	-5.38218300	2.92100700
H	-2.54966800	-4.69268000	-0.59435400
H	-1.92312700	-6.14592000	1.32925000

12b

SCF energy: -2851.682566

SCF energy in solution: -2850.88366208

Free energy in solution: -2850.24335708

P	1.97659300	-1.27287300	0.47273400
C	-1.27236400	-2.82417600	1.30527400
H	-0.70887300	-2.71121700	2.23672600
H	-2.18111400	-3.38358900	1.55036000
C	1.79892100	-2.89453600	1.41303000
H	2.80869300	-3.27601600	1.60175100
H	1.38353500	-2.63855200	2.39414900
C	-0.42976400	-3.56830600	0.24184400
H	-0.30000600	-2.94493400	-0.65124900
H	-0.96946800	-4.45859700	-0.09922700
C	0.96008200	-3.99631600	0.74145600
H	0.85358400	-4.81529700	1.46668200
H	1.52231500	-4.40505200	-0.10604600
P	-1.75065400	-1.11028400	0.73843900
C	-3.14555300	-1.54565700	-0.39422800
C	-2.96643500	-1.48611500	-1.78374000
C	-4.36554900	-2.01330900	0.12050700
C	-3.98940200	-1.90385900	-2.64020900
H	-2.05693000	-1.06835800	-2.20531600
C	-5.38623200	-2.42125100	-0.73824000
H	-4.52530000	-2.04813000	1.19505700
C	-5.19752200	-2.37198100	-2.12224700
H	-3.84034300	-1.84616400	-3.71506800
H	-6.32839000	-2.77457800	-0.32697800
H	-5.99294400	-2.68925200	-2.79162600
C	-2.56629800	-0.38447500	2.23167200
C	-3.00326400	0.95164000	2.17625000
C	-2.73390000	-1.09754200	3.43022600
C	-3.59081600	1.55041000	3.29038500
H	-2.89283200	1.51133900	1.25323800
C	-3.31810500	-0.49109400	4.54567000
H	-2.41662200	-2.13189500	3.50848700
C	-3.74664900	0.83427300	4.47967200
H	-3.92474700	2.58294600	3.22893900
H	-3.43808200	-1.05986100	5.46414800
H	-4.19942300	1.30589900	5.34781200
C	3.43597000	-0.57082900	1.35810400
C	4.53091500	-0.02872200	0.66986200
C	3.42708700	-0.51482100	2.76187300
C	5.59815400	0.53602500	1.36969900
H	4.54617100	-0.03197500	-0.41431200
C	4.49609300	0.04836700	3.45933200
H	2.58200200	-0.90526100	3.32290000
C	5.58761400	0.57253100	2.76447300
H	6.43591100	0.95466900	0.81875300
H	4.47318700	0.07835800	4.54556400
H	6.42006400	1.01277400	3.30678400
C	2.63283900	-1.86549300	-1.14783400
C	3.77810900	-2.67797600	-1.21966900
C	1.94400000	-1.55587000	-2.33111900
C	4.22386800	-3.16784200	-2.44686400
H	4.33328900	-2.91984000	-0.31710600
C	2.39232200	-2.05063600	-3.55910900
H	1.06225400	-0.91982800	-2.30114500
C	3.52971300	-2.85569000	-3.61941400
H	5.11271900	-3.79198300	-2.48784400
H	1.84996300	-1.79692200	-4.46561500
H	3.87829800	-3.23754500	-4.57539200
P	-1.09377100	1.58694300	-1.47111800
C	-3.67583200	2.08721100	-1.94033600
H	-3.45413100	3.11453300	-2.25574200
H	-3.60976700	1.44233500	-2.82238700
C	-0.96089200	4.07675800	-0.48215500
H	-2.03936800	4.21143000	-0.32212400
H	-0.53522400	3.63601800	0.42849900
O	-0.96483500	0.98840800	-2.84892100
O	-0.75463900	3.19866200	-1.59582800
O	-2.68784500	1.66257900	-0.97665500
C	-5.04738400	1.99645100	-1.29261900
H	-5.25923800	0.96877800	-0.98094300
H	-5.82059700	2.31010900	-2.00411800
H	-5.10984300	2.64531000	-0.41173500
C	-0.28509400	5.40288600	-0.79090000
H	-0.45682300	6.11402500	0.02626400
H	-0.68560100	5.83288300	-1.71520300
H	0.79298300	5.26144700	-0.91160500
Pd	0.12820200	0.26247300	-0.00153900
C	1.60577900	1.68251300	-0.31877600
C	1.98175200	2.45637200	0.79214300
C	2.25434100	1.92231300	-1.53863000
C	2.98074500	3.43073700	0.69023000
H	1.50017900	2.29993300	1.75556800

C	3.26141500	2.88885000	-1.64075300
H	1.95432400	1.37944900	-2.42987500
C	3.62936800	3.64734200	-0.52767100
H	3.25260000	4.01615400	1.56626400
H	3.74634700	3.05734700	-2.60017500
H	4.40780200	4.40226800	-0.60905700

TS9b

SCF energy: -2851.653840

SCF energy in solution: -2850.85755851

Free energy in solution: -2850.21875251

P	2.10192200	-1.29390700	0.25147000
C	-1.15214600	-3.13382700	0.89954700
H	-0.62274800	-3.12740700	1.85914400
H	-2.02187000	-3.78884600	1.02024200
C	1.99257100	-3.01737200	1.00542100
H	3.00753800	-3.40116800	1.16378400
H	1.56660500	-2.86719400	2.00484200
C	-0.23122600	-3.64844400	-0.23457900
H	-0.13316600	-2.88812000	-1.01895100
H	-0.70097100	-4.51175600	-0.71989100
C	1.17794100	-4.06563700	0.22322400
H	1.10277100	-4.96120700	0.85678400
H	1.74790900	-4.36627600	-0.66435000
P	-1.71608600	-1.37729600	0.58954500
C	-3.04474400	-1.66072000	-0.66942000
C	-2.81441100	-1.27853500	-1.99979900
C	-4.25586400	-2.29116800	-0.33921600
C	-3.77484000	-1.54061200	-2.98224700
H	-1.90368100	-0.74738600	-2.26389100
C	-5.21406100	-2.54372900	-1.32086700
H	-4.45745100	-2.57619500	0.69027700
C	-4.97256900	-2.17270400	-2.64691700
H	-3.58429900	-1.23838900	-4.00881100
H	-6.14933600	-3.02792000	-1.05108100
H	-5.71956900	-2.37008900	-3.41164500
C	-2.66239600	-0.95947200	2.12437400
C	-3.07761400	0.37405100	2.29185800
C	-2.96346200	-1.88817700	3.13303000
C	-3.78487300	0.75988700	3.43007000
H	-2.84273500	1.10238900	1.52060800
C	-3.66302300	-1.49585500	4.27826600
H	-2.65703300	-2.92506300	3.03765900
C	-4.07729900	-0.17277000	4.42902700
H	-4.10278900	1.79359500	3.54091300
H	-3.88425000	-2.22877000	5.05009200
H	-4.62176500	0.13109600	5.31924500
C	3.49362200	-0.61896000	1.26578400
C	4.73373700	-0.23162400	0.73778800
C	3.26541100	-0.43628400	2.64155400
C	5.72493000	0.30084900	1.56622300
H	4.93143500	-0.34468800	-0.32292600
C	4.25850700	0.08562200	3.46892500
H	2.29869000	-0.69218800	3.06970900
C	5.49464900	0.45549300	2.93315500
H	6.68022900	0.59370100	1.13778800
H	4.06308500	0.21217700	4.53074100
H	6.26830600	0.86686400	3.57609800
C	2.83289500	-1.64143100	-1.40854900
C	3.93154900	-2.50155600	-1.58510200
C	2.23947500	-1.05909100	-2.54074600
C	4.42999300	-2.76654900	-2.86066500
H	4.40721300	-2.96234500	-0.72297800
C	2.74199700	-1.32655100	-3.81793000
H	1.37810900	-0.40245100	-2.43140500
C	3.83536700	-2.17750300	-3.98035500
H	5.28041300	-3.43292200	-2.98092000
H	2.27076900	-0.86748100	-4.68274500
H	4.22354900	-2.38517800	-4.97420100
P	-0.76584600	1.89285400	-1.24171200
C	-3.38379200	2.37674300	-1.54191100
H	-3.20531000	3.41510600	-1.84120900
H	-3.36288000	1.75463100	-2.44244700
C	-0.85786200	4.59675900	-0.80009300
H	-1.79113800	4.45020400	-0.23962400
H	-0.03882400	4.66632800	-0.07471600
O	-0.56305000	1.15409800	-2.54020500
O	-0.63019100	3.49112400	-1.67750800
O	-2.32404700	1.93867800	-0.65221500
C	-4.70673900	2.23343900	-0.81002800
H	-4.88021300	1.19184500	-0.52317200
H	-5.52872600	2.55534300	-1.46041000
H	-4.72388900	2.85148100	0.09467900
C	-0.92885500	5.85992800	-1.64573900
H	-1.08279300	6.73669400	-1.00566800
H	-1.75322500	5.80414400	-2.36461800
H	0.00223300	5.99670900	-2.20492200
Pd	0.08808500	0.09784700	0.09290100
C	0.96262400	2.07219800	0.01494400
C	0.82496000	2.61729000	1.30754000
C	2.11474700	2.39105800	-0.73177700

C	1.84750100	3.39290200	1.86500000
H	-0.07876700	2.42949700	1.88175300
C	3.11611000	3.18803700	-0.18157800
H	2.21606300	2.01356800	-1.74522800
C	2.99222300	3.68264300	1.12227700
H	1.73680700	3.78437900	2.87354100
H	4.00296400	3.41743800	-0.76750700
H	3.77908300	4.29894700	1.54891900

2c

SCF energy: -2638.859583

SCF energy in solution: -2638.0194170300

Free energy in solution: -2637.4065360300

P	2.61710900	-0.13305000	-0.61415100
C	0.23514300	1.95953200	-2.67827200
H	0.41723700	1.08483200	-3.31204600
H	-0.34764200	2.66181500	-3.28362900
C	2.99015500	0.39204000	-2.37249400
H	4.01203900	0.09328600	-2.63450600
H	2.31806000	-0.20061800	-3.00550300
C	1.56485800	2.59708900	-2.20329900
H	1.58888200	2.65166100	-1.10833600
H	1.60379800	3.63813500	-2.54481900
C	2.84747100	1.89589800	-2.68179200
H	2.94315400	2.01567700	-3.77028400
H	3.70129500	2.42398900	-2.23956400
P	-0.78963300	1.36235000	-1.22894200
C	-1.21338700	2.96126900	-0.40095600
C	-1.67790600	4.07806500	-1.11780600
C	-1.05238500	3.07109800	0.98728900
C	-1.96279600	5.27531900	-0.46268700
H	-1.82893400	4.01373800	-2.19222800
C	-1.34281700	4.26989300	1.64500800
H	-0.70826900	2.21063100	1.55314900
C	-1.79349400	5.37376800	0.92191100
H	-2.31866000	6.13094700	-1.03099200
H	-1.22102500	4.33219900	2.72279200
H	-2.01721900	6.30723700	1.43193200
C	-2.37712600	0.87680500	-2.04450900
C	-3.62380700	1.31001100	-1.56407300
C	-2.35265100	-0.02933500	-3.11940900
C	-4.80984200	0.86053300	-2.15000600
H	-3.66998800	2.00463700	-0.73147900
C	-3.53749600	-0.46867900	-3.71017000
H	-1.40551700	-0.41177900	-3.48754700
C	-4.77188800	-0.02597100	-3.22718400
H	-5.76433100	1.21140100	-1.76557000
H	-3.49546500	-1.15995500	-4.54830500
H	-5.69480000	-0.36926800	-3.68725700
C	3.40757200	-1.80223000	-0.50615000
C	3.35972000	-2.44959800	0.74199900
C	4.00537300	-2.46959900	-1.58550100
C	3.92384200	-3.71240100	0.90984700
H	2.85850200	-1.97051900	1.57767900
C	4.55948200	-3.74227300	-1.41739500
H	4.04152700	-2.01271100	-2.56902500
C	4.52747600	-4.36347100	-0.16973600
H	3.87867900	-4.19457900	1.88268900
H	5.01721800	-4.24389500	-2.26638300
H	4.96074200	-5.35176800	-0.03985700
C	3.78410900	0.91648400	0.36729600
C	5.17188800	0.89792600	0.15107600
C	3.26439400	1.76293000	1.35673800
C	6.01677900	1.71599500	0.90043200
H	5.59653500	0.23035900	-0.59466100
C	4.11107800	2.58169800	2.10919800
H	2.19222100	1.76864000	1.53712600
C	5.48706600	2.56111000	1.88038500
H	7.08922100	1.69100600	0.72461100
H	3.69400500	3.23063100	2.87487700
H	6.14735600	3.19569800	2.46575200
O	0.23671500	-1.72052500	1.58693700
C	-0.98211100	-1.38754900	1.37543300
C	-1.70941800	-0.44766900	2.28379200
C	-3.02093100	-0.01422300	2.02996700
C	-1.04924800	0.03279700	3.42658200
C	-3.65117300	0.88105500	2.89233400
H	-3.54214200	-0.37032300	1.14570200
C	-1.68207300	0.92986800	4.28551100
H	-0.04560900	-0.32420900	3.63267700
C	-2.98590200	1.36093400	4.02394400
H	-4.66681900	1.20629200	2.68011800
H	-1.16022800	1.28231800	5.17216800
H	-3.48119900	2.05499200	4.69784400
C	-2.62195600	-3.82325300	-1.19013700
C	-3.54031400	-4.26636800	1.05867400
C	-3.91200600	-3.98740600	-0.39336900
H	-2.79999800	-3.52930100	-2.22831100
H	-3.05675700	-5.25008400	1.14437400
H	-4.51185000	-3.07111300	-0.46281900
N	-1.85740600	-2.41770000	0.73485200

C	-2.57388100	-3.24494700	1.64322500
C	-1.68451200	-2.77126500	-0.61259700
O	-2.42286600	-3.13736500	2.84246800
O	-0.82877300	-2.26339900	-1.31906900
H	-4.40553200	-4.28795900	1.72819700
H	-4.52026600	-4.80151600	-0.80257300
H	-2.06891500	-4.77325400	-1.22052500
Pd	0.31339300	-0.23908300	0.04077600

TS1c

SCF energy: -2638.835531

SCF energy in solution: -2637.9974260000

Free energy in solution: -2637.3850890000

P	2.43905500	-0.19026500	-1.04871500
C	0.43758200	2.54495300	-2.15547700
H	0.48099500	1.71622500	-2.86871500
H	-0.02324500	3.38475100	-2.68609700
C	2.95394900	0.76187400	-2.58672600
H	3.92113100	0.38951200	-2.94413900
H	2.22438200	0.46922000	-3.35177000
C	1.84634700	2.91361900	-1.63691300
H	1.95595800	2.60524300	-0.58953600
H	1.95753300	4.00361000	-1.63179200
C	3.00429100	2.29533700	-2.43924600
H	3.03994500	2.73426700	-3.44612100
H	3.94368100	2.57575600	-1.94740300
P	-0.69983400	1.97901600	-0.77915400
C	-0.86345200	3.55101100	0.17991700
C	-1.23390500	4.75214200	-0.45282500
C	-0.53943500	3.57556400	1.54436800
C	-1.28385100	5.94693500	0.26313300
H	-1.49527600	4.75672000	-1.50761800
C	-0.58817200	4.77749000	2.25825600
H	-0.26820000	2.65588500	2.05331200
C	-0.95869000	5.96174600	1.62281100
H	-1.57489000	6.86574900	-0.23953800
H	-0.33696500	4.77999400	3.31557600
H	-0.99582900	6.89390300	2.18068400
C	-2.29582400	1.81022200	-1.69557800
C	-3.46310300	2.50013600	-1.34180100
C	-2.34725100	0.91275600	-2.77699400
C	-4.64327300	2.31614600	-2.06627100
H	-3.45995400	3.17459100	-0.49283600
C	-3.52327600	0.73550900	-3.50353700
H	-1.46552900	0.33657900	-3.04694400
C	-4.67666200	1.44190000	-3.15209200
H	-5.53915700	2.85723100	-1.77361500
H	-3.54044800	0.04227400	-4.34067500
H	-5.59540700	1.30306800	-3.71573800
C	2.76252300	-1.90872700	-1.64667900
C	3.85016100	-2.69298300	-1.23929900
C	1.83856000	-2.45845900	-2.55150400
C	4.01796300	-3.98753800	-1.73771800
H	4.56816800	-2.29896000	-0.52730900
C	2.01253300	-3.74590000	-3.05744600
H	0.96475100	-1.88233600	-2.84814700
C	3.10530300	-4.51591600	-2.65121100
H	4.86642300	-4.58247100	-1.40900400
H	1.28826900	-4.15229400	-3.75880600
H	3.23895400	-5.52244700	-3.03869600
C	3.79572300	0.17949000	0.14740700
C	5.14141600	0.32331800	-0.23266800
C	3.45636400	0.35338300	1.49962000
C	6.12081100	0.62805000	0.71369200
H	5.43417800	0.19219200	-1.27096300
C	4.43777000	0.65603500	2.44648300
H	2.41798600	0.26127500	1.80991900
C	5.77033100	0.79422600	2.05603300
H	7.15660100	0.73668800	0.40241600
H	4.15510100	0.78873800	3.48725100
H	6.53337300	1.03399100	2.79190000
O	-0.48199400	0.60494800	2.74942200
C	-1.11103800	0.00782700	1.87459400
C	-2.59117700	0.16698700	1.64706500
C	-3.29641600	-0.63604800	0.74297700
C	-3.27174800	1.16283700	2.35824900
C	-4.66745100	-0.46326500	0.56995700
H	-2.76383500	-1.40388500	0.18875400
C	-4.64392800	1.34129100	2.17674400
H	-2.72030100	1.76580000	3.07151800
C	-5.34693000	0.52627400	1.28759400
H	-5.20780100	-1.09719500	-0.12839900
H	-5.16684900	2.10723500	2.74449900
H	-6.41764600	0.65879200	1.15375500
C	0.36104000	-3.95767500	2.08066500
C	-1.30865500	-3.73917700	3.91095000
C	-0.78766600	-4.65797800	2.80695600
H	0.68669300	-4.49109900	1.18297500
H	-0.54198700	-3.61620600	4.69062500
H	-1.59438800	-4.87828300	2.09535800
N	-0.98819800	-1.86689400	2.26831200

C	-1.66216400	-2.33864100	3.40165200
C	-0.00658700	-2.54244000	1.66697700
O	-2.48649000	-1.65631300	3.98186400
O	0.66088600	-2.02146300	0.73394600
H	-2.20154300	-4.13260400	4.40435000
H	-0.45505000	-5.61743700	3.21877500
H	1.23920900	-3.88240800	2.73873400
Pd	0.16362400	0.01899400	0.18335700

3c

SCF energy: -2638.856499

SCF energy in solution: -2638.01672273

Free energy in solution: -2637.4056747300

P	2.00758800	-1.08902900	0.67704000
C	-1.11889600	-2.02812900	2.29359200
H	-0.58739100	-1.30445000	2.91908000
H	-1.97833300	-2.37214800	2.87840100
C	1.99212300	-1.89438900	2.37799300
H	3.02919700	-2.06446500	2.68924700
H	1.61297900	-1.10954700	3.04396700
C	-0.20181300	-3.20571400	1.88674600
H	-0.05806400	-3.22123600	0.79906500
H	-0.70085100	-4.15153300	2.12506400
C	1.18220600	-3.19266900	2.55157400
H	1.07962800	-3.38222800	3.62921300
H	1.75801200	-4.03238200	2.14538200
P	-1.74972500	-1.09535200	0.80717800
C	-2.76088900	-2.39892100	-0.01538200
C	-3.78691600	-3.06540300	0.67962200
C	-2.45454400	-2.79930500	-1.32397300
C	-4.49207900	-4.10469800	0.07573400
H	-4.04497100	-2.76681400	1.69219500
C	-3.16316100	-3.84390300	-1.92528700
H	-1.68167300	-2.28032300	-1.87998700
C	-4.17923000	-4.49724500	-1.22935300
H	-5.28440800	-4.60876100	0.62285200
H	-2.91853600	-4.13987300	-2.94167700
H	-4.72926700	-5.30841500	-1.69910300
C	-2.95994900	0.07292200	1.55867600
C	-4.28421300	0.18100600	1.10999500
C	-2.51490200	0.93805800	2.57307000
C	-5.14977500	1.11664400	1.68040600
H	-4.64381600	-0.46210600	0.31344300
C	-3.38265600	1.86771300	3.14398900
H	-1.48057400	0.90882200	2.90493200
C	-4.70458600	1.95698500	2.70113100
H	-6.17264800	1.18879400	1.32066700
H	-3.02054200	2.52960700	3.92572800
H	-5.37968200	2.68474100	3.14308500
C	3.42266600	0.06911600	0.95170200
C	4.68077500	-0.10802800	0.35836000
C	3.22820400	1.15633300	1.82031300
C	5.72807100	0.77239800	0.64288800
H	4.84940900	-0.93230500	-0.32679000
C	4.27910300	2.02565500	2.11283400
H	2.24702000	1.35740800	2.23854900
C	5.53307100	1.83513200	1.52620000
H	6.69664700	0.62290000	0.17267500
H	4.10547200	2.86428900	2.78127900
H	6.34984300	2.51656400	1.74979800
C	2.68846600	-2.39378000	-0.43521900
C	3.58069300	-3.38398700	0.00964000
C	2.29997100	-2.39116900	-1.78575100
C	4.06231000	-4.35521800	-0.86934800
H	3.91298800	-3.39596900	1.04368400
C	2.78869500	-3.36012900	-2.66504000
H	1.62304800	-1.62327600	-2.14936500
C	3.66525700	-4.34572500	-2.20854800
H	4.74907800	-5.11647000	-0.50852700
H	2.48073400	-3.34195400	-3.70693500
H	4.04054500	-5.10222600	-2.89268000
O	-1.51352800	-0.13558600	-2.76511600
C	-1.41123500	0.56162400	-1.77423000
C	-2.14071100	1.86681700	-1.66378400
C	-1.97933900	2.72590100	-0.56905700
C	-3.01932800	2.22280600	-2.70379600
C	-2.68563600	3.92875900	-0.51622700
H	-1.27918200	2.46560500	0.21604200
C	-3.72478200	3.42024100	-2.64480700
H	-3.12965800	1.54650600	-3.54559500
C	-3.55788700	4.27594600	-1.54941300
H	-2.54722800	4.59263300	0.33241600
H	-4.40240800	3.69175300	-3.45037900
H	-4.10779700	5.21295500	-1.50503600
C	2.51021100	3.00419700	-2.08809100
C	2.10027400	4.77290300	-0.37110100
C	3.15803400	4.12396100	-1.26878700
H	3.24923100	2.37330400	-2.59158000
H	1.35042800	5.28671200	-0.99179800
H	3.95723200	3.70374400	-0.64476300
N	1.13579500	2.47534000	-0.05123000

C	1.36784500	3.72894900	0.47959500
C	1.62354500	2.11592500	-1.22723200
O	0.97100800	4.01786900	1.60676900
O	1.34284900	0.96382900	-1.70983000
H	2.52430300	5.51992800	0.30580600
H	3.62312400	4.86521500	-1.92969400
H	1.87118400	3.42708700	-2.87757900
Pd	-0.05430800	-0.09135000	-0.40235000

4c

SCF energy: -2638.872183

SCF energy in solution: -2638.03425282

Free energy in solution: -2637.4216598200

P	-1.97379000	0.65131500	0.95891100
C	1.18179800	2.27464500	2.18906300
H	1.00469200	1.54678500	2.98846200
H	2.04450100	2.87187100	2.50262200
C	-1.80184200	1.34808400	2.69847700
H	-2.76737900	1.26633800	3.21019000
H	-1.12716800	0.65139300	3.21047300
C	-0.06442700	3.16416500	1.96881600
H	-0.36361400	3.15710400	0.91414800
H	0.20087200	4.20571900	2.18326200
C	-1.27928000	2.79202900	2.83116100
H	-1.04068000	2.96195500	3.89073100
H	-2.08797700	3.48831100	2.58393900
P	1.66876300	1.31290700	0.66465300
C	2.02539200	2.65129600	-0.55021600
C	2.86800700	3.72742400	-0.22036300
C	1.43139700	2.61209800	-1.82024600
C	3.10099300	4.74980300	-1.13814700
H	3.35412900	3.76446800	0.75112800
C	1.66987100	3.63871100	-2.73864500
H	0.80893600	1.76827100	-2.09872500
C	2.49861800	4.70752200	-2.39946800
H	3.75332200	5.57720600	-0.87146100
H	1.20927700	3.59340200	-3.72155100
H	2.68223100	5.50440500	-3.11545000
C	3.33632800	0.67778500	1.13438600
C	4.39267300	0.67439700	0.21045400
C	3.55033000	0.12248900	2.40640000
C	5.63555800	0.14331500	0.55788800
H	4.24410400	1.08326200	-0.78382200
C	4.79466600	-0.40475600	2.75224400
H	2.74542800	0.09032900	3.13539400
C	5.84188800	-0.39408800	1.82923000
H	6.44222300	0.14829200	-0.17015700
H	4.94310100	-0.82670700	3.74270100
H	6.81029700	-0.80745000	2.09749100
C	-3.28770500	-0.61955200	1.24290800
C	-4.44301000	-0.67284700	0.44831100
C	-3.12213100	-1.57575200	2.25796200
C	-5.41732400	-1.64781300	0.67602200
H	-4.58822000	0.05002400	-0.34773300
C	-4.10074700	-2.54223500	2.48959300
H	-2.21673400	-1.58832400	2.85590700
C	-5.25253100	-2.58089300	1.70100900
H	-6.30840000	-1.67044400	0.05382300
H	-3.95403300	-3.27360400	3.27971700
H	-6.01314800	-3.33605300	1.88098600
C	-2.87345800	1.96572800	0.02940000
C	-3.86623200	2.76133700	0.62842000
C	-2.57307800	2.15753900	-1.32821000
C	-4.52367500	3.74728900	-0.10653000
H	-4.14020500	2.60376700	1.66808700
C	-3.24136700	3.14155300	-2.06334500
H	-1.85054900	1.50837200	-1.81563800
C	-4.20733600	3.94250300	-1.45423700
H	-5.28590200	4.35837300	0.37000000
H	-3.00541500	3.27404000	-3.11572200
H	-4.72109500	4.71019600	-2.02710300
O	1.87556200	-0.51940100	-2.31137800
C	1.63704100	-1.04024100	-1.23896600
C	2.38494300	-2.27206000	-0.80709700
C	2.21157000	-2.84542900	0.45739200
C	3.30304000	-2.84201300	-1.70722500
C	2.94614100	-3.97609400	0.81939600
H	1.47558800	-2.42474700	1.13302700
C	4.03045200	-3.97141100	-1.34583200
H	3.42669500	-2.38076500	-2.68212100
C	3.85391700	-4.53952400	-0.07855800
H	2.80028000	-4.42187300	1.79970600
H	4.73523000	-4.41182900	-2.04686100
H	4.42187500	-5.42268400	0.20417100
C	-2.23661400	-2.77257400	-2.95030600
C	-1.91616200	-4.16666200	-0.90822100
C	-2.91756700	-3.74063600	-1.98174500
H	-2.93152000	-2.34557400	-3.67871300
H	-1.13481100	-4.80093700	-1.35373400
H	-3.77408800	-3.24516000	-1.50647200
N	-1.03490900	-1.82463200	-0.97274100

C	-1.20579600	-2.98317200	-0.25317500
C	-1.55988100	-1.61098700	-2.22620600
O	-0.77837600	-3.08710100	0.89932800
O	-1.47490300	-0.50786400	-2.77128400
H	-2.38145000	-4.74968900	-0.10868100
H	-3.30913700	-4.61430800	-2.51649600
H	-1.45732900	-3.30000400	-3.52098300
Pd	0.11675600	-0.24229400	-0.11136700

TS2c

SCF energy: -2638.807877

SCF energy in solution: -2637.9711702200

Free energy in solution: -2637.3605342200

P	1.51251800	0.55109400	-1.21360000
C	-2.00047500	0.30582400	-2.77524700
H	-1.59166900	-0.58844600	-3.25929500
H	-3.02068300	0.41073100	-3.16095900
C	1.15727100	0.27772000	-3.05015200
H	2.11110700	0.27990600	-3.58878900
H	0.76042400	-0.74165600	-3.12373200
C	-1.14485700	1.55275600	-3.09397100
H	-0.98402400	2.15024600	-2.19130800
H	-1.70973200	2.20383300	-3.77288600
C	0.21112400	1.26628800	-3.75668300
H	0.03663800	0.87541600	-4.76956000
H	0.72933800	2.22349700	-3.88288600
P	-2.13253000	-0.11972600	-0.95995800
C	-3.11697800	1.26315500	-0.24367200
C	-3.72958200	2.25608800	-1.02567800
C	-3.27443000	1.30067100	1.15266600
C	-4.47686600	3.27097000	-0.42460800
H	-3.63403300	2.25033100	-2.10602100
C	-4.03550300	2.30990400	1.74550300
H	-2.80955300	0.53925500	1.77521000
C	-4.63239700	3.29989000	0.96216500
H	-4.93946600	4.03550000	-1.04336100
H	-4.15582300	2.32027600	2.82550200
H	-5.21696500	4.08879900	1.42836000
C	-3.34302800	-1.51559200	-1.07177900
C	-4.68368400	-1.39308000	-0.68226700
C	-2.90481000	-2.73706900	-1.60920700
C	-5.56360200	-2.46850100	-0.82827100
H	-5.04414700	-0.46159800	-0.25926200
C	-3.78649700	-3.80521600	-1.76555000
H	-1.86242500	-2.85939200	-1.89500900
C	-5.12036500	-3.67391600	-1.37202200
H	-6.59796600	-2.35974600	-0.51317400
H	-3.42872700	-4.74335000	-2.18135500
H	-5.80658300	-4.50914800	-1.48242300
C	3.28261200	0.02131700	-1.13558800
C	4.20240900	0.68074500	-0.30382500
C	3.72724700	-1.06922300	-1.90108300
C	5.53606800	0.27143000	-0.26577900
H	3.86874500	1.49385600	0.32752700
C	5.06093800	-1.47805400	-1.85499400
H	3.03641600	-1.61481900	-2.53626600
C	5.97204400	-0.80402800	-1.04162700
H	6.23559700	0.79727300	0.37900000
H	5.38425600	-2.32369900	-2.45651900
H	7.01219400	-1.11799600	-1.00868400
C	1.59070000	2.38943200	-1.09629800
C	2.48846400	3.13063300	-1.88059600
C	0.70419800	3.07040300	-0.25097600
C	2.49366000	4.52539700	-1.82557600
H	3.19610700	2.61985600	-2.52828000
C	0.70593600	4.46563800	-0.20143900
H	0.02567300	2.50296900	0.37782300
C	1.59958200	5.19537900	-0.98749500
H	3.19702700	5.08670300	-2.43520800
H	0.01417100	4.98043300	0.45998800
H	1.60373800	6.28143100	-0.94404800
O	-1.29277300	-3.24203100	1.38332700
C	-0.69166100	-2.35213100	0.95061300
C	1.27338600	-2.45576800	0.64573800
C	1.56669400	-3.42616000	-0.32311900
C	2.09573700	-2.32463900	1.77038700
C	2.69993800	-4.23074000	-0.18765400
H	0.90584700	-3.56653900	-1.17463200
C	3.22877900	-3.13072900	1.90025800
H	1.84927900	-1.59121300	2.52933100
C	3.53358200	-4.08116200	0.92288200
H	2.92479400	-4.97950800	-0.94348100
H	3.87295000	-3.01637000	2.76844000
H	4.41345300	-4.70987200	1.03132000
C	-0.51981800	0.55480000	4.77471900
C	1.52667400	1.72835200	4.02694600
C	0.23520300	1.88115700	4.82577000
H	-1.51038500	0.60842000	5.23511000
H	2.21619300	1.05452300	4.55811400
H	-0.38284900	2.67500500	4.38373400
N	0.18965400	0.37905300	2.36110700

C	1.29639600	1.13441700	2.63043800
C	-0.71004200	0.05243400	3.33810700
O	2.15578700	1.34906300	1.76532700
O	-1.69075800	-0.66768500	3.09870600
H	2.05901400	2.67461100	3.89223600
H	0.44298400	2.17973700	5.86049700
H	0.04223000	-0.21551700	5.32449100
Pd	-0.07332300	-0.76359100	0.13154300

TS3c

SCF energy: -3364.976436

SCF energy in solution: -3364.0415340500

Free energy in solution: -3363.2837760500

P	-1.43108800	1.55061600	1.14992900
C	2.01684400	2.33026300	1.90894500
H	1.61599900	1.63898400	2.65520600
H	3.00671400	2.64827200	2.25321800
C	-0.96647900	2.37834800	2.76621700
H	-1.88391000	2.61452500	3.31750800
H	-0.45063200	1.59084500	3.32464200
C	1.08392700	3.54228000	1.67887600
H	0.67068600	3.52486900	0.66298600
H	1.67085900	4.46646300	1.73094200
C	-0.08499900	3.63683300	2.66963400
H	0.29801500	3.85291500	3.67672100
H	-0.70275000	4.49625000	2.38207100
P	2.23617700	1.30210400	0.37450900
C	2.87614500	2.54310500	-0.83572000
C	4.01618100	3.31148800	-0.53807700
C	2.19172700	2.78145000	-2.03541600
C	4.45746200	4.29607000	-1.42008400
H	4.56779500	3.13544200	0.38152000
C	2.63777000	3.76917600	-2.91920100
H	1.32472800	2.18026500	-2.28628900
C	3.76657100	4.52803200	-2.61353500
H	5.33991000	4.88230500	-1.17710400
H	2.09996500	3.93871400	-3.84810000
H	4.11168300	5.29582000	-3.30114100
C	3.71965600	0.28607500	0.78289900
C	4.75092500	0.08871100	-0.14859000
C	3.80688300	-0.33772400	2.03990900
C	5.85523800	-0.70104800	0.17411500
H	4.69763200	0.55523200	-1.12724500
C	4.91700400	-1.12182700	2.35773100
H	3.00019700	-0.23418500	2.76009400
C	5.94415600	-1.30463400	1.42944000
H	6.64563400	-0.84292100	-0.55821900
H	4.97616800	-1.59195800	3.33614400
H	6.80678900	-1.91604300	1.68135400
C	-2.91400200	0.59269700	1.70692700
C	-4.11282300	0.60214600	0.97765100
C	-2.84586200	-0.18065900	2.87874700
C	-5.21670100	-0.13658600	1.41248300
H	-4.19055400	1.18729400	0.06797200
C	-3.95159100	-0.91261700	3.31246200
H	-1.92806600	-0.20934600	3.45537600
C	-5.14149700	-0.89538000	2.58086300
H	-6.13992700	-0.10738200	0.83865900
H	-3.88264700	-1.49617500	4.22718900
H	-6.00222600	-1.46468600	2.92203300
C	-2.18933600	2.90826200	0.15000300
C	-2.98308300	3.91320300	0.72960200
C	-1.97359900	2.93413000	-1.23642900
C	-3.53258800	4.92699400	-0.05513700
H	-3.18250700	3.90183600	1.79777400
C	-2.53104500	3.94603300	-2.02281700
H	-1.38504900	2.14742000	-1.69855000
C	-3.30569900	4.94588200	-1.43416600
H	-4.14056300	5.69963700	0.40859600
H	-2.35946900	3.94794100	-3.09598800
H	-3.73556000	5.73523000	-2.04543600
O	1.10648600	-0.14142200	-2.81823100
C	1.29639700	-0.65613200	-1.73281800
C	2.11226500	-1.91188800	-1.62102300
C	2.29264700	-2.58248000	-0.40694400
C	2.71727700	-2.41344000	-2.78838300
C	3.06511900	-3.74367900	-0.35890600
H	1.81372900	-2.19268200	0.48369000
C	3.48679900	-3.57164700	-2.73682700
H	2.57094100	-1.87819000	-3.72125100
C	3.66132400	-4.23973900	-1.51946500
H	3.20436200	-4.25967500	0.58726000
H	3.95316000	-3.95492800	-3.64096200
H	4.26387700	-5.14380000	-1.47801800
C	-0.59899700	-4.17395800	2.32164300
C	0.46751600	-2.69791700	4.00371400
C	-0.61865600	-3.75045400	3.78830600
H	-1.44377500	-4.81545700	2.05403800
H	1.46039400	-3.16002800	3.88792200
H	-1.60010800	-3.32163700	4.03400500
N	-0.11576000	-1.76232500	1.73702400

C	0.37016700	-1.55135000	2.98777500
C	-0.60188700	-2.97848900	1.35918600
O	0.77033700	-0.42681600	3.35532700
O	-1.03959600	-3.17472100	0.21214500
H	0.43955600	-2.25793500	5.00480800
H	-0.47415200	-4.61134000	4.45258500
H	0.31322800	-4.75395300	2.11181800
Pd	0.27462300	0.21417600	-0.21088100
P	-2.63300800	-1.47390500	-1.51395300
H	-3.04820200	-2.05579900	-0.31999400
C	-1.06258700	-3.18763400	-2.88998300
H	-0.48985600	-2.37648800	-3.34665400
H	-0.57313100	-3.50549700	-1.96917000
C	-5.15340300	-1.61196500	-2.32459600
H	-4.93065500	-2.37099300	-3.08175500
H	-5.41695300	-2.12414300	-1.38859500
O	-1.57577500	-0.41851200	-1.40933200
O	-3.97724100	-0.80344600	-2.11166300
O	-2.38231900	-2.66866500	-2.54790900
C	-1.26402100	-4.33967400	-3.85533800
H	-1.84700300	-5.14120900	-3.39001900
H	-0.28781500	-4.74593200	-4.14358800
H	-1.78343300	-4.01074600	-4.76178200
C	-6.27830800	-0.69706700	-2.77479000
H	-7.18758100	-1.28170400	-2.95450300
H	-6.00648700	-0.18203700	-3.70144000
H	-6.49476500	0.05807200	-2.01224900

5c

SCF energy: -3364.980548

SCF energy in solution: -3364.0409706300

Free energy in solution: -3363.2867386300

P	-1.50575600	1.74751300	0.76398800
C	1.94665600	2.20016500	1.95992500
H	1.53749300	1.37886600	2.55748500
H	2.93746200	2.42837400	2.36718600
C	-1.12398500	2.11435400	2.56440800
H	-2.07427100	2.23792500	3.09599800
H	-0.67670000	1.17964000	2.92628600
C	1.03174600	3.44715300	1.97714100
H	0.69579800	3.70286700	0.96450400
H	1.61356800	4.31489600	2.30897500
C	-0.20134100	3.30727100	2.87772400
H	0.11716300	3.20945500	3.92457600
H	-0.77110100	4.24189200	2.81492400
P	2.18412400	1.50505700	0.25736100
C	2.82265100	2.93590400	-0.71442800
C	3.86634800	3.73024900	-0.20710500
C	2.26220000	3.26195400	-1.95710500
C	4.32941500	4.83223100	-0.92354100
H	4.32549400	3.48581300	0.74694200
C	2.73161100	4.36582400	-2.67500200
H	1.48077000	2.63621800	-2.37362200
C	3.75991700	5.15367400	-2.15937900
H	5.13490700	5.43923400	-0.51875300
H	2.29209100	4.60351500	-3.63989100
H	4.12217500	6.01290300	-2.71769500
C	3.65449600	0.41567100	0.45890200
C	4.66081800	0.37732200	-0.51905800
C	3.76278100	-0.41045500	1.59079900
C	5.76460400	-0.46190500	-0.36287300
H	4.58713400	1.00530300	-1.40178500
C	4.87422000	-1.24162500	1.74153300
H	2.97920300	-0.42306500	2.34423000
C	5.87639000	-1.27000600	0.76986400
H	6.53742200	-0.48021100	-1.12678200
H	4.95299600	-1.87125100	2.62407900
H	6.73842900	-1.92047100	0.89281600
C	-3.09899900	0.83235300	0.98455200
C	-4.34731100	1.37015800	0.63704700
C	-3.04176900	-0.44075100	1.57517500
C	-5.51965200	0.65785600	0.89916400
H	-4.41359800	2.34591200	0.16806400
C	-4.21813800	-1.15017200	1.82924000
H	-2.07984600	-0.89112800	1.82135100
C	-5.45985200	-0.60138500	1.50046000
H	-6.48079100	1.09293800	0.63584300
H	-4.15208200	-2.13866000	2.27587200
H	-6.37473600	-1.15096900	1.70845100
C	-2.02848400	3.34574800	0.00880600
C	-2.67511900	4.36090100	0.73387600
C	-1.79076000	3.54297900	-1.36113800
C	-3.05725100	5.54875400	0.10857600
H	-2.89536500	4.22108500	1.78821800
C	-2.18132700	4.72795700	-1.98839100
H	-1.30379100	2.75963600	-1.93660300
C	-2.80906700	5.73504100	-1.25352000
H	-3.55271000	6.32625200	0.68421400
H	-1.99284700	4.86257500	-3.05009200
H	-3.10751600	6.66012100	-1.73955600
O	1.65606100	0.30244000	-3.05385500

C	1.45873100	-0.30277300	-2.02023600
C	1.92554700	-1.71460700	-1.82853500
C	1.69914900	-2.40694000	-0.63268700
C	2.60745000	-2.34463300	-2.88498000
C	2.15591900	-3.71923200	-0.49472700
H	1.15335300	-1.93328700	0.18067800
C	3.05879600	-3.65329000	-2.74241000
H	2.77033400	-1.78932800	-3.80340500
C	2.83471600	-4.34207100	-1.54368000
H	1.97580400	-4.25393200	0.43351600
H	3.58591000	-4.13883600	-3.55977000
H	3.18966300	-5.36357900	-1.43109200
C	-0.41501800	-4.49592300	3.02259700
C	0.92517100	-2.80628700	4.25906400
C	-0.08948600	-3.93979900	4.40891200
H	-1.23218200	-5.22317400	3.03852600
H	1.89757600	-3.21687800	3.94451900
H	-1.00703400	-3.55141600	4.87222200
N	-0.31087700	-2.12401400	2.17112300
C	0.49715100	-1.77590600	3.20359600
C	-0.79565600	-3.38647100	2.03195300
O	0.93987900	-0.61443900	3.32398600
O	-1.55277900	-3.69144700	1.08825200
H	1.10053000	-2.26999900	5.19643700
H	0.29068700	-4.72641800	5.07249000
H	0.46456600	-5.02028700	2.61700000
Pd	0.26339900	0.57261200	-0.62698400
P	-2.18690100	-1.68474500	-1.60324300
H	-2.10340500	-2.30855600	-0.34737500
C	-1.02704900	-3.96853300	-2.39228300
H	-0.03258400	-3.66598900	-2.72873600
H	-0.99868400	-4.15509700	-1.31370200
C	-4.76986800	-2.21517200	-1.96900800
H	-4.49167000	-3.02810100	-2.64687000
H	-4.90951700	-2.62384400	-0.96134700
O	-1.30494000	-0.47101300	-1.76265400
O	-3.69276000	-1.24663400	-1.93140100
O	-1.94270400	-2.86664600	-2.66710700
C	-1.52034300	-5.18458000	-3.15391400
H	-2.50896700	-5.49588200	-2.80055200
H	-0.82407800	-6.01773800	-3.00544300
H	-1.58288300	-4.97330500	-4.22644400
C	-6.01896000	-1.49824700	-2.44641200
H	-6.85786600	-2.20234000	-2.48882300
H	-5.86419100	-1.07987400	-3.44593000
H	-6.27799100	-0.68471000	-1.76277400

6c

SCF energy: -3364.978443

SCF energy in solution: -3364.0384128200

Free energy in solution: -3363.2822138200

P	-0.66794300	2.35006100	-0.91316100
C	-2.93493500	-0.11000300	-2.29826800
H	-1.98968000	-0.10864500	-2.84984800
H	-3.61705600	-0.76769800	-2.84713100
C	-1.27981900	2.51204200	-2.68212600
H	-0.90276000	3.45802800	-3.08787400
H	-0.72612500	1.72566800	-3.20968600
C	-3.52014900	1.31379400	-2.14731900
H	-3.51925000	1.61998800	-1.09364700
H	-4.57611900	1.30081900	-2.43894700
C	-2.79003200	2.39269400	-2.95651400
H	-2.92399000	2.20951600	-4.03160500
H	-3.27602300	3.35239300	-2.74583100
P	-2.56998200	-0.88819500	-0.64684900
C	-4.20225200	-0.77806600	0.20008100
C	-5.36605500	-1.26518100	-0.42251200
C	-4.31088400	-0.14416000	1.44614600
C	-6.60947600	-1.12086300	0.19020900
H	-5.30204200	-1.76747100	-1.38405700
C	-5.56020400	-0.00122600	2.05716400
H	-3.41952700	0.21610800	1.94785400
C	-6.70831600	-0.48617700	1.43222600
H	-7.50066500	-1.50269800	-0.30074600
H	-5.62918100	0.48753700	3.02500100
H	-7.67843800	-0.37384000	1.90904900
C	-2.35752600	-2.66562900	-1.07086700
C	-3.09081300	-3.67714200	-0.43208700
C	-1.40813600	-3.01592600	-2.04702400
C	-2.89958200	-5.01501000	-0.78265000
H	-3.81388400	-3.42646500	0.33719400
C	-1.23080800	-4.35462700	-2.39728600
H	-0.76665000	-2.26453900	-2.49999800
C	-1.97665600	-5.35615400	-1.77198100
H	-3.47438400	-5.78832300	-0.27997600
H	-0.49455100	-4.61235700	-3.15391200
H	-1.83159700	-6.39771800	-2.04651900
C	1.05618500	2.93913600	-1.19879600
C	1.45458800	4.26750800	-0.99130900
C	1.97154000	2.01723400	-1.72878700
C	2.74578500	4.67312500	-1.33244700

H	0.76175500	4.98714800	-0.56681800
C	3.26181700	2.42974400	-2.06753700
H	1.68443900	0.97806500	-1.87135300
C	3.64907000	3.75779600	-1.87832600
H	3.04478500	5.70577100	-1.17085800
H	3.96289300	1.70220100	-2.46559300
H	4.65241100	4.07790300	-2.14832400
C	-1.47839100	3.71032200	0.02813400
C	-2.03257500	4.84951700	-0.57801600
C	-1.53276100	3.59481500	1.42856000
C	-2.63865100	5.84252500	0.19462200
H	-1.98713500	4.97430700	-1.65577100
C	-2.13225600	4.59246400	2.19877100
H	-1.09124100	2.72858800	1.91377800
C	-2.69150000	5.71466700	1.58385600
H	-3.06611300	6.71643200	-0.29006700
H	-2.16189400	4.48968100	3.28011500
H	-3.16363700	6.48785300	2.18414800
O	-1.56503800	-0.99578100	2.84039200
C	-0.90500700	-1.25617600	1.85579400
C	-0.06985500	-2.49427100	1.76280600
C	0.72562400	-2.76454700	0.64231400
C	-0.09773400	-3.40078100	2.83874200
C	1.48506500	-3.93578000	0.59810500
H	0.75800200	-2.06733500	-0.19068700
C	0.65549300	-4.56889700	2.78545800
H	-0.71470400	-3.16741600	3.70071200
C	1.44711200	-4.83870700	1.66152800
H	2.10858000	-4.13469900	-0.26818600
H	0.63087900	-5.27006100	3.61570600
H	2.03648900	-5.75142200	1.62082100
C	5.23464600	-2.21847500	-2.22451400
C	3.09510400	-2.33214900	-3.49395000
C	4.59684400	-2.06075100	-3.60535800
H	6.28240200	-1.90380200	-2.20390200
H	2.92657600	-3.39789000	-3.27285300
H	4.75562500	-1.03571300	-3.96866600
N	3.16359300	-1.13035600	-1.28707100
C	2.44651800	-1.51276700	-2.36975800
C	4.48614900	-1.42661800	-1.14300600
O	1.23459900	-1.22135600	-2.47923100
O	5.11511900	-1.08340700	-0.12663200
H	2.55776800	-2.11513600	-4.42225100
H	5.06584100	-2.73016900	-4.33711300
H	5.21996600	-3.27829000	-1.92635300
Pd	-0.82659100	0.18290700	0.42142700
P	2.29756300	0.58607800	1.58678500
H	2.71497900	-0.12194100	0.43797300
C	3.47397200	-1.52776600	2.78630100
H	2.77318300	-2.36468100	2.74077800
H	4.07876000	-1.51340300	1.87396300
C	4.60553400	1.83911400	1.85543800
H	4.83109600	1.42154900	2.84312200
H	4.99380100	1.15765700	1.08986600
O	0.83348700	0.98916100	1.59028400
O	3.15892600	1.93469300	1.72499300
O	2.67580500	-0.30507800	2.87043300
C	4.33899500	-1.61184600	4.03062000
H	5.05427800	-0.78383100	4.07253600
H	4.90412700	-2.55110200	4.02046100
H	3.72424700	-1.58628700	4.93637800
C	5.17663300	3.23693600	1.71165800
H	6.26647700	3.20374800	1.82366700
H	4.76773500	3.90275000	2.47879200
H	4.93606600	3.65053900	0.72842600

TS4c

SCF energy: -3364.966743

SCF energy in solution: -3364.0235310500

Free energy in solution: -3363.2731420500

P	-0.48915500	2.26387600	0.89130500
C	2.65535200	0.91367400	2.19595500
H	1.83356400	0.47470800	2.77006800
H	3.58946300	0.59748200	2.67279800
C	0.01292900	2.54870400	2.68076000
H	-0.72004000	3.22322000	3.13777700
H	-0.14977100	1.56347000	3.13492900
C	2.55484900	2.45607900	2.12842700
H	2.40906800	2.79322100	1.09474600
H	3.51214000	2.89162400	2.43652700
C	1.43587200	3.05453900	2.98811300
H	1.63712500	2.85553500	4.04988200
H	1.47112000	4.14369200	2.86963000
P	2.57177100	0.14179700	0.50908800
C	3.92610800	0.99597600	-0.40361800
C	5.24709200	0.95587900	0.07656000
C	3.64162200	1.74143800	-1.55573900
C	6.25947000	1.65165900	-0.58140400
H	5.48821300	0.37163500	0.96075400
C	4.65962300	2.43743100	-2.21407000
H	2.63053300	1.75866600	-1.94714600

C	5.96604100	2.39548200	-1.72867000
H	7.27684900	1.61275100	-0.20106400
H	4.42678100	3.00708300	-3.10944300
H	6.75663300	2.93629300	-2.24226100
C	3.23578200	-1.55499000	0.78195300
C	4.02870100	-2.17699800	-0.19586300
C	2.91705000	-2.26195100	1.95338000
C	4.50596300	-3.47312300	-0.00069900
H	4.27857200	-1.64832800	-1.11078300
C	3.40191800	-3.55744200	2.14412500
H	2.27719800	-1.81761100	2.70949500
C	4.19714000	-4.16581200	1.17143800
H	5.11951800	-3.94011600	-0.76644800
H	3.15591600	-4.09068700	3.05894800
H	4.57218000	-5.17437400	1.32431900
C	-2.32226800	2.29267700	1.13870800
C	-3.11234200	3.41416700	0.85037300
C	-2.92263000	1.16517400	1.71872000
C	-4.47492400	3.41483900	1.15619900
H	-2.67069200	4.29115200	0.38931800
C	-4.28420700	1.17237500	2.02628200
H	-2.32940000	0.27470800	1.91110500
C	-5.06388300	2.29772100	1.75140900
H	-5.07439600	4.29334900	0.93054800
H	-4.73580600	0.29137200	2.47572700
H	-6.12360700	2.30301700	1.99397000
C	-0.15368100	3.83545500	-0.01116300
C	-0.05025500	5.08764400	0.61630900
C	-0.01769900	3.76662700	-1.40868400
C	0.20375500	6.23929800	-0.13163200
H	-0.17952700	5.17338700	1.69116900
C	0.22632500	4.92042400	-2.15559700
H	-0.11735500	2.80697700	-1.90971900
C	0.34520700	6.15731600	-1.51837200
H	0.28621100	7.20021600	0.36971400
H	0.32282500	4.85002900	-3.23571000
H	0.54186700	7.05441900	-2.09951600
O	1.65819200	-0.42228500	-2.88661900
C	1.14532300	-0.92935300	-1.90985300
C	0.88916100	-2.40669600	-1.84121200
C	0.31749600	-2.99840100	-0.70954700
C	1.24681600	-3.20462500	-2.94161200
C	0.10499800	-4.37766000	-0.67789600
H	0.03593600	-2.37508700	0.13536800
C	1.03214100	-4.57951500	-2.90664900
H	1.68814900	-2.72445600	-3.80946100
C	0.46079100	-5.16841400	-1.77236900
H	-0.33841400	-4.83573600	0.20225100
H	1.30764300	-5.19495300	-3.75930500
H	0.29441900	-6.24244600	-1.74431800
C	-2.88801700	-3.79522300	2.68177800
C	-0.94426000	-3.13725300	4.09785600
C	-2.40831900	-3.58479700	4.11860200
H	-3.97206800	-3.92606300	2.61218100
H	-0.30964200	-3.95588300	3.72449300
H	-3.01982800	-2.81020300	4.60032000
N	-1.50196600	-1.79742700	2.03697300
C	-0.73671900	-1.93281400	3.17589400
C	-2.49011200	-2.63684200	1.77706800
O	0.13677600	-1.10501700	3.45047200
O	-3.19305500	-2.53204700	0.70610500
H	-0.57161800	-2.87014900	5.09038300
H	-2.53340300	-4.49968600	4.70871100
H	-2.43893500	-4.70646900	2.25862400
Pd	0.48250000	0.32319700	-0.45594700
P	-2.65269300	-0.55954900	-1.42757000
H	-2.88153700	-1.65236600	-0.10188200
C	-2.65767300	-2.78451300	-2.95222600
H	-1.62732500	-2.92988700	-3.29422800
H	-2.75833500	-3.26748600	-1.97144300
C	-5.19324300	0.20323100	-1.71878000
H	-5.30102700	-0.56045100	-2.49790700
H	-5.53404500	-0.22554100	-0.76541500
O	-1.35618600	0.26798300	-1.54807300
O	-3.81554900	0.58712400	-1.60853400
O	-2.91888800	-1.37627600	-2.84403600
C	-3.64045500	-3.38373200	-3.94646800
H	-4.67126100	-3.26957700	-3.59368200
H	-3.43711200	-4.45244500	-4.08388900
H	-3.55314100	-2.88681600	-4.91834000
C	-6.00184700	1.44229400	-2.06728100
H	-7.06513100	1.18861300	-2.15539200
H	-5.66313300	1.86249400	-3.01979500
H	-5.88571900	2.20524800	-1.29177600

TS5c

SCF energy: -3364.971213

SCF energy in solution: -3364.0253718400

Free energy in solution: -3363.2734088400

P	-0.54822600	2.39015300	-0.95922000
C	-3.11325200	0.23113500	-2.27860000

H	-2.20082300	0.19884900	-2.88242000
H	-3.87426500	-0.32940400	-2.83182400
C	-1.29064400	2.74158300	-2.65174100
H	-0.87395100	3.68867700	-3.01391600
H	-0.84136400	1.96671100	-3.28546200
C	-3.56898900	1.68240700	-2.00013600
H	-3.45069300	1.92455500	-0.93630600
H	-4.64360600	1.76593700	-2.19600700
C	-2.82295300	2.74815300	-2.81205000
H	-3.05224600	2.63425400	-3.88071200
H	-3.21802400	3.72723000	-2.51824100
P	-2.72599800	-0.67900900	-0.69974000
C	-4.33745000	-0.56717900	0.18621200
C	-5.53084100	-0.98146100	-0.43400200
C	-4.40027300	0.01792700	1.45930700
C	-6.75651200	-0.82059200	0.20972600
H	-5.50543100	-1.43829400	-1.41974300
C	-5.63231000	0.17888900	2.10042100
H	-3.48919700	0.32980400	1.95764000
C	-6.80889800	-0.23826100	1.47984700
H	-7.67006700	-1.14739300	-0.27988200
H	-5.66493900	0.62974900	3.08834800
H	-7.76517800	-0.11210500	1.98057400
C	-2.57637200	-2.42305800	-1.26979100
C	-3.37863400	-3.45984200	-0.77114400
C	-1.58622700	-2.72256200	-2.22192100
C	-3.21520500	-4.76566800	-1.23872700
H	-4.13122300	-3.25418900	-0.01725600
C	-1.43426300	-4.02657300	-2.69134600
H	-0.89561100	-1.95773300	-2.56483700
C	-2.25119700	-5.05049500	-2.20617000
H	-3.84351100	-5.55903500	-0.84269100
H	-0.66282800	-4.24132500	-3.42571600
H	-2.12790000	-6.06691800	-2.57061900
C	1.19921300	2.80618600	-1.38268000
C	1.70991900	4.10785500	-1.27363800
C	2.00958000	1.79204200	-1.91340000
C	3.00553700	4.39414700	-1.70532300
H	1.10103500	4.89992900	-0.84876700
C	3.30523100	2.08470700	-2.34453200
H	1.64006300	0.77123100	-1.97749400
C	3.80455100	3.38430000	-2.24653500
H	3.39091300	5.40661200	-1.61530800
H	3.92808700	1.28841800	-2.74177400
H	4.81414400	3.60831700	-2.58141100
C	-1.10448500	3.77505500	0.12248600
C	-1.66228600	4.96678000	-0.36833600
C	-0.95286800	3.61845300	1.51260800
C	-2.07285100	5.97377100	0.50835800
H	-1.77212600	5.12420400	-1.43685900
C	-1.35819000	4.63036000	2.38394000
H	-0.49747800	2.71345800	1.90528900
C	-1.92413000	5.80613000	1.88603200
H	-2.50530700	6.88905500	0.11242400
H	-1.23028200	4.49591000	3.45460100
H	-2.24408300	6.58988700	2.56764800
O	-1.65598200	-0.78069800	2.82282700
C	-1.06760100	-1.16439900	1.83275600
C	-0.41984200	-2.51269800	1.77711600
C	0.32593500	-2.92748400	0.66766000
C	-0.58236000	-3.37756300	2.87478000
C	0.90173800	-4.19965200	0.65522400
H	0.46518600	-2.25964500	-0.17789100
C	-0.00726200	-4.64425000	2.85631400
H	-1.16053000	-3.03405200	3.72676100
C	0.73551100	-5.05770100	1.74366500
H	1.47683100	-4.51899500	-0.20942600
H	-0.13464700	-5.31143500	3.70489800
H	1.18288900	-6.04848800	1.72867900
C	5.51818200	-2.49042400	-1.72438800
C	3.38570300	-2.69612300	-2.99787600
C	4.88969500	-2.44198600	-3.11760800
H	6.57091900	-2.19375100	-1.72331800
H	3.20784000	-3.73696600	-2.68663400
H	5.06035900	-1.45333800	-3.56544800
N	3.45370100	-1.31298100	-0.91574000
C	2.72007500	-1.78680400	-1.96096300
C	4.78726800	-1.59273600	-0.72381400
O	1.51550400	-1.50980800	-2.08801100
O	5.39183600	-1.14432800	0.25191300
H	2.85752700	-2.55663100	-3.94582300
H	5.35782000	-3.17502800	-3.78505200
H	5.47920400	-3.51797400	-1.33206200
Pd	-0.87086900	0.20773500	0.34709600
P	2.35616900	0.38493100	1.39703600
H	2.88723700	-0.51954300	0.14215200
C	3.01274800	-1.73947600	2.93110900
H	2.24408300	-2.15617600	3.59053900
H	2.91078800	-2.22369400	1.95372300
C	4.55526800	1.82019200	1.86421400
H	4.69374700	1.47185900	2.89362200
H	5.08561600	1.13112700	1.19806600

O	0.87217300	0.81502300	1.42447200
O	3.14169500	1.80455700	1.56009600
O	2.75363400	-0.32538000	2.82235400
C	4.40830400	-1.96366300	3.49117700
H	5.16001900	-1.60625400	2.78182600
H	4.57403500	-3.03393400	3.66719500
H	4.52962000	-1.43627100	4.44372100
C	5.05006900	3.24665600	1.69877800
H	6.11773900	3.30329800	1.94230500
H	4.50548900	3.92420400	2.36521300
H	4.90630600	3.58784100	0.66901400

7c

SCF energy: -2965.002221

SCF energy in solution: -2964.1691861400

Free energy in solution: -2963.5304041400

P	1.41492600	-1.70754300	0.86949600
C	-2.10457000	-2.70483400	1.39988000
H	-1.70712000	-2.40619300	2.37514300
H	-3.10605100	-3.11094900	1.57814200
C	0.92556000	-3.05600800	2.08233100
H	1.83551600	-3.48131000	2.52215600
H	0.44088500	-2.50490500	2.89846300
C	-1.18436800	-3.75083400	0.72448800
H	-0.80267000	-3.37054300	-0.23088100
H	-1.77723600	-4.63509300	0.46596400
C	0.01049900	-4.19031000	1.58312300
H	-0.35076500	-4.74173900	2.46276400
H	0.59947200	-4.90342200	0.99561800
P	-2.27521600	-1.16223900	0.36965800
C	-3.07967400	-1.82124600	-1.14996300
C	-4.35611000	-2.40721300	-1.09489900
C	-2.38674400	-1.80252900	-2.36874700
C	-4.92417200	-2.96857200	-2.23715300
H	-4.91323400	-2.41488400	-0.16166100
C	-2.95866900	-2.36840900	-3.51123500
H	-1.41303300	-1.32736700	-2.42718100
C	-4.22406700	-2.95121100	-3.44739600
H	-5.91260900	-3.41722000	-2.18413000
H	-2.41459700	-2.34262300	-4.45114400
H	-4.66879300	-3.38727200	-4.33801200
C	-3.61271700	-0.22116200	1.21791000
C	-4.46680900	0.61014400	0.47419300
C	-3.75434800	-0.25881100	2.61416400
C	-5.44347500	1.37406900	1.11250700
H	-4.36880600	0.66048600	-0.60603000
C	-4.73298300	0.50718700	3.25017500
H	-3.10505200	-0.88570600	3.21815600
C	-5.58056100	1.32447600	2.50123300
H	-6.09551300	2.01161800	0.52192600
H	-4.83203500	0.46174900	4.33144800
H	-6.34156700	1.92113600	2.99662100
C	2.61329400	-0.80638600	1.94658400
C	3.93975100	-1.22903400	2.10989400
C	2.16171300	0.30745300	2.66884900
C	4.79149200	-0.55814300	2.98866500
H	4.31526200	-2.07382500	1.54014000
C	3.01221600	0.97569100	3.55050300
H	1.14699800	0.66720700	2.52079300
C	4.32921400	0.54288600	3.71316900
H	5.81905400	-0.89359600	3.10295600
H	2.65029900	1.84325400	4.09575400
H	4.99537500	1.06622500	4.39398800
C	2.44948400	-2.55833400	-0.39620400
C	2.97552300	-3.84916200	-0.21857000
C	2.71701500	-1.87114100	-1.59447200
C	3.74169000	-4.44783700	-1.22109500
H	2.80196500	-4.39621100	0.70296800
C	3.48780600	-2.47428000	-2.58956000
H	2.34267700	-0.85793400	-1.72090200
C	3.99626000	-3.76240300	-2.41015300
H	4.13976400	-5.44797200	-1.06946000
H	3.69227400	-1.92920300	-3.50718300
H	4.59231300	-4.22910600	-3.19020900
O	-1.73583100	1.29666300	-2.09487700
C	-1.37726600	1.40782000	-0.93949100
C	-1.62915400	2.67680300	-0.17140300
C	-1.28275100	2.80582400	1.17821600
C	-2.23322600	3.75729000	-0.83530600
C	-1.53581700	3.99503400	1.86069200
H	-0.80824100	1.96799900	1.68157200
C	-2.48108400	4.94671100	-0.15589300
H	-2.49357000	3.64205300	-1.88276100
C	-2.13356500	5.06672700	1.19406700
H	-1.26109800	4.08913400	2.90780700
H	-2.94315100	5.78258100	-0.67491800
H	-2.32634100	5.99622200	1.72375000
Pd	-0.28804000	-0.07902700	-0.07084500
P	2.10407700	2.28427900	-0.65385800
C	1.22903500	3.60051800	-2.81065100
H	0.40699300	2.94148200	-3.12313100

H	0.82210400	4.30003100	-2.06260400
C	4.71584300	2.72848100	-0.46374200
H	4.80480800	3.23160200	-1.43584500
H	4.46656900	3.49935500	0.28399500
O	1.40340000	0.87000700	-0.82863200
O	3.68862900	1.74230700	-0.52330900
O	2.28500500	2.82684600	-2.24892300
C	1.77052200	4.37126500	-4.00689100
H	2.57454000	5.04798300	-3.69722300
H	0.97638000	4.96458000	-4.47689600
H	2.17585400	3.68130100	-4.75488500
C	6.02351700	2.04360200	-0.09356900
H	6.84076800	2.77392400	-0.04513300
H	6.28065300	1.28395800	-0.83964900
H	5.93457400	1.54965600	0.87957000

8c

SCF energy: -2965.025613

SCF energy in solution: -2964.1967967700

Free energy in solution: -2963.5531257700

P	1.88834700	-0.95338200	0.97969900
C	-1.38021700	-2.90389100	1.82683500
H	-1.24480100	-2.49379300	2.83339700
H	-2.25022700	-3.56694500	1.87772900
C	1.52899500	-1.99418300	2.50473300
H	2.41551500	-1.97223700	3.14878800
H	0.74922300	-1.44767500	3.04840900
C	-0.11773200	-3.67599700	1.37697900
H	0.14086500	-3.42298100	0.34119300
H	-0.34083300	-4.74908900	1.36509800
C	1.10688300	-3.45440700	2.27698800
H	0.90724000	-3.89433100	3.26478400
H	1.95256400	-4.01202800	1.85821100
P	-1.81486200	-1.50348600	0.66248000
C	-2.38844300	-2.46204600	-0.80650900
C	-3.46723200	-3.35795000	-0.71079300
C	-1.70489400	-2.34548900	-2.02624200
C	-3.85307400	-4.12230100	-1.81073700
H	-4.01898800	-3.45102500	0.22113800
C	-2.09098400	-3.11835800	-3.12484800
H	-0.87873400	-1.64738200	-2.12987500
C	-3.16241100	-4.00476700	-3.02056300
H	-4.69201300	-4.80794400	-1.72413900
H	-1.55285500	-3.01480200	-4.06281200
H	-3.46338100	-4.60093900	-3.87813000
C	-3.35605600	-0.82152600	1.41445100
C	-4.44535900	-0.44150700	0.61333200
C	-3.42500300	-0.58842600	2.79827300
C	-5.57804400	0.13764600	1.18714500
H	-4.40439700	-0.59108900	-0.46015000
C	-4.55958100	-0.01074700	3.36905000
H	-2.59245000	-0.85514800	3.44369000
C	-5.64150500	0.35174200	2.56494700
H	-6.41215600	0.42316100	0.55171300
H	-4.59602100	0.15550600	4.44247400
H	-6.52522500	0.80199600	3.00884400
C	2.79691900	0.42262000	1.82075800
C	4.15009900	0.70467300	1.59105400
C	2.08592800	1.22331500	2.73203900
C	4.78035600	1.75153800	2.26917600
H	4.71431600	0.11085600	0.87995600
C	2.71786700	2.26524200	3.41148600
H	1.02959200	1.03655100	2.91074400
C	4.06995500	2.53175300	3.18236300
H	5.83095800	1.95569700	2.07987900
H	2.15320200	2.86941200	4.11698300
H	4.56380900	3.34371500	3.70924700
C	3.18401400	-1.93538200	0.11326400
C	4.19013600	-2.61572600	0.82544000
C	3.15570500	-2.03068300	-1.28689900
C	5.14251600	-3.37993800	0.15321800
H	4.24035400	-2.54510200	1.90870400
C	4.11643200	-2.79714100	-1.95468600
H	2.40849300	-1.49075200	-1.86453600
C	5.10467500	-3.47397200	-1.24134000
H	5.91319900	-3.89984500	0.71648400
H	4.08609300	-2.85564700	-3.03916600
H	5.84701500	-4.07022400	-1.76574800
O	-2.39899900	0.84523900	-1.73449100
C	-1.66406200	1.18669500	-0.82487100
C	-1.93070000	2.47712800	-0.08648800
C	-1.05332100	2.97253800	0.88465900
C	-3.10166500	3.19250400	-0.38232800
C	-1.33604900	4.16486000	1.55161000
H	-0.13923000	2.42299300	1.09515500
C	-3.38690700	4.38108300	0.28469400
H	-3.76955700	2.79775200	-1.14136100
C	-2.50458000	4.86969800	1.25408200
H	-0.64360800	4.54676800	2.29756100
H	-4.29529800	4.93062100	0.05060100
H	-2.72664900	5.79899700	1.77276300

Pd	-0.10658400	0.02058900	-0.13676600
P	1.07205700	1.05749900	-1.88329100
C	-0.26479700	2.37714000	-3.82110200
H	0.31640600	1.71708400	-4.47103400
H	-1.27804000	1.96894100	-3.72957100
C	2.68173300	3.02138400	-0.90131900
H	1.95165700	3.70093200	-1.35100000
H	2.49178900	2.96721000	0.17828100
O	1.30302100	0.00735300	-2.94212500
O	2.53665400	1.71193100	-1.47415800
O	0.33405500	2.40374400	-2.50912000
C	-0.29934700	3.79963100	-4.35644000
H	-0.86481600	4.45422900	-3.68440600
H	-0.78130100	3.81801400	-5.34155200
H	0.71376700	4.20318100	-4.45948400
C	4.09946000	3.50156500	-1.17110600
H	4.25418500	4.49171500	-0.72519000
H	4.28325200	3.57054000	-2.24818700
H	4.83068900	2.81050200	-0.74023800

TS6c

SCF energy: -2964.958412

SCF energy in solution: -2964.12778756

Free energy in solution: -2963.4892445600

P	1.94696500	-1.48785800	-0.37411900
C	-1.34844100	-3.36342800	0.03693400
H	-1.10076100	-3.61941100	-0.99856100
H	-2.23727900	-3.94742800	0.29585900
C	1.66598400	-3.27964300	-0.84675500
H	2.62108500	-3.69926500	-1.18329800
H	1.00442700	-3.26782500	-1.72074700
C	-0.16527100	-3.69442100	0.97760700
H	0.09626800	-2.82426200	1.59166800
H	-0.47717800	-4.46627900	1.69015100
C	1.09680400	-4.19202700	0.25658700
H	0.89011700	-5.16877600	-0.20343600
H	1.87574000	-4.36379200	1.00797800
P	-1.79796000	-1.55021500	0.08031900
C	-2.54621900	-1.39778100	1.75973900
C	-2.04789500	-0.45005300	2.66524100
C	-3.60602000	-2.23713700	2.15079000
C	-2.60390600	-0.35518300	3.94675100
H	-1.23252400	0.21063400	2.37111400
C	-4.15356600	-2.13508400	3.42736600
H	-4.01742400	-2.96225300	1.45320900
C	-3.65022600	-1.19217300	4.33013600
H	-2.21141100	0.38186700	4.64249500
H	-4.97307900	-2.78740900	3.71788700
H	-4.07805900	-1.11260300	5.32633900
C	-3.26993700	-1.48170800	-1.03454400
C	-3.31301100	-2.22268800	-2.22643400
C	-4.34414100	-0.62842700	-0.73656900
C	-4.40926700	-2.12998800	-3.08573100
H	-2.49175000	-2.88042000	-2.49585400
C	-5.43667100	-0.53238000	-1.59873100
H	-4.32945200	-0.03895200	0.17475700
C	-5.47586900	-1.28581900	-2.77334200
H	-4.42825800	-2.71998500	-3.99846400
H	-6.25892700	0.13284100	-1.34931000
H	-6.33005600	-1.21417900	-3.44128800
C	3.27216600	-0.96485600	-1.54847800
C	4.03970300	0.16656800	-1.22439800
C	3.49657800	-1.60616600	-2.77557400
C	5.02343400	0.62659200	-2.09790900
H	3.85556800	0.69922500	-0.29554800
C	4.48110400	-1.13953000	-3.65046000
H	2.90761700	-2.47126100	-3.06450500
C	5.25030800	-0.02653800	-3.31183200
H	5.60743800	1.50326500	-1.83190600
H	4.64452400	-1.65042900	-4.59580300
H	6.01629400	0.33535600	-3.99230100
C	2.86445400	-1.63060100	1.21908400
C	4.02137600	-2.42732200	1.29762800
C	2.40587700	-0.96255300	2.36238000
C	4.69911200	-2.56545400	2.50709900
H	4.40132800	-2.93077300	0.41208100
C	3.09558400	-1.10280000	3.57195100
H	1.54310900	-0.30244900	2.28956800
C	4.23362500	-1.90414900	3.64868600
H	5.59218100	-3.18289900	2.55877400
H	2.74097000	-0.57115200	4.45082800
H	4.76590300	-2.00911800	4.59064700
O	1.40171100	1.82773000	-2.55628500
C	0.73454100	1.22991200	-1.82091100
C	-1.21437700	1.41321900	-1.72305900
C	-1.67425200	2.54351200	-1.03464700
C	-1.81411800	1.02027000	-2.92873000
C	-2.76752100	3.25044700	-1.54428000
H	-1.18584200	2.87450600	-0.12249600
C	-2.90197200	1.73700900	-3.42849600
H	-1.43069500	0.16564000	-3.47809100

C	-3.38058100	2.85158700	-2.73440200
H	-3.13030600	4.12504000	-1.00977900
H	-3.37017100	1.42779300	-4.35924200
H	-4.22330100	3.41461000	-3.12789800
Pd	0.01431500	-0.03395500	-0.60996400
P	0.93359800	2.54507900	1.93885900
C	-1.15787200	3.98275700	2.80842700
H	-1.99863100	3.27092700	2.81595500
H	-0.60947000	3.84475600	3.75495000
C	2.35418100	4.27064200	0.47858100
H	1.58530900	5.02088600	0.25187100
H	2.77463000	4.52503600	1.46479400
O	0.30278200	1.18469900	1.52554700
O	1.75787800	2.97499300	0.51456100
O	-0.30832900	3.72224300	1.70048400
C	-1.68406900	5.40987500	2.71844600
H	-0.85520900	6.12544600	2.74334900
H	-2.36109300	5.62964400	3.55341100
H	-2.23266000	5.56011500	1.78168300
C	3.45086000	4.29324500	-0.57693400
H	3.89574500	5.29371800	-0.64669500
H	3.04807000	4.02248800	-1.55834200
H	4.24440700	3.58028900	-0.32507400

9c

SCF energy: -2965.006762

SCF energy in solution: -2964.1604512000

Free energy in solution: -2963.5225632000

P	0.64385600	-1.85127200	-0.21796300
C	-2.83645600	0.48007300	-1.37293700
H	-2.79907700	1.48830200	-1.80166000
H	-2.45219800	0.56894200	-0.35156200
C	-1.20054800	-2.14749400	-0.38757700
H	-1.37488400	-3.19620600	-0.11832400
H	-1.71195700	-1.54090100	0.36724000
C	-1.92732400	-0.42438500	-2.22594300
H	-0.93033100	0.03783400	-2.25447400
H	-2.29625400	-0.41854400	-3.25993800
C	-1.80258300	-1.89081300	-1.78203600
H	-2.79918700	-2.34997800	-1.78992000
H	-1.21661200	-2.43556800	-2.53166600
P	-4.65238100	-0.00677500	-1.37211400
C	-4.75158700	-1.12950900	0.11202600
C	-4.42929600	-0.72288700	1.41755300
C	-5.16640200	-2.45429100	-0.09094500
C	-4.50179000	-1.62038400	2.48390700
H	-4.13347400	0.30608900	1.60603100
C	-5.23731500	-3.35690000	0.97400100
H	-5.43557300	-2.78012100	-1.09299200
C	-4.90224800	-2.94210500	2.26330800
H	-4.25341600	-1.28702600	3.48855500
H	-5.55881100	-4.37990600	0.79595200
H	-4.96130200	-3.63999300	3.09447800
C	-5.44376100	1.53071800	-0.69617100
C	-6.84004500	1.63080600	-0.82572700
C	-4.75502200	2.59616900	-0.09301700
C	-7.52950800	2.74722200	-0.35314500
H	-7.39031100	0.82553500	-1.30728800
C	-5.44392400	3.71984800	0.37155300
H	-3.67517500	2.56103000	0.01813200
C	-6.83149300	3.79798900	0.24649600
H	-8.60971800	2.80133800	-0.46189300
H	-4.89234400	4.53452400	0.83442500
H	-7.36489100	4.67311500	0.60828400
C	1.05013800	-2.72874200	1.35337800
C	2.38792800	-3.08119000	1.60837300
C	0.07668900	-2.99403900	2.33012400
C	2.73211900	-3.70220500	2.80878200
H	3.15650000	-2.85167800	0.87593000
C	0.43110900	-3.61122500	3.53246000
H	-0.96242600	-2.72713500	2.16620200
C	1.75754800	-3.96978900	3.77349800
H	3.76917000	-3.97079000	2.99104300
H	-0.33449400	-3.81327100	4.27716500
H	2.03119900	-4.45197900	4.70838700
C	1.31330900	-2.93722500	-1.54347100
C	1.18189000	-4.33288300	-1.47020900
C	1.89868600	-2.36565300	-2.68059500
C	1.62423500	-5.13935800	-2.51864500
H	0.74507400	-4.79273400	-0.58779800
C	2.33510900	-3.17367500	-3.73192500
H	2.03452800	-1.29043500	-2.72979700
C	2.19896400	-4.56016700	-3.65277100
H	1.52269500	-6.21919300	-2.44876000
H	2.79347700	-2.71905100	-4.60599900
H	2.54532700	-5.18929900	-4.46852600
O	-0.32852300	2.20097600	-0.10833800
C	0.87729500	2.45925100	-0.02122000
C	1.38545900	3.83751100	0.11879900
C	2.76343300	4.09549000	0.16081100
C	0.46823000	4.90272400	0.21359700

C	3.21846200	5.40733800	0.29847700
H	3.46182100	3.26948700	0.07490800
C	0.92911700	6.20681700	0.35223800
H	-0.59467700	4.68586400	0.17766900
C	2.30579300	6.45978900	0.39516100
H	4.28581900	5.60788700	0.33119400
H	0.22216300	7.02858600	0.42688300
H	2.66424200	7.48015100	0.50389800
Pd	1.26575800	0.50895200	-0.14445200
P	3.50690200	0.12556600	0.04179200
C	4.68667800	1.49683400	-1.90940800
H	5.00351100	0.51696900	-2.28052500
H	3.76047300	1.78109400	-2.43071100
C	3.63626600	1.23216600	2.50951300
H	4.25570600	2.09942100	2.24867300
H	2.58171800	1.51716500	2.39669500
O	3.96315300	-1.16284000	-0.57767400
O	3.94287000	0.15028800	1.61993300
O	4.42705500	1.40078600	-0.49712900
C	5.76848900	2.54180800	-2.12880100
H	5.44571500	3.52555400	-1.77102000
H	5.99795400	2.62510400	-3.19751800
H	6.68405000	2.26304200	-1.59745100
C	3.91893600	0.76872900	3.92913100
H	3.70162000	1.57540300	4.63911500
H	4.96981000	0.48215800	4.03938700
H	3.29809500	-0.09723500	4.18044500

TS7c

SCF energy: -2964.968598

SCF energy in solution: -2964.1306125400

Free energy in solution: -2963.4923735400

P	-0.68374900	-1.50535700	0.30004800
C	3.14248300	0.61636200	1.28856900
H	3.22108000	1.62066900	1.72333200
H	2.75620300	0.74906200	0.27409100
C	1.16618500	-1.82722600	0.33905300
H	1.28536500	-2.87285800	0.03181000
H	1.63358500	-1.21562500	-0.43937800
C	2.16032800	-0.19948100	2.15043500
H	1.21390700	0.35595100	2.20753700
H	2.55005300	-0.24643100	3.17562200
C	1.88353200	-1.64000400	1.69178000
H	2.83724500	-2.17668000	1.61868600
H	1.31289800	-2.15475300	2.47254400
P	4.90088300	-0.05172400	1.25402800
C	4.85702700	-1.18042700	-0.22883300
C	4.50825200	-0.75702500	-1.52222700
C	5.19239400	-2.52922500	-0.03651100
C	4.48018800	-1.65973400	-2.58620900
H	4.27109500	0.28775300	-1.70519300
C	5.16396300	-3.43659600	-1.09954000
H	5.47893200	-2.87018500	0.95562900
C	4.80514900	-3.00361400	-2.37634100
H	4.21307700	-1.31304200	-3.58150500
H	5.42675600	-4.47761300	-0.92974400
H	4.78639400	-3.70524600	-3.20625600
C	5.82473900	1.40338600	0.56566400
C	7.21870100	1.40709000	0.74505800
C	5.23660800	2.49393000	-0.09695400
C	8.00400600	2.45475900	0.26358000
H	7.69079700	0.58134800	1.27261700
C	6.02112400	3.54866000	-0.57029100
H	4.16210900	2.53228100	-0.25021100
C	7.40567700	3.53112400	-0.39487400
H	9.08075200	2.43535700	0.41132100
H	5.54660400	4.38418900	-1.07880800
H	8.01371600	4.35297400	-0.76379900
C	-1.25647700	-2.57124300	-1.08640500
C	-2.58282700	-3.03610000	-1.09699300
C	-0.41234600	-2.87525500	-2.16749600
C	-3.04091400	-3.81123900	-2.16249900
H	-3.25843100	-2.77462400	-0.28772600
C	-0.88180400	-3.64543200	-3.23312900
H	0.61386800	-2.52095200	-2.18788700
C	-2.19505300	-4.11848800	-3.23064800
H	-4.06772000	-4.16592100	-2.15837500
H	-0.21749000	-3.87723100	-4.06143900
H	-2.55845500	-4.72073500	-4.05918700
C	-1.26389500	-2.33999000	1.82700400
C	-1.16533800	-3.73464400	1.95625500
C	-1.72925800	-1.58255000	2.90862900
C	-1.52432000	-4.35677900	3.15152000
H	-0.82021300	-4.33768200	1.12095800
C	-2.08176700	-2.20673200	4.10575400
H	-1.84064400	-0.50860600	2.80335100
C	-1.98039500	-3.59281000	4.22872700
H	-1.45102000	-5.43738300	3.23988300
H	-2.45212100	-1.61012800	4.93465100
H	-2.26316400	-4.07917800	5.15849300
O	1.14936200	2.23852300	-0.88202900

C	0.13665000	1.83202400	-0.44200300
C	-1.31311000	2.93430900	-0.34154000
C	-1.44608700	3.65556600	0.85605900
C	-1.78505500	3.48980400	-1.54161100
C	-2.06828500	4.90503800	0.85683900
H	-1.05477200	3.24460400	1.78357100
C	-2.40303900	4.73881400	-1.53849100
H	-1.65970100	2.94978600	-2.47595100
C	-2.54812800	5.44440100	-0.33940100
H	-2.17255000	5.45910100	1.78590000
H	-2.77083200	5.16447900	-2.46833000
H	-3.02626900	6.42025400	-0.34014200
Pd	-1.37924800	0.71261400	-0.01635200
P	-3.71643600	0.17795300	0.10595700
C	-4.91483500	2.02045000	1.62272500
H	-5.35194300	1.19004200	2.18784600
H	-3.99480400	2.33664800	2.13794800
C	-4.16470400	0.65360700	-2.51642700
H	-4.69062000	1.59021400	-2.29567800
H	-3.10742900	0.89252100	-2.70426800
O	-4.15546500	-0.88946000	1.07164600
O	-4.27135600	-0.23176300	-1.39844100
O	-4.60060000	1.58010400	0.29634500
C	-5.88374500	3.18767800	1.52117400
H	-5.43415100	4.01553500	0.96253400
H	-6.15177400	3.54738700	2.52197300
H	-6.79984900	2.88093600	1.00587100
C	-4.76955600	-0.03898600	-3.72777700
H	-4.70398900	0.60892600	-4.61022100
H	-5.82334600	-0.27447200	-3.54670100
H	-4.24012600	-0.97373900	-3.93961500

10c

SCF energy: -2964.989376

SCF energy in solution: -2964.1490236400

Free energy in solution: -2963.5128566400

P	-0.68517700	-1.37759100	0.29859400
C	3.28942400	0.72906700	1.11525800
H	3.42711900	1.76022300	1.46284200
H	2.93907100	0.79172900	0.07961100
C	1.17404100	-1.67742200	0.35090700
H	1.30431100	-2.73663600	0.10148300
H	1.63901900	-1.10989500	-0.46245000
C	2.23847300	0.05596400	2.02005500
H	1.32552000	0.66816100	2.00601800
H	2.60504500	0.08583500	3.05416800
C	1.89080500	-1.40455500	1.68995900
H	2.81812900	-1.99019500	1.67975500
H	1.29088700	-1.81656800	2.50830700
P	4.99538500	-0.06700000	1.18053800
C	4.90597700	-1.27209600	-0.23759700
C	4.62352200	-0.89749700	-1.56174500
C	5.13427700	-2.62879100	0.03749600
C	4.55452800	-1.85353900	-2.57588900
H	4.47508800	0.15070500	-1.80860400
C	5.06458500	-3.58962600	-0.97550900
H	5.36948700	-2.93357400	1.05452900
C	4.77177000	-3.20373700	-2.28385800
H	4.34062400	-1.54467900	-3.59615000
H	5.24400700	-4.63596000	-0.74213400
H	4.72115600	-3.94762500	-3.07462200
C	6.05230000	1.26796500	0.44214300
C	7.43857300	1.15620500	0.64554200
C	5.57421900	2.37351200	-0.28025700
C	8.32078500	2.10512300	0.12882500
H	7.82800200	0.31840400	1.21952900
C	6.45561400	3.33049000	-0.78932400
H	4.50933600	2.50074200	-0.45111800
C	7.83046800	3.19758300	-0.58984200
H	9.38931700	1.99689600	0.29602400
H	6.06480300	4.18006400	-1.34358700
H	8.51466300	3.94310100	-0.98621800
C	-1.21430900	-2.49581900	-1.06720600
C	-2.52143400	-3.01199400	-1.07535000
C	-0.35596200	-2.79118200	-2.13955800
C	-2.94504500	-3.82634000	-2.12559300
H	-3.20931700	-2.75949700	-0.27427400
C	-0.79121500	-3.59872700	-3.19246300
H	0.65839400	-2.40427300	-2.16301700
C	-2.08482000	-4.12218200	-3.18553000
H	-3.95719100	-4.22127100	-2.11723300
H	-0.11432000	-3.82156800	-4.01307800
H	-2.42154700	-4.75472800	-4.00269400
C	-1.22776800	-2.21783000	1.84057200
C	-1.12106800	-3.61043800	1.97976700
C	-1.67077900	-1.45478300	2.92853300
C	-1.45240100	-4.22530800	3.18720400
H	-0.79175300	-4.21864700	1.14197800
C	-1.99420900	-2.07057700	4.13820100
H	-1.78510300	-0.38104400	2.82063300
C	-1.88707200	-3.45579900	4.26894700

H	-1.37337200	-5.30507900	3.28150900
H	-2.34516800	-1.46842500	4.97167300
H	-2.14726600	-3.93617000	5.20839600
O	1.11603600	2.34576100	-1.05162000
C	0.28597400	1.77870300	-0.50186500
C	-2.09773500	2.94238100	0.03602800
C	-2.08768000	3.59835200	1.27732900
C	-2.45373900	3.67955300	-1.10096200
C	-2.44963000	4.94651100	1.38187200
H	-1.79992200	3.06204900	2.17970600
C	-2.81170700	5.02828600	-0.99884900
H	-2.46351900	3.20860700	-2.07991300
C	-2.81557700	5.66598300	0.24298200
H	-2.44192400	5.43132600	2.35570000
H	-3.08772600	5.57932000	-1.89528700
H	-3.09465200	6.71355900	0.32161800
Pd	-1.44267000	0.96275700	0.02370600
P	-3.70296000	0.28457000	0.02726800
C	-5.32147800	1.91937700	1.37995000
H	-5.75097500	1.04909200	1.88715300
H	-4.50766600	2.31677800	1.99964500
C	-3.97873900	0.64467800	-2.64459400
H	-4.64331800	1.49847500	-2.47234100
H	-2.95710800	1.02298600	-2.78537700
O	-4.01949900	-0.82410200	0.98958700
O	-4.01183100	-0.22425300	-1.50256500
O	-4.79854000	1.50754000	0.10416200
C	-6.36547000	2.99458400	1.13048900
H	-5.91396500	3.85977800	0.63458500
H	-6.79922000	3.32506600	2.08169700
H	-7.17159700	2.60994900	0.49695300
C	-4.41892600	-0.15992300	-3.85689200
H	-4.39334800	0.46735800	-4.75583900
H	-5.43980500	-0.53122100	-3.72084300
H	-3.75743000	-1.01873800	-4.00939500

11c

SCF energy: -2964.996686

SCF energy in solution: -2964.1567356900

Free energy in solution: -2963.5208876900

P	-1.67623600	-1.63399500	-0.76040000
C	2.75176700	-1.48990700	-0.58070500
H	2.34235100	-1.20991100	-1.55929900
H	3.42473300	-2.34294400	-0.74105500
C	-0.24586800	-2.74394400	-1.25285900
H	-0.67759000	-3.68649400	-1.61053900
H	0.26307900	-2.27847500	-2.10561800
C	1.62155000	-1.88990000	0.38093200
H	0.98827000	-1.01781200	0.59277200
H	2.06595100	-2.18284600	1.33947600
C	0.75501700	-3.05991600	-0.12251000
H	1.41561700	-3.86212000	-0.48009100
H	0.20195100	-3.48232600	0.72391900
P	3.70300300	0.00428300	0.04766000
C	4.52700500	-0.71998800	1.54536100
C	5.53597900	-1.69597000	1.48166800
C	4.10003400	-0.27720900	2.80682000
C	6.09542600	-2.21776800	2.64787200
H	5.89392400	-2.03955800	0.51462900
C	4.65609900	-0.80267000	3.97637100
H	3.33025900	0.48818700	2.87163700
C	5.65499200	-1.77344000	3.89822400
H	6.87745200	-2.97015400	2.58263000
H	4.31337200	-0.44798700	4.94494200
H	6.09355900	-2.17962700	4.80597600
C	5.11929800	0.10121500	-1.14057600
C	6.16551700	0.99146300	-0.83448700
C	5.17257500	-0.58680100	-2.36248000
C	7.23463800	1.17215300	-1.70917100
H	6.14321000	1.54493000	0.10152200
C	6.23984500	-0.39771300	-3.24576500
H	4.38331500	-1.27865300	-2.63908800
C	7.27501500	0.47817200	-2.92195300
H	8.03460400	1.85995500	-1.44746900
H	6.25975800	-0.94142600	-4.18693600
H	8.10477200	0.62351000	-3.60841800
C	-2.86704600	-1.77843700	-2.15683200
C	-4.11365000	-1.13794400	-2.01612200
C	-2.56399700	-2.43464100	-3.35985100
C	-5.03582300	-1.17416500	-3.06183700
H	-4.34654100	-0.61162000	-1.09173900
C	-3.49188400	-2.45762600	-4.40472100
H	-1.60938700	-2.93224200	-3.49749300
C	-4.72901400	-1.83036700	-4.25709300
H	-5.99636500	-0.68036300	-2.94177300
H	-3.24430900	-2.96907300	-5.33120500
H	-5.44975400	-1.84994700	-5.07031400
C	-2.42429400	-2.61227400	0.60596300
C	-3.27721200	-3.69413000	0.34164000
C	-2.06315700	-2.33225300	1.93142300
C	-3.75995400	-4.48196500	1.38743000

H	-3.57490200	-3.91642800	-0.67875800
C	-2.54104100	-3.12823200	2.97392900
H	-1.43278800	-1.47595000	2.14874400
C	-3.39102800	-4.20247300	2.70468300
H	-4.42682700	-5.31246700	1.17158100
H	-2.25642100	-2.90117700	3.99795500
H	-3.76911700	-4.81608900	3.51803000
O	0.79111800	0.71384500	-3.12953800
C	0.12308600	0.65783500	-2.20302300
C	-0.62624000	2.78243200	-0.71228100
C	0.52867200	3.24786400	-0.06897400
C	-1.38757100	3.68098400	-1.47263200
C	0.90075900	4.59439700	-0.16388500
H	1.14992300	2.56581000	0.50643100
C	-1.01170400	5.02533900	-1.56987100
H	-2.28961600	3.34468600	-1.97739100
C	0.13167800	5.48687300	-0.91296100
H	1.79700800	4.94042600	0.34630200
H	-1.61736400	5.71112800	-2.15823700
H	0.42224800	6.53172000	-0.98811900
Pd	-1.10347100	0.76349800	-0.65393200
P	-2.71622900	1.23157400	0.99209900
C	-2.78731900	0.78655500	3.62082400
H	-3.42319700	1.67122200	3.74743300
H	-3.44274700	-0.07901600	3.47907900
C	-2.51639100	3.83376700	1.84437000
H	-1.86619500	3.40322100	2.61348300
H	-1.88891400	4.36530300	1.12469000
O	-3.95436000	0.39574900	0.80743500
O	-3.22648900	2.78608200	1.16077100
O	-1.96171700	0.94810800	2.44554800
C	-1.87223400	0.60542100	4.82035100
H	-1.23533300	-0.27757800	4.69638900
H	-2.46627400	0.47678000	5.73284900
H	-1.22172300	1.47679700	4.95122300
C	-3.54263100	4.77426300	2.45934100
H	-3.03618200	5.60708800	2.96204900
H	-4.16796100	4.25295700	3.19222800
H	-4.19803100	5.18548100	1.68463600

TS8c

SCF energy: -2964.984214

SCF energy in solution: -2964.15713167

Free energy in solution: -2963.5150186700

P	2.01219200	1.28983100	-0.19251700
C	-1.36190000	3.20977600	0.75977400
H	-1.11558800	3.73512200	-0.16954400
H	-2.20912800	3.74152500	1.20669200
C	1.62776800	3.13230200	-0.22652800
H	2.54661100	3.64667100	-0.52999300
H	0.89867200	3.29316700	-1.02939900
C	-0.14183900	3.20770800	1.71090700
H	0.05691400	2.19781100	2.08870700
H	-0.37675300	3.80584500	2.59906800
C	1.14062800	3.77551200	1.08536800
H	0.98769000	4.84440700	0.87788900
H	1.94607500	3.71927900	1.82612900
P	-1.90431700	1.47618800	0.30221500
C	-2.69918700	0.96840000	1.89663200
C	-3.92851200	1.49728300	2.32410400
C	-2.02378200	0.06781000	2.73408900
C	-4.46386300	1.13899600	3.56112800
H	-4.47408600	2.18487300	1.68351600
C	-2.55820500	-0.28557800	3.97627100
H	-1.08733300	-0.37670800	2.40705200
C	-3.77787200	0.24863100	4.39196900
H	-5.41785100	1.55390300	3.87639300
H	-2.02433200	-0.98816900	4.61082900
H	-4.19714300	-0.03104300	5.35490400
C	-3.35257400	1.78730500	-0.80459200
C	-4.19841000	0.71056400	-1.13095000
C	-3.60638200	3.03528000	-1.39840400
C	-5.26405600	0.88228500	-2.01309100
H	-4.02113500	-0.26791500	-0.69702200
C	-4.67194700	3.20294200	-2.28695600
H	-2.98375900	3.89385200	-1.17050300
C	-5.50467000	2.12831800	-2.59695700
H	-5.90279300	0.03531800	-2.24869900
H	-4.85004300	4.17886400	-2.73137300
H	-6.33323100	2.25924500	-3.28784500
C	3.26577500	1.15972800	-1.54835900
C	4.17295500	0.08516800	-1.55948800
C	3.29235000	2.07985900	-2.61027800
C	5.09483100	-0.04281200	-2.59896900
H	4.12476900	-0.65941400	-0.77179800
C	4.21395800	1.94069200	-3.65050300
H	2.59707400	2.91247700	-2.64365900
C	5.12193700	0.88190700	-3.64505500
H	5.79036000	-0.87788700	-2.59144500
H	4.21866500	2.66326100	-4.46245000
H	5.84051400	0.77472800	-4.45344900

C	2.99872200	1.17821600	1.36081300
C	4.24940700	1.80662600	1.45955400
C	2.46927100	0.53832700	2.48868700
C	4.95198400	1.79992600	2.66567700
H	4.68511800	2.29125200	0.59027600
C	3.16871600	0.53897700	3.69636800
H	1.52097400	0.01689400	2.41457000
C	4.41103500	1.16901700	3.78771800
H	5.92280600	2.28478700	2.72604400
H	2.74776300	0.03513600	4.56249000
H	4.95860000	1.16267400	4.72648500
O	0.09272200	0.72163900	-3.74904900
C	-0.04003100	0.64366400	-2.61360600
C	-1.40881600	-1.61568800	-1.12611000
C	-2.22823100	-2.14948400	-0.11831100
C	-1.67452800	-2.00496200	-2.45014000
C	-3.29473000	-3.00424600	-0.42333000
H	-2.03616400	-1.91495700	0.92144000
C	-2.74235900	-2.85627700	-2.75846500
H	-1.04579500	-1.66130800	-3.26520800
C	-3.56317800	-3.35695700	-1.74690800
H	-3.91111700	-3.39648700	0.38314400
H	-2.92342100	-3.13010200	-3.79569500
H	-4.39050600	-4.02073900	-1.98518800
Pd	0.07715600	-0.22256100	-0.68722500
P	1.26323900	-2.05323700	0.11462200
C	1.25887300	-3.32065900	2.46046500
H	1.48860600	-4.29031500	2.00045400
H	2.20934100	-2.82495400	2.68206000
C	0.23370800	-4.46719300	-0.75487000
H	-0.28041000	-4.46067600	0.21119600
H	-0.50984500	-4.27684000	-1.53391200
O	2.72061600	-1.76901900	0.36772100
O	1.22346300	-3.42712100	-0.79218700
O	0.50869900	-2.51155600	1.52940800
C	0.41797000	-3.50682100	3.71248500
H	0.20230300	-2.54038100	4.18230100
H	0.95328700	-4.12944500	4.43900500
H	-0.53465700	-3.99295000	3.47615600
C	0.93498200	-5.79694000	-0.99448000
H	0.20085300	-6.61182400	-1.00928900
H	1.66948700	-6.00297800	-0.20847100
H	1.45994500	-5.78705400	-1.95537900

12c

SCF energy: -2851.682240

SCF energy in solution: -2850.8764302200

Free energy in solution: -2850.2386532200

P	-1.86095300	-1.12434000	-0.74544900
C	1.50983500	-3.05514800	-1.19778000
H	1.33610600	-2.97578900	-2.27611500
H	2.42371300	-3.64579300	-1.07573900
C	-1.45360600	-2.48719500	-1.97400700
H	-2.35294900	-2.68360600	-2.56865200
H	-0.71006000	-2.07263100	-2.66504500
C	0.30806100	-3.73779900	-0.50695600
H	0.06476300	-3.23276300	0.43615900
H	0.58941200	-4.75952800	-0.22605500
C	-0.95021700	-3.81532300	-1.38465100
H	-0.75048500	-4.49182800	-2.22815700
H	-1.75615200	-4.27776800	-0.80401800
P	1.86713700	-1.34128400	-0.52412500
C	2.63987200	-1.80160500	1.08931800
C	3.81989700	-2.56183000	1.15287800
C	1.99722600	-1.44907100	2.28477900
C	4.34350700	-2.95625600	2.38348300
H	4.34074300	-2.83590100	0.23924500
C	2.51795800	-1.85163600	3.51739500
H	1.09273700	-0.84719800	2.24421500
C	3.69151500	-2.60371100	3.56868800
H	5.26019200	-3.53908700	2.41777000
H	2.00802100	-1.56985900	4.43462800
H	4.10026300	-2.91296500	4.52698600
C	3.27690800	-0.80212000	-1.58438300
C	4.38483600	-0.13419900	-1.03992800
C	3.21519800	-0.97489000	-2.97719900
C	5.41329600	0.32316300	-1.86431800
H	4.43938700	0.04497000	0.02831700
C	4.24497000	-0.51712600	-3.80005200
H	2.36033400	-1.46452800	-3.43515100
C	5.35056400	0.12919500	-3.24494300
H	6.26068700	0.84065900	-1.42318400
H	4.18088500	-0.66668200	-4.87465200
H	6.15295200	0.48587200	-3.88509200
C	-3.02963300	-0.10814100	-1.75667600
C	-4.08880900	0.57961000	-1.14250300
C	-2.83670200	0.03763700	-3.14081500
C	-4.94736800	1.37073500	-1.90646800
H	-4.20963700	0.52564900	-0.06628300
C	-3.69500600	0.83648400	-3.89840900
H	-2.01753100	-0.46921100	-3.64227900

C	-4.75715600	1.50077200	-3.28343900
H	-5.76226900	1.89676700	-1.41643700
H	-3.53255500	0.93515900	-4.96870900
H	-5.42753600	2.12094000	-3.87286200
C	-2.93722700	-2.02476500	0.44691800
C	-4.08249700	-2.71002300	0.00941900
C	-2.58347500	-2.08702000	1.80087000
C	-4.85113400	-3.45048600	0.90761300
H	-4.38482200	-2.65688600	-1.03328900
C	-3.35102800	-2.83228900	2.69814300
H	-1.72989400	-1.52116600	2.15597400
C	-4.48325000	-3.51604400	2.25394100
H	-5.73768800	-3.97255500	0.55716400
H	-3.07035100	-2.86489700	3.74745200
H	-5.08300500	-4.09142000	2.95436700
C	1.55315300	1.66147400	0.10851500
C	2.26810800	1.99361300	1.26844900
C	1.89874200	2.32278300	-1.08329600
C	3.29297600	2.94691800	1.23852800
H	2.01342600	1.52826800	2.21491000
C	2.91324400	3.28546300	-1.11525800
H	1.37430200	2.08760700	-2.00788700
C	3.61796900	3.60030000	0.04806700
H	3.83024400	3.18503900	2.15467400
H	3.15300700	3.78395800	-2.05231500
H	4.40876300	4.34646900	0.02765100
Pd	0.06162900	0.23317000	-0.04798000
P	-1.39533400	1.67589200	1.06940000
C	-1.31126900	2.99261400	3.37821000
H	-1.81509700	3.88298200	2.97949100
H	-2.08330900	2.30299200	3.73487100
C	-1.05135600	4.06706000	-0.18601800
H	-0.36689300	4.32354600	0.63079600
H	-0.44540900	3.74628300	-1.03995600
O	-2.63777400	0.99046300	1.58174300
O	-1.91650900	2.99607800	0.21967800
O	-0.55794300	2.36072000	2.32446400
C	-0.34401500	3.37257000	4.48709800
H	0.14671700	2.48180000	4.89448000
H	-0.87917900	3.87508600	5.30171900
H	0.43144600	4.04877500	4.11186000
C	-1.92427200	5.25441500	-0.56331500
H	-1.30062700	6.09128700	-0.89995100
H	-2.52070900	5.58689500	0.29304500
H	-2.61071500	4.98434700	-1.37275400

TS9c

SCF energy: -2851.659052

SCF energy in solution: -2850.8565232500

Free energy in solution: -2850.2207432500

P	1.64370900	-1.58536400	0.24485500
C	-1.94501600	-3.11143600	-0.37204500
H	-1.80981700	-3.58689300	0.60717100
H	-2.87650900	-3.50853500	-0.79009000
C	1.05308200	-3.33527300	0.59552900
H	1.88833300	-3.91824200	1.00156600
H	0.32232000	-3.24029900	1.40773700
C	-0.75371900	-3.43891000	-1.30413400
H	-0.41497400	-2.53594700	-1.82660000
H	-1.09217600	-4.12456900	-2.09015500
C	0.44242100	-4.09733000	-0.59448400
H	0.13156600	-5.08559400	-0.22554800
H	1.22727000	-4.28229000	-1.33793200
P	-2.15730200	-1.26956800	-0.07318800
C	-3.06710900	-0.79247100	-1.61759900
C	-4.43544800	-1.04566200	-1.80239600
C	-2.34335600	-0.18722200	-2.65866700
C	-5.06378100	-0.70951200	-3.00224900
H	-5.01696300	-1.49730500	-1.00342300
C	-2.97286800	0.13927000	-3.86290300
H	-1.28946900	0.04810900	-2.52324100
C	-4.33306200	-0.11997300	-4.03702200
H	-6.12553100	-0.90663500	-3.12793900
H	-2.39740500	0.60658900	-4.65765500
H	-4.82432000	0.14171300	-4.97066800
C	-3.46186600	-1.23030000	1.23823700
C	-3.63771500	-0.03006700	1.94803100
C	-4.26155700	-2.33365600	1.58221400
C	-4.59395500	0.06762500	2.95920000
H	-3.01931000	0.82928300	1.71249200
C	-5.21251200	-2.23699600	2.60096700
H	-4.15201800	-3.27754600	1.05760400
C	-5.38331100	-1.03558700	3.29039900
H	-4.71369200	1.00673900	3.49291900
H	-5.82022000	-3.10242700	2.85307900
H	-6.12327500	-0.96158400	4.08304300
C	2.65265200	-1.29174100	1.76919700
C	4.02938600	-1.02970400	1.74698100
C	1.98652300	-1.26816600	3.00722200
C	4.72367900	-0.76534300	2.93078700
H	4.56511800	-1.02757600	0.80366700

C	2.68120100	-1.01233900	4.18901300
H	0.91242900	-1.43332200	3.04828300
C	4.05495600	-0.75955100	4.15517100
H	5.79148500	-0.56468200	2.89194200
H	2.14716000	-1.00368000	5.13584400
H	4.59679100	-0.55563300	5.07488200
C	2.87719500	-1.87015500	-1.09997000
C	3.83565100	-2.89740300	-1.02647700
C	2.82638600	-1.06973900	-2.25175100
C	4.72538100	-3.11677600	-2.07765600
H	3.89609100	-3.52541000	-0.14140700
C	3.72065500	-1.29358500	-3.30363700
H	2.09891400	-0.26509700	-2.32491000
C	4.66818300	-2.31362200	-3.22059800
H	5.46148300	-3.91350000	-2.00564300
H	3.67109200	-0.66369300	-4.18790800
H	5.36075200	-2.48538800	-4.04071900
C	-0.76844400	2.09450400	0.38241300
C	-1.86666100	2.59680300	-0.34441200
C	-0.64021500	2.45587500	1.74091900
C	-2.82893500	3.39369000	0.28030800
H	-1.97462700	2.34841600	-1.39594200
C	-1.60956900	3.24379900	2.36343100
H	0.22829800	2.12475100	2.30382000
C	-2.70656800	3.71550600	1.63542100
H	-3.67908300	3.75840600	-0.29133100
H	-1.50177600	3.50132500	3.41448700
H	-3.45397000	4.34065200	2.11726200
Pd	-0.09007000	0.05274100	0.06847300
P	1.06533600	1.99951300	-0.69196800
C	0.62884700	4.54738100	-1.47417500
H	0.79844300	4.17685000	-2.49045700
H	-0.45401200	4.58272700	-1.29771600
C	3.68331900	2.42101700	-0.05164400
H	4.46233300	1.67553200	-0.24341900
H	3.60741100	3.07448900	-0.92411100
O	0.97295200	1.68946000	-2.16788100
O	2.46031100	1.65991700	0.11169900
O	1.23435300	3.65138700	-0.53294900
C	1.24292500	5.92503800	-1.27564500
H	1.07522100	6.28112300	-0.25365600
H	0.79084600	6.64265900	-1.97052300
H	2.32256800	5.90096700	-1.45892400
C	3.98453800	3.21525300	1.20833000
H	4.94769600	3.73190900	1.10919200
H	4.03772300	2.54891600	2.07590700
H	3.20393900	3.96117800	1.38220400

2d

SCF energy: -2638.858576

SCF energy in solution: -2638.01716823

Free energy in solution: -2637.40445923

P	-2.41585900	-0.36652000	-0.31018400
C	0.04337600	1.40218700	-2.88755300
H	-0.30314700	2.33907700	-3.34125500
H	1.01112900	1.15973100	-3.33739700
C	-2.99448000	0.76983200	-1.66947700
H	-4.08950400	0.76500700	-1.73668500
H	-2.70315400	1.77760300	-1.35481400
C	-0.91220500	0.24053600	-3.23176700
H	-0.59756700	-0.64660100	-2.66996900
H	-0.74876300	-0.00104200	-4.29134400
C	-2.42773500	0.45914500	-3.07109900
H	-2.74105400	1.27799200	-3.73467600
H	-2.92405800	-0.44340000	-3.44987900
P	0.43160800	1.64028000	-1.06677100
C	2.10805700	2.42645400	-1.08684400
C	2.79754100	2.49905600	0.13312700
C	2.69906900	2.99125300	-2.22688300
C	4.04174800	3.12488000	0.21313500
H	2.36697500	2.04969300	1.02283700
C	3.94743800	3.61246800	-2.14770700
H	2.19417600	2.95606200	-3.18726100
C	4.62148600	3.68333400	-0.92766000
H	4.55970800	3.16257300	1.16757400
H	4.39059400	4.04309800	-3.04227100
H	5.59284500	4.16739000	-0.86769900
C	-0.57148300	3.11600400	-0.54311100
C	-0.68323100	4.27510800	-1.32858200
C	-1.19435000	3.09507300	0.71349200
C	-1.41515900	5.37349700	-0.87818000
H	-0.18227000	4.33276600	-2.29134200
C	-1.92343000	4.19712100	1.16919400
H	-1.11028500	2.20526100	1.33163800
C	-2.03899200	5.33618500	0.37235200
H	-1.49281100	6.26202200	-1.49964600
H	-2.40259600	4.15846000	2.14370200
H	-2.60742000	6.19365800	0.72303500
C	-3.47811100	0.07825000	1.13421600
C	-3.21905600	-0.59653000	2.34111600
C	-4.48227600	1.05680200	1.11114600

C	-3.96134200	-0.31442000	3.48646600
H	-2.42526500	-1.33908100	2.38039300
C	-5.21770800	1.34595400	2.26439000
H	-4.69779200	1.60634800	0.20044900
C	-4.96330000	0.65981500	3.45182300
H	-3.75152200	-0.84949700	4.40887500
H	-5.99184100	2.10842600	2.22985800
H	-5.53749700	0.88501200	4.34662200
C	-3.08339300	-2.01827800	-0.81008100
C	-4.38738900	-2.17803900	-1.30722900
C	-2.26486200	-3.14936900	-0.66978900
C	-4.85894000	-3.43935800	-1.66923600
H	-5.04499600	-1.31793500	-1.40428900
C	-2.74301400	-4.41363800	-1.02712500
H	-1.26177200	-3.03789700	-0.26572600
C	-4.03546100	-4.56052300	-1.53092900
H	-5.86955500	-3.54865100	-2.05441600
H	-2.10218900	-5.28326300	-0.90667500
H	-4.40472500	-5.54390300	-1.81030900
O	0.39914600	-2.05281400	1.18259800
C	1.55639200	-1.52827600	0.93746800
C	2.32854700	-0.82544700	2.00206700
C	3.65991800	-0.41969700	1.81975500
C	1.70693100	-0.55684400	3.23518200
C	4.34854300	0.24049700	2.83845900
H	4.15833100	-0.61252500	0.87513400
C	2.39515600	0.10707300	4.24673300
H	0.68580900	-0.89055900	3.38566600
C	3.72049300	0.51222000	4.05516400
H	5.38103700	0.54158100	2.67816700
H	1.90009900	0.29930300	5.19552500
H	4.25799400	1.02523800	4.84829900
C	3.52054700	-4.53622200	-0.43846900
C	3.43370500	-2.83573800	-2.23461900
C	4.34332900	-3.81920100	-1.50385300
H	4.11858900	-5.19984600	0.19111700
H	2.66203200	-3.38676700	-2.79313300
H	5.17840300	-3.28185500	-1.03577200
N	2.39428900	-2.32073900	-0.01741900
C	2.70618400	-1.86973800	-1.30633100
C	2.80213000	-3.58081600	0.50248200
O	2.40452300	-0.75544800	-1.70306400
O	2.56873700	-3.88367100	1.65357200
H	3.97137200	-2.21956800	-2.95972800
H	4.78009500	-4.53709300	-2.20671100
H	2.74970000	-5.15685400	-0.91921800
Pd	-0.05418800	-0.32846600	0.09902800

TS1d

SCF energy: -2638.832927

SCF energy in solution: -2637.99202351

Free energy in solution: -2637.38025951

P	-2.44820500	-1.07697600	0.30977100
C	0.51255000	-3.00155900	1.39396300
H	0.03865800	-3.62199500	0.62651900
H	1.31215300	-3.61007000	1.82817900
C	-2.54775600	-2.86234200	0.87142500
H	-3.59291500	-3.19235200	0.88332900
H	-2.04136200	-3.44909700	0.09528500
C	-0.51003500	-2.58527900	2.47779600
H	-0.56867700	-1.49225000	2.53610000
H	-0.16082700	-2.92204100	3.46119000
C	-1.93056200	-3.13819900	2.25554300
H	-1.92762000	-4.22640500	2.40883900
H	-2.58722900	-2.72053500	3.02896000
P	1.31522700	-1.58162700	0.44922700
C	2.79953000	-1.26240600	1.51011300
C	4.11326900	-1.34536900	1.02941900
C	2.59890800	-0.91196200	2.85699300
C	5.19692100	-1.10907000	1.87874100
H	4.29752600	-1.58697600	-0.01125800
C	3.68129000	-0.68451400	3.70531800
H	1.59042900	-0.80822100	3.24784700
C	4.98703800	-0.78649500	3.21883800
H	6.20766700	-1.17510100	1.48490900
H	3.50419400	-0.42305400	4.74555700
H	5.83205400	-0.60672200	3.87819200
C	1.98698400	-2.49927400	-1.00618100
C	2.72762400	-3.68587400	-0.85409400
C	1.69712500	-2.04102600	-2.30015800
C	3.16548000	-4.39720800	-1.97030200
H	2.97413100	-4.05274700	0.13846200
C	2.13947200	-2.75705400	-3.41702600
H	1.14243600	-1.11724700	-2.43344500
C	2.87016000	-3.93368700	-3.25581300
H	3.73747300	-5.31192600	-1.83725900
H	1.91069500	-2.38748500	-4.41302800
H	3.21197800	-4.48870800	-4.12565800
C	-3.28835200	-1.14523200	-1.33708600
C	-2.88232000	-0.22114300	-2.31524100
C	-4.28412800	-2.07920900	-1.67169800

C	-3.46911500	-0.21890700	-3.58198400
H	-2.08875500	0.48582700	-2.09114500
C	-4.86793300	-2.07813000	-2.93988800
H	-4.60960900	-2.82081100	-0.94857800
C	-4.46455700	-1.14503600	-3.89687100
H	-3.13626800	0.50116300	-4.32459200
H	-5.63531200	-2.80972500	-3.17969200
H	-4.91747300	-1.14684800	-4.88483700
C	-3.67349700	-0.27822900	1.44641900
C	-5.06291200	-0.39068000	1.28314400
C	-3.18098100	0.44235600	2.54600800
C	-5.93664700	0.18998400	2.20380000
H	-5.46887800	-0.92065500	0.42668000
C	-4.05510400	1.01419100	3.47250300
H	-2.10955400	0.57687500	2.66095200
C	-5.43494400	0.88889200	3.30397500
H	-7.01013600	0.09762600	2.05956500
H	-3.65652300	1.56910100	4.31798400
H	-6.11630600	1.34038200	4.02040500
O	0.80386600	1.09009800	-2.22701900
C	1.09726800	1.38701600	-1.06960200
C	2.49695900	1.66616400	-0.60247700
C	2.77230100	2.14727900	0.68216800
C	3.55177800	1.43042200	-1.49297500
C	4.08380400	2.41954500	1.06273600
H	1.94942900	2.32038200	1.36979100
C	4.86593800	1.69478100	-1.10669400
H	3.32287400	1.07450600	-2.49188400
C	5.13525200	2.19581600	0.16827100
H	4.28917400	2.80092300	2.05956100
H	5.67857800	1.52504100	-1.80891700
H	6.15839900	2.41134100	0.46585100
C	-0.12719400	5.50758900	-1.24636800
C	-1.84772000	4.26539900	0.04753500
C	-1.03013400	5.55555900	-0.01479200
H	0.56294500	6.35390200	-1.30041700
H	-2.58683400	4.24257800	-0.76666800
H	-0.41757300	5.64981700	0.89164900
N	0.22998400	3.08705800	-0.67767500
C	-0.97557300	3.02949800	-0.10803000
C	0.72306800	4.23460100	-1.30971700
O	-1.44300100	1.93814900	0.31432300
O	1.78080700	4.22518100	-1.91289100
H	-2.40877100	4.15979800	0.98075700
H	-1.69089900	6.42925500	-0.04526400
H	-0.73827100	5.53583200	-2.16093600
Pd	-0.21302500	0.15199100	0.03617800

3d

SCF energy: -2638.856103

SCF energy in solution: -2638.0118791700

Free energy in solution: -2637.3999231700

P	-1.94344000	-0.82727700	0.23260400
C	0.96154800	-2.75019300	1.96220100
H	0.66546100	-3.74603600	1.61413100
H	1.87081900	-2.89025900	2.55313900
C	-2.01090600	-2.51258600	1.04283600
H	-3.03629700	-2.89211500	0.97312000
H	-1.38689000	-3.17282900	0.42765100
C	-0.14349300	-2.12849600	2.84415500
H	-0.07329300	-1.03519300	2.79372400
H	0.05479800	-2.39966400	3.88915900
C	-1.57815000	-2.57723900	2.51629300
H	-1.70032600	-3.62038400	2.84103100
H	-2.27480900	-1.98657700	3.12430700
P	1.47224000	-1.72316400	0.46388600
C	3.31426100	-1.69063200	0.61851200
C	4.14556800	-1.95364000	-0.47993200
C	3.90394100	-1.32438300	1.84017900
C	5.53342800	-1.87275500	-0.35237900
H	3.71333800	-2.22052500	-1.43821800
C	5.29072200	-1.24925300	1.96613500
H	3.28459800	-1.07931700	2.69883300
C	6.11010400	-1.52613000	0.86985900
H	6.16253400	-2.08156500	-1.21339600
H	5.72848900	-0.96571100	2.91931000
H	7.19065000	-1.46528300	0.96687700
C	1.20068100	-2.78860500	-1.01190400
C	1.45800400	-4.17068800	-0.99960100
C	0.76621000	-2.18617700	-2.20230200
C	1.26466200	-4.93415200	-2.15023100
H	1.82382100	-4.65468800	-0.09798500
C	0.57846100	-2.95300300	-3.35505300
H	0.57240400	-1.11793800	-2.22624100
C	0.82222500	-4.32599700	-3.32899400
H	1.46333000	-6.00239900	-2.12816500
H	0.22954900	-2.47234600	-4.26408800
H	0.67027300	-4.92356800	-4.22383000
C	-2.60092400	-1.18197700	-1.45536600
C	-2.34155900	-0.23422700	-2.45820800
C	-3.33331800	-2.33596100	-1.78543700

C	-2.81870900	-0.42415500	-3.75627000
H	-1.75652100	0.65430600	-2.23522500
C	-3.80220800	-2.52624300	-3.08688200
H	-3.54187000	-3.09853100	-1.04177200
C	-3.54960600	-1.56999500	-4.07402300
H	-2.60213800	0.33736900	-4.49965400
H	-4.36607800	-3.42431600	-3.32709900
H	-3.91969600	-1.72270200	-5.08492700
C	-3.31760700	0.05190100	1.10246100
C	-4.66623200	-0.23795000	0.83753300
C	-3.00810200	1.00360000	2.08670800
C	-5.68098500	0.39965200	1.55099500
H	-4.92616300	-0.95194200	0.06113000
C	-4.02723700	1.63599400	2.80409400
H	-1.97349800	1.27703400	2.26433300
C	-5.36346400	1.33491400	2.53955700
H	-6.72035300	0.16956400	1.33136000
H	-3.77289300	2.37422700	3.56021100
H	-6.15557200	1.83265600	3.09287400
O	2.64215100	1.33668800	-0.85009500
C	2.09055700	1.27743700	0.22700300
C	2.64507500	1.98749900	1.43274900
C	2.00069800	1.95572100	2.67547800
C	3.85692100	2.68420600	1.30052100
C	2.56079000	2.60637200	3.77513100
H	1.05326100	1.43292100	2.76430400
C	4.41548300	3.33382300	2.39827000
H	4.34231200	2.69859100	0.32977800
C	3.76884400	3.29461900	3.63816200
H	2.05247400	2.58407900	4.73562600
H	5.35483600	3.87026800	2.29135600
H	4.20475100	3.80282600	4.49464600
C	-1.45028400	4.75040100	-2.48679500
C	-1.14160100	4.43656600	-0.03400700
C	-0.80330500	5.33195200	-1.22999000
H	-1.10205800	5.23650000	-3.40330300
H	-2.21920900	4.48416300	0.18306500
H	0.28708700	5.36846400	-1.35544700
N	-0.82084900	2.47913300	-1.56073100
C	-0.78125000	2.98933900	-0.34482300
C	-1.21703500	3.24010900	-2.64667900
O	-0.43660600	2.27715000	0.66489400
O	-1.41473600	2.72064500	-3.74220100
H	-0.61652700	4.73859700	0.87654300
H	-1.13882300	6.36077000	-1.05255700
H	-2.53997700	4.89955600	-2.45139700
Pd	0.31914000	0.28811700	0.33929600

4d

SCF energy: -2638.873415

SCF energy in solution: -2638.0321829000

Free energy in solution: -2637.4188499000

P	-2.06513800	-0.77150100	0.14371400
C	0.78729300	-2.52160300	2.15206500
H	0.60785800	-3.58504600	1.95535600
H	1.66228500	-2.47724000	2.80678700
C	-2.14037800	-2.44473700	0.97689100
H	-3.14280100	-2.86845200	0.84776400
H	-1.44529200	-3.08939600	0.42530200
C	-0.41998500	-1.89112500	2.87870800
H	-0.39247900	-0.80110300	2.76248600
H	-0.29850800	-2.08229000	3.95315700
C	-1.79815500	-2.44391900	2.47637000
H	-1.87590300	-3.48405900	2.82469200
H	-2.56807900	-1.88444900	3.02195900
P	1.33516900	-1.67843400	0.55514400
C	3.17279300	-1.64265300	0.77470600
C	4.05200400	-2.18400000	-0.17361300
C	3.70903700	-1.01300100	1.91089000
C	5.43347300	-2.11193700	0.01938800
H	3.66410800	-2.66342800	-1.06565600
C	5.08804600	-0.94712400	2.10394400
H	3.05067000	-0.55566000	2.64471500
C	5.95536100	-1.49874000	1.15827500
H	6.10022600	-2.53841600	-0.72535600
H	5.48334600	-0.45463200	2.98807800
H	7.03050000	-1.44414500	1.30617400
C	1.11303700	-2.89891800	-0.80856600
C	1.21822400	-4.28800100	-0.62722500
C	0.87847400	-2.39689900	-2.09896100
C	1.06744500	-5.15607300	-1.70918800
H	1.43169400	-4.70182600	0.35420400
C	0.73704000	-3.26803300	-3.18130600
H	0.81712000	-1.32359700	-2.25278600
C	0.82408100	-4.64715000	-2.98760500
H	1.14540400	-6.22896700	-1.55406200
H	0.54790100	-2.86365200	-4.17140900
H	0.70594900	-5.32502200	-3.82882200
C	-2.48823900	-1.16505500	-1.60990600
C	-2.13425800	-0.22781300	-2.59659900
C	-3.13585500	-2.34904300	-2.00023800

C	-2.43033200	-0.47388900	-3.93911200
H	-1.61965100	0.69131700	-2.32318500
C	-3.42298900	-2.59260000	-3.34471900
H	-3.42189100	-3.09243600	-1.26324900
C	-3.07177100	-1.65477700	-4.31770300
H	-2.14934900	0.26189900	-4.68787800
H	-3.92221900	-3.51541900	-3.62911100
H	-3.29662700	-1.84495700	-5.36415800
C	-3.59053300	0.04459800	0.80015100
C	-4.81400700	0.01313700	0.11155900
C	-3.53200600	0.68572000	2.04965200
C	-5.95400500	0.59939100	0.66446300
H	-4.87907000	-0.46640300	-0.85972000
C	-4.67762800	1.26342600	2.60207200
H	-2.58639800	0.76779200	2.57612200
C	-5.89080200	1.22168800	1.91259200
H	-6.89220400	0.56937300	0.11625500
H	-4.61448700	1.75511000	3.56940500
H	-6.77964600	1.67759800	2.34100400
O	2.27414900	0.94317300	-1.50072100
C	1.93620600	1.19830800	-0.36133500
C	2.74006800	2.13816200	0.49137300
C	2.45325300	2.33709800	1.84705900
C	3.82804300	2.80808300	-0.09409200
C	3.24728900	3.19461800	2.61113400
H	1.59892300	1.83500600	2.29093700
C	4.61394700	3.66713300	0.66865300
H	4.03670600	2.63828700	-1.14567100
C	4.32616800	3.85982000	2.02469600
H	3.01797100	3.34735800	3.66262800
H	5.45209600	4.18663300	0.21096800
H	4.94148200	4.52978700	2.62037200
C	-1.46019300	4.48873400	-0.57765500
C	-1.47505500	4.14145300	1.87952500
C	-1.08818200	5.11289400	0.76557900
H	-1.09212500	5.06617000	-1.43055400
H	-2.56956000	4.03495900	1.92442300
H	-0.00681500	5.30071700	0.80096300
N	-0.65066200	2.31260000	0.38220400
C	-0.89162700	2.74813600	1.65835500
C	-0.92988300	3.06357600	-0.73902000
O	-0.66333300	2.02334000	2.63764400
O	-0.77823500	2.59997800	-1.86978100
H	-1.14692800	4.47693000	2.86746100
H	-1.58553300	6.08083100	0.89900100
H	-2.55476300	4.43933600	-0.67883400
Pd	0.18377500	0.33801600	0.21408000

TS2d

SCF energy: -2638.807635

SCF energy in solution: -2637.963813

Free energy in solution: -2637.353171

P	-1.58514200	0.59453900	-1.17658700
C	1.77423900	-0.42758600	-2.92030400
H	1.66358500	0.58162400	-3.33005300
H	2.69153900	-0.82656900	-3.36562000
C	-1.09362700	0.73754600	-2.97789700
H	-1.91174000	1.23678700	-3.51000600
H	-0.27077700	1.46197400	-2.96829600
C	0.54779900	-1.30243400	-3.26301500
H	0.25527400	-1.89000800	-2.38528900
H	0.81876500	-2.02783300	-4.04083200
C	-0.67617700	-0.51589000	-3.77100700
H	-0.46772200	-0.17484700	-4.79527900
H	-1.51962500	-1.21175700	-3.84972200
P	2.06541100	-0.20683100	-1.07458300
C	3.30600500	-1.52366000	-0.69858000
C	4.09079900	-1.41553600	0.46358000
C	3.43783800	-2.66821600	-1.50121500
C	4.99958000	-2.42141200	0.79224400
H	3.96589200	-0.55871500	1.11685200
C	4.34399100	-3.67566400	-1.16120300
H	2.83472400	-2.79139300	-2.39556100
C	5.13187500	-3.55225800	-0.01690700
H	5.60123400	-2.32202700	1.69182200
H	4.43335100	-4.55380100	-1.79560100
H	5.83898700	-4.33444400	0.24631000
C	3.07377000	1.33765900	-1.08458500
C	4.38383200	1.34575400	-1.58996900
C	2.50032800	2.54426200	-0.66545000
C	5.09988200	2.53982400	-1.67756500
H	4.85093700	0.41723100	-1.90540400
C	3.21565000	3.73958800	-0.75911500
H	1.49702400	2.54723000	-0.25635500
C	4.51641000	3.73988900	-1.26407100
H	6.11480100	2.53177800	-2.06657000
H	2.75662000	4.66758100	-0.42856700
H	5.07609700	4.66916000	-1.33098400
C	-1.84542700	2.39152700	-0.81238900
C	-1.12280300	3.02359600	0.20670400
C	-2.76550000	3.14375700	-1.56214800

C	-1.29678700	4.38866300	0.45334600
H	-0.44783100	2.43725400	0.82166000
C	-2.93800600	4.50451800	-1.31372100
H	-3.36666900	2.66531900	-2.33080100
C	-2.19881200	5.13195600	-0.30716700
H	-0.73205000	4.86622200	1.25001200
H	-3.65449700	5.07323300	-1.90070500
H	-2.33561900	6.19233700	-0.11177800
C	-3.31986300	-0.02679500	-1.19394900
C	-3.98911200	-0.43541000	-2.35683500
C	-4.00614000	-0.04378900	0.03331600
C	-5.32103500	-0.85438000	-2.29705600
H	-3.48879700	-0.42496900	-3.31946300
C	-5.33743500	-0.45528100	0.08374200
H	-3.49449300	0.26764900	0.94069300
C	-5.99810200	-0.86297600	-1.07781100
H	-5.82677800	-1.16828400	-3.20664300
H	-5.85858800	-0.45890800	1.03731500
H	-7.03512200	-1.18550100	-1.03277300
O	1.25874900	-2.75624500	1.96189800
C	0.66734700	-2.04552400	1.26747400
C	-1.28485100	-2.35166500	0.77131300
C	-1.40666900	-3.40221200	-0.14921300
C	-2.18046400	-2.25515600	1.84282600
C	-2.44923600	-4.32409800	-0.02640700
H	-0.68785300	-3.51144900	-0.95658600
C	-3.21434500	-3.18760900	1.96477500
H	-2.09860300	-1.43543300	2.54761800
C	-3.35306500	-4.21852400	1.03298700
H	-2.54442500	-5.13039800	-0.74971200
H	-3.91518600	-3.10268600	2.79175400
H	-4.15774100	-4.94201900	1.13566800
C	1.63494000	1.63254700	4.13349200
C	-0.82599500	1.72920000	4.41589100
C	0.48815800	1.37503400	5.10861300
H	2.60031300	1.28381700	4.51116300
H	-0.87774800	2.81594100	4.24742500
H	0.47993500	0.31499800	5.39729600
N	0.13898500	0.72143400	2.31856800
C	-0.97005500	1.04821300	3.04958800
C	1.40885300	0.96355000	2.77244000
O	-2.11428400	0.83326900	2.62359100
O	2.40187900	0.67343700	2.09272800
H	-1.70529600	1.46157900	5.00872400
H	0.61690300	1.95418700	6.03097600
H	1.73734500	2.71415200	3.95576400
Pd	-0.00327400	-0.63227000	0.21184500

TS3d

SCF energy: -3364.967799

SCF energy in solution: -3363.2692315700

Free energy in solution: -3363.2692315700

P	1.81573400	1.29817200	0.98318800
C	-1.71368400	2.58999400	2.16454100
H	-2.05822100	3.63087400	2.17448800
H	-2.50607100	1.99903600	2.62551000
C	1.54717300	3.07826000	1.50188200
H	2.51776700	3.58451300	1.56915300
H	1.03303800	3.53150800	0.64764700
C	-0.46879200	2.40555300	3.04466500
H	-0.18160900	1.35063600	3.01322600
H	-0.80080300	2.58729500	4.07598800
C	0.74743100	3.30752300	2.79835500
H	0.43923000	4.36308200	2.82420700
H	1.42137800	3.17215800	3.65236300
P	-1.70368000	1.97216900	0.39531400
C	-3.52796300	1.76858400	0.11680300
C	-4.18015400	2.33679500	-0.98801800
C	-4.28007500	0.99603300	1.02050400
C	-5.55065500	2.14889600	-1.17904800
H	-3.62504200	2.93300600	-1.70343100
C	-5.65013100	0.81873600	0.82889400
H	-3.79222300	0.51424500	1.86226300
C	-6.29154100	1.39429700	-0.26977100
H	-6.03681800	2.59954000	-2.04044700
H	-6.21550500	0.22101300	1.53918900
H	-7.35882600	1.25180800	-0.41750200
C	-1.32091000	3.43993100	-0.67683800
C	-1.39651600	4.77060400	-0.23535900
C	-0.96962200	3.19718200	-2.01800100
C	-1.11558200	5.82895500	-1.10266200
H	-1.67393500	4.99935600	0.78798600
C	-0.70728600	4.25859100	-2.88709700
H	-0.91380000	2.17432600	-2.38109600
C	-0.77207400	5.57694300	-2.43140500
H	-1.17133200	6.85110400	-0.73714400
H	-0.44800000	4.05042500	-3.92198000
H	-0.55850700	6.40156300	-3.10631600
C	3.05844400	1.59248400	-0.36233200
C	2.61272100	2.15959800	-1.56717800
C	4.42435500	1.31106100	-0.21674700

C	3.51383500	2.46558500	-2.58697700
H	1.55541600	2.35625900	-1.71293200
C	5.32423900	1.60295600	-1.24593500
H	4.79317000	0.86666600	0.70181200
C	4.87471100	2.18830800	-2.43017600
H	3.14972000	2.91472000	-3.50760800
H	6.38002500	1.37960400	-1.11364300
H	5.57729100	2.42568000	-3.22496700
C	2.83961500	0.56472000	2.33044500
C	3.55372100	1.33212600	3.26571900
C	2.93590700	-0.83504400	2.38855200
C	4.32989400	0.71449600	4.24851200
H	3.52073100	2.41640900	3.22818500
C	3.72441200	-1.44896000	3.36419400
H	2.39713500	-1.44643300	1.67106200
C	4.41573800	-0.67827700	4.30087700
H	4.87100000	1.32302700	4.96862700
H	3.79086400	-2.53357200	3.39050700
H	5.02133700	-1.15820800	5.06543500
O	-1.40007900	-0.03170400	-2.46454000
C	-1.55425900	-0.52935000	-1.36787200
C	-2.49505800	-1.68339400	-1.18399500
C	-3.03684500	-2.02758800	0.05814100
C	-2.86608700	-2.40863500	-2.33021800
C	-3.94485300	-3.08371800	0.15404900
H	-2.76029200	-1.45508600	0.93271800
C	-3.75607500	-3.47376500	-2.22696700
H	-2.44150000	-2.12530200	-3.28731100
C	-4.29913400	-3.81289300	-0.98279900
H	-4.37766000	-3.33550600	1.11900800
H	-4.03200100	-4.03752800	-3.11452200
H	-5.00041500	-4.64000000	-0.90305900
C	0.02369500	-4.09638300	2.68430200
C	-1.23629800	-2.43269900	4.00943700
C	-1.23086600	-3.88321100	3.52544400
H	-0.01098600	-5.02438500	2.10398300
H	-0.36814900	-2.25547200	4.66206100
H	-2.12659500	-4.06774000	2.91683300
N	-0.32618300	-1.75946500	1.76749000
C	-1.15439900	-1.47801800	2.81645300
C	0.32094600	-2.95333000	1.69928900
O	-1.85728300	-0.45233700	2.83526700
O	1.20412300	-3.17613600	0.85010500
H	-2.13363500	-2.17852900	4.57959900
H	-1.26751100	-4.58500300	4.36753400
H	0.90523300	-4.17686200	3.33726600
Pd	-0.25799100	0.15438000	0.02310600
P	1.79863900	-2.30824400	-1.81366800
H	2.74104100	-2.88818100	-0.96058800
C	3.48528100	-1.26263100	-3.57481400
H	2.97156200	-0.30036700	-3.50935300
H	4.30224900	-1.26152000	-2.84076100
C	0.92716400	-4.81022600	-1.81723400
H	1.72263900	-5.14628200	-2.49376300
H	1.25401400	-4.91735700	-0.77924100
O	1.31423100	-0.95162500	-1.42024600
O	0.66492300	-3.40424400	-2.06277000
O	2.54832400	-2.31631700	-3.25234400
C	4.01512800	-1.52258100	-4.97330400
H	4.52788700	-2.48873000	-5.02481700
H	4.72559300	-0.73687800	-5.25406400
H	3.19622800	-1.52714100	-5.69979700
C	-0.35876500	-5.57224500	-2.07551600
H	-0.19783500	-6.64069700	-1.89019300
H	-0.68600900	-5.44457900	-3.11219700
H	-1.15544400	-5.21583700	-1.41624500

5d

SCF energy: -3364.977346

SCF energy in solution: -3364.0357665300

Free energy in solution: -3363.2803775300

P	1.89194700	1.20887500	0.92926500
C	-1.62078800	1.93221900	2.44679500
H	-2.06035900	2.85803800	2.83721000
H	-2.33880400	1.13117900	2.63725900
C	1.65225900	2.74277600	1.96539700
H	2.62648600	3.18310300	2.21019900
H	1.15319000	3.45723200	1.30305700
C	-0.34573700	1.54502000	3.21121000
H	-0.02294900	0.56165900	2.85536400
H	-0.66567800	1.38028000	4.24894500
C	0.84193800	2.52176900	3.26147800
H	0.50322600	3.50291500	3.62379100
H	1.52866900	2.13860600	4.02572300
P	-1.60228900	2.03903000	0.58439600
C	-3.40484800	1.88780200	0.20914000
C	-4.10257700	2.86584300	-0.51472900
C	-4.08784100	0.73905300	0.64840000
C	-5.46247600	2.70451100	-0.78806200
H	-3.59263000	3.75554600	-0.86785000
C	-5.44749800	0.58975300	0.37527800

H	-3.55861300	-0.03960700	1.19221800
C	-6.13855900	1.56865100	-0.34212400
H	-5.99067000	3.47144000	-1.34858100
H	-5.96462200	-0.30193800	0.71929100
H	-7.19720300	1.44496000	-0.55519200
C	-1.21694900	3.78922200	0.12835500
C	-1.33400400	4.86059200	1.02828200
C	-0.81759800	4.05687400	-1.19365300
C	-1.04337600	6.16492600	0.62289900
H	-1.65029700	4.69067000	2.05208300
C	-0.53943500	5.36405300	-1.59769200
H	-0.74245700	3.24178700	-1.90831600
C	-0.64461600	6.41997000	-0.69021300
H	-1.13234900	6.98087500	1.33525400
H	-0.23783700	5.55407600	-2.62427000
H	-0.42023000	7.43576700	-1.00446500
C	3.20514000	1.75264300	-0.25994100
C	2.79421300	2.23968200	-1.51226700
C	4.57934300	1.70902100	0.02437400
C	3.72920200	2.69414000	-2.44363000
H	1.73891400	2.23894500	-1.76984800
C	5.51414500	2.15690800	-0.91118500
H	4.92889500	1.31058200	0.97092400
C	5.09207100	2.65564400	-2.14514700
H	3.38994200	3.06222800	-3.40812800
H	6.57412200	2.11278200	-0.67397700
H	5.82144400	3.00165200	-2.87278600
C	2.72877900	0.02768000	2.06992100
C	3.69417300	0.42468300	3.01332000
C	2.38309200	-1.32944500	1.98830200
C	4.32177000	-0.52047500	3.82584400
H	3.95964800	1.47316600	3.11997500
C	3.02232400	-2.27749200	2.79253500
H	1.57877600	-1.65266300	1.33606000
C	3.99574400	-1.87490400	3.70737700
H	5.06509100	-0.19911600	4.55103300
H	2.74204600	-3.32177400	2.68952500
H	4.49206900	-2.60917600	4.33674700
O	-1.33531300	1.22244600	-2.86707300
C	-1.43396700	0.39349400	-1.98176800
C	-2.35562000	-0.77747100	-2.09164700
C	-2.40526000	-1.76605100	-1.10173600
C	-3.18562400	-0.87292100	-3.22269900
C	-3.28146700	-2.84364100	-1.24384600
H	-1.76840600	-1.70229700	-0.22264600
C	-4.06212300	-1.94477800	-3.35505400
H	-3.12726800	-0.09793500	-3.98036900
C	-4.11190400	-2.93270600	-2.36326000
H	-3.31211400	-3.60984700	-0.47393100
H	-4.70750800	-2.01488400	-4.22697500
H	-4.79975200	-3.76881200	-2.46594400
C	-0.51523500	-4.97240900	2.77100600
C	-2.05904500	-3.21215400	3.59597700
C	-1.93833100	-4.69777400	3.25492000
H	-0.39138200	-5.98047500	2.36318800
H	-1.44303500	-2.98237100	4.47904400
H	-2.65397900	-4.95047200	2.45991800
N	-0.62769600	-2.75168000	1.57384100
C	-1.57679400	-2.31844400	2.44448000
C	-0.05760400	-3.97484000	1.69780900
O	-2.07268400	-1.17898900	2.34789200
O	0.88734000	-4.32595700	0.95712000
H	-3.08352900	-2.91673300	3.84147100
H	-2.19180100	-5.32533400	4.11838900
H	0.18673500	-4.88950100	3.61496400
Pd	-0.11471900	0.59561700	-0.44899400
P	1.37609800	-2.27046900	-1.67322600
H	1.15483700	-2.98868900	-0.47925900
C	4.02626000	-2.15062900	-1.49891700
H	4.04074300	-1.05975900	-1.58101200
H	3.95953700	-2.41981300	-0.43772200
C	0.37176100	-4.38610300	-2.88094600
H	1.34125300	-4.76360400	-3.22287000
H	0.17198000	-4.78805300	-1.88065900
O	1.17838900	-0.77560300	-1.58680000
O	0.45247800	-2.93461900	-2.79792300
O	2.85521600	-2.65189400	-2.19399700
C	5.24959800	-2.77513000	-2.14357100
H	5.22369600	-3.86565500	-2.05210300
H	6.15683200	-2.40643700	-1.65203600
H	5.30007400	-2.51583700	-3.20586900
C	-0.73579500	-4.73392100	-3.85638600
H	-0.81931000	-5.82316700	-3.94583500
H	-0.52165700	-4.31934600	-4.84659700
H	-1.69316800	-4.33415100	-3.51025600

6d

SCF energy: -3364.980829

SCF energy in solution: -3364.0379390100

Free energy in solution: -3363.2835900100

P	-0.94640600	2.33743800	0.76830500

C	-2.75606000	-0.48391500	2.57534800
H	-3.64649000	0.15242500	2.62678700
H	-3.01134000	-1.41583400	3.08873500
C	-2.09954100	2.53840800	2.21877200
H	-2.13246400	3.59789500	2.49963500
H	-3.10357900	2.27037800	1.86623700
C	-1.55226200	0.19687700	3.26258000
H	-0.62461500	-0.02226200	2.72548700
H	-1.41867500	-0.25124700	4.25449800
C	-1.72117800	1.71324000	3.46232200
H	-2.50288900	1.89023700	4.21479400
H	-0.79189400	2.11160500	3.88622600
P	-2.54761300	-0.95528200	0.76120500
C	-2.37578000	-2.78619900	0.87132100
C	-3.18885600	-3.65725200	0.13234800
C	-1.36870000	-3.31593800	1.69781900
C	-3.01586900	-5.03927600	0.23654800
H	-3.95839000	-3.26245300	-0.52310400
C	-1.20740900	-4.69750100	1.79967800
H	-0.68388900	-2.66139100	2.23304800
C	-2.03080400	-5.56225200	1.07461600
H	-3.65405100	-5.70430600	-0.33927800
H	-0.42607200	-5.09702800	2.44060600
H	-1.89846100	-6.63790700	1.15565100
C	-4.23223400	-0.66635600	0.07854600
C	-5.37442800	-1.14608100	0.74497100
C	-4.39198100	0.07866000	-1.09884000
C	-6.64812800	-0.87927000	0.24531600
H	-5.27027800	-1.73669900	1.65123100
C	-5.67079000	0.34430800	-1.59635100
H	-3.51618200	0.43244800	-1.63278400
C	-6.79784700	-0.13094700	-0.92620000
H	-7.52291600	-1.25581300	0.76876100
H	-5.78014300	0.92018300	-2.51106200
H	-7.79135500	0.07628800	-1.31490700
C	-1.51269400	3.63712800	-0.41316100
C	-0.83299000	3.74990000	-1.64104200
C	-2.60742300	4.48151300	-0.16765500
C	-1.23246600	4.69588300	-2.58447600
H	-0.00317700	3.08487400	-1.85947500
C	-3.00798200	5.42204100	-1.12053500
H	-3.16077700	4.41707700	0.76316200
C	-2.32044700	5.53419400	-2.32877000
H	-0.69588600	4.76965700	-3.52657900
H	-3.85814900	6.06671900	-0.91291400
H	-2.63284500	6.26633200	-3.06872000
C	0.63315300	2.98478200	1.46004500
C	0.88448400	4.36137600	1.58430100
C	1.57766800	2.06490400	1.94189700
C	2.05520400	4.80986600	2.19606500
H	0.16818400	5.08213000	1.19960600
C	2.74670200	2.52135600	2.55812600
H	1.41536100	0.99387000	1.84225500
C	2.98574700	3.88995000	2.68978900
H	2.24132500	5.87700800	2.28686100
H	3.47280100	1.79618500	2.91316800
H	3.89727100	4.24191900	3.16613500
O	-1.80796500	-1.19625000	-2.67487900
C	-0.98665100	-1.35169700	-1.79434200
C	0.00262200	-2.47247000	-1.81380700
C	0.93861800	-2.64672500	-0.78773700
C	-0.01171300	-3.35585700	-2.90760000
C	1.86032900	-3.69260200	-0.86030300
H	0.94794400	-1.97756100	0.06866200
C	0.90195800	-4.40248800	-2.97011900
H	-0.74212400	-3.19914200	-3.69499500
C	1.84156900	-4.57117000	-1.94508000
H	2.59347400	-3.81327000	-0.06835700
H	0.88879300	-5.08591000	-3.81535300
H	2.55765300	-5.38792200	-1.99533900
C	5.40132200	-1.90598900	2.15222400
C	3.28228600	-2.33174400	3.39235200
C	4.55860500	-2.97621600	2.84791500
H	6.25860100	-2.32486300	1.61674400
H	3.53275900	-1.65784300	4.22601300
H	4.29266500	-3.76034100	2.12476600
N	3.23731500	-0.92897800	1.30616100
C	2.55454500	-1.49934100	2.32790500
C	4.58240700	-1.08028300	1.15081800
O	1.31964700	-1.34652100	2.44577400
O	5.18452400	-0.53954400	0.20582600
H	2.57502100	-3.06729200	3.78781900
H	5.12510200	-3.46749400	3.64867900
H	5.80948500	-1.20878000	2.90018200
Pd	-0.89140300	0.14778800	-0.41503300
P	2.24886000	0.65127000	-1.59273800
H	2.70769300	0.05526400	-0.39659800
C	4.11233500	2.46469400	-0.89748300
H	3.60060900	3.10517300	-0.17403700
H	4.55718500	1.60981300	-0.37869800
C	3.98663200	-0.65802100	-3.09263000
H	4.48426100	0.22643800	-3.50517800

H	4.47622300	-0.92522800	-2.14942100
O	0.76029800	0.95090500	-1.61677200
O	2.59628100	-0.30620000	-2.83247500
O	3.11203200	1.98331500	-1.84900800
C	5.15356600	3.24357000	-1.67932500
H	5.66979000	2.59571500	-2.39517700
H	5.89925100	3.65452900	-0.98903500
H	4.69420000	4.07281600	-2.22752400
C	3.99443400	-1.80908200	-4.08004600
H	5.02872700	-2.08707700	-4.31350300
H	3.49199400	-1.52544900	-5.01067200
H	3.48272800	-2.68020700	-3.66067000

TS4d

SCF energy: -3364.970174

SCF energy in solution: -3364.0261843500

Free energy in solution: -3363.2751483500

P	-0.69116000	2.28305300	0.70166600
C	-2.14334200	-0.76718800	2.62326900
H	-3.13060200	-0.57241200	3.05952500
H	-1.85746500	-1.77868000	2.91910400
C	-1.89826600	2.44534900	2.11207700
H	-2.02026500	3.50123200	2.38106200
H	-2.86551500	2.09347500	1.73424200
C	-1.08655800	0.19206700	3.19796000
H	-0.17134300	0.10093600	2.60536200
H	-0.82425800	-0.19188700	4.19185700
C	-1.48849600	1.66383800	3.37448600
H	-2.32342000	1.72703200	4.08707100
H	-0.64598400	2.18401100	3.84726300
P	-2.32898200	-0.87219900	0.75551800
C	-2.73849600	-2.65734900	0.52064900
C	-3.84002200	-3.06783600	-0.24478100
C	-1.88661900	-3.62973700	1.07376600
C	-4.09812700	-4.42650400	-0.43719600
H	-4.50001900	-2.33209700	-0.69184200
C	-2.15507900	-4.98495000	0.88201900
H	-1.00630100	-3.33432500	1.63911600
C	-3.26026500	-5.38767300	0.12922100
H	-4.95691100	-4.72998200	-1.03018400
H	-1.49009600	-5.72658600	1.31616400
H	-3.46353200	-6.44492300	-0.01987300
C	-3.91046000	-0.01817500	0.33135500
C	-5.05384400	-0.10452100	1.14444500
C	-3.98538900	0.70854700	-0.86759400
C	-6.23593600	0.53771100	0.77594800
H	-5.03420800	-0.68480700	2.06258200
C	-5.17267600	1.34555000	-1.23766300
H	-3.11450700	0.76547400	-1.51394300
C	-6.29674500	1.26624900	-0.41535600
H	-7.11086500	0.46445000	1.41651000
H	-5.21218100	1.90428500	-2.16842900
H	-7.21913700	1.76478300	-0.70134400
C	-1.29500400	3.49877400	-0.54902100
C	-0.71637500	3.44585700	-1.83142200
C	-2.30364700	4.44263600	-0.29950000
C	-1.12853700	4.33166400	-2.82729400
H	0.04374000	2.69913100	-2.04688300
C	-2.71713400	5.32248100	-1.30331100
H	-2.78152200	4.49941100	0.67311400
C	-2.12844900	5.27202000	-2.56727300
H	-0.67287300	4.27716300	-3.81242500
H	-3.50056300	6.04628100	-1.09342600
H	-2.45129100	5.95693700	-3.34702400
C	0.83407800	3.06243700	1.38876700
C	0.94542900	4.45172700	1.56254800
C	1.90364500	2.23868600	1.77057500
C	2.10047000	5.00432400	2.11607500
H	0.13324100	5.10430100	1.25326500
C	3.06080500	2.79582700	2.32247200
H	1.84163700	1.16303200	1.62939800
C	3.16047800	4.17676600	2.49776400
H	2.17555300	6.08118100	2.24398300
H	3.88883600	2.14579500	2.59089600
H	4.06280400	4.60964500	2.92189700
O	-1.50013400	-1.14612100	-2.72181000
C	-0.74112900	-1.41650900	-1.81281000
C	0.06135800	-2.67759500	-1.79256900
C	0.97109300	-2.94680900	-0.76487000
C	-0.11610600	-3.60513400	-2.83279200
C	1.70210800	-4.13552800	-0.77886000
H	1.11223700	-2.23385600	0.04339600
C	0.61025400	-4.79208900	-2.83965800
H	-0.82426100	-3.37386000	-3.62216000
C	1.52222900	-5.05905900	-1.81088800
H	2.41010800	-4.33804000	0.02036500
H	0.46968000	-5.51074000	-3.64314900
H	2.08909500	-5.98711700	-1.81655600
C	4.76970900	-1.56377200	2.78974500
C	2.86122400	-2.55469300	4.04304400
C	4.29599700	-2.79251700	3.56674200

H	5.70963600	-1.73546700	2.25670400
H	2.84696400	-1.74264300	4.78624100
H	4.32398300	-3.67477000	2.91314400
N	2.44315800	-1.38802400	1.84412900
C	1.94341400	-2.14461000	2.88741300
C	3.73047400	-1.09567900	1.77811000
O	0.75627600	-2.47221400	2.91745300
O	4.20134900	-0.35512100	0.83768700
H	2.42377700	-3.43438900	4.52260300
H	4.96391800	-3.00183000	4.41013500
H	4.95311100	-0.72662400	3.48010400
Pd	-0.56532400	0.05526000	-0.42056700
P	2.62301200	0.39531700	-1.53600900
H	3.42140200	-0.06565900	-0.10038000
C	3.67754300	2.84981600	-1.57230900
H	2.73165100	3.40057900	-1.50001500
H	4.02444900	2.64518200	-0.55062200
C	4.05326300	-1.27230700	-3.02921400
H	4.69611900	-0.48098000	-3.43261200
H	4.51856300	-1.65267700	-2.10857000
O	1.13534400	0.80520000	-1.51548200
O	2.76000600	-0.71874400	-2.72808200
O	3.45738300	1.61713200	-2.27569100
C	4.71433300	3.65516000	-2.33821400
H	5.66286700	3.11067100	-2.39322300
H	4.89212200	4.61547600	-1.84035000
H	4.37105900	3.85107600	-3.35938900
C	3.86635500	-2.39129000	-4.03955000
H	4.83722400	-2.82957600	-4.29994100
H	3.40228100	-2.00639200	-4.95341400
H	3.22367100	-3.17638700	-3.63020400

TS5d

SCF energy: -3364.974927

SCF energy in solution: -3364.028773

Free energy in solution: -3363.2783487600

P	0.99249300	-2.19476500	0.68546200
C	2.49406400	0.74974100	2.72448300
H	3.47561500	0.39056800	3.05554600
H	2.38306900	1.75695800	3.13546500
C	2.16042300	-2.37189800	2.12705700
H	2.29879600	-3.43375100	2.36302300
H	3.13185500	-1.98614600	1.79348100
C	1.36855800	-0.14459600	3.28192200
H	0.45091700	0.01246900	2.70490400
H	1.13958600	0.21198300	4.29459500
C	1.69746600	-1.64271300	3.40225600
H	2.48802900	-1.77202700	4.15534100
H	0.81141100	-2.15179300	3.80057000
P	2.55712700	0.99414000	0.85618800
C	2.88855900	2.80728000	0.72385900
C	3.92323900	3.31615200	-0.07426300
C	2.03822600	3.70886700	1.38657000
C	4.11649400	4.69454300	-0.18728100
H	4.58085100	2.64076600	-0.61077600
C	2.23631100	5.08421300	1.27475200
H	1.20368700	3.34235500	1.97821400
C	3.27874000	5.58129600	0.48946000
H	4.92516200	5.07207700	-0.80727500
H	1.56784800	5.76618100	1.79283800
H	3.43118700	6.65344300	0.40020400
C	4.14249600	0.23402500	0.29756000
C	5.32563800	0.33596700	1.05035000
C	4.17962800	-0.43162900	-0.93759200
C	6.51185800	-0.23109600	0.58561500
H	5.33244200	0.87098500	1.99607100
C	5.37086300	-0.99433500	-1.40320900
H	3.27632100	-0.50350400	-1.53611900
C	6.53579500	-0.89937300	-0.64191800
H	7.41815900	-0.14655400	1.17933800
H	5.38061900	-1.50905100	-2.35961000
H	7.46129200	-1.34003900	-1.00279900
C	1.70481500	-3.29110600	-0.61424500
C	1.13157800	-3.22324400	-1.89855300
C	2.79144400	-4.15324500	-0.39998500
C	1.63073800	-4.01385800	-2.93381100
H	0.30380100	-2.54285000	-2.08279100
C	3.29078900	-4.93774800	-1.44316200
H	3.26127700	-4.22066600	0.57603300
C	2.71060400	-4.87199600	-2.71042900
H	1.17791700	-3.95067800	-3.91966300
H	4.13329500	-5.60011000	-1.26112100
H	3.09998800	-5.48297700	-3.52065100
C	-0.50240600	-3.10018300	1.27176800
C	-0.58594300	-4.50148400	1.22134700
C	-1.56776300	-2.36805400	1.81820700
C	-1.71106400	-5.15944800	1.71865900
H	0.22353800	-5.07938700	0.78465200
C	-2.69033800	-3.03366200	2.31897200
H	-1.53345100	-1.28183200	1.84812300
C	-2.76484800	-4.42629400	2.27133900

H	-1.76627200	-6.24397900	1.67065100
H	-3.51338000	-2.45478400	2.72836900
H	-3.64285300	-4.93993600	2.65441300
O	1.46839500	1.66744300	-2.47298500
C	0.74076400	1.72149100	-1.50349300
C	-0.18474200	2.87374200	-1.26187300
C	-1.03080300	2.91055700	-0.14760200
C	-0.18413400	3.94021000	-2.17587400
C	-1.87163000	4.00697900	0.05049500
H	-1.04019400	2.08535600	0.56102800
C	-1.02156300	5.03287700	-1.97304400
H	0.47796300	3.88866300	-3.03428100
C	-1.86772200	5.06772600	-0.85792000
H	-2.52976900	4.02967700	0.91500900
H	-1.01951700	5.85796200	-2.68077800
H	-2.52259800	5.92142000	-0.70079200
C	-6.08454100	1.10286100	1.98551500
C	-4.03403500	1.55311900	3.33070200
C	-5.35584800	2.14429800	2.83638100
H	-6.97705200	1.50352000	1.49628100
H	-4.23341600	0.74323500	4.04887500
H	-5.15451200	3.03803600	2.22986500
N	-3.82682100	0.48365800	1.08127800
C	-3.19955000	0.96125600	2.19172800
C	-5.18754700	0.51436500	0.89396100
O	-1.96420400	0.90790500	2.31170700
O	-5.69170400	0.05743100	-0.13526200
H	-3.41120700	2.28659300	3.85140500
H	-5.97833600	2.46812500	3.67888500
H	-6.42051100	0.26911000	2.62065500
Pd	0.76651600	0.08992200	-0.28986500
P	-2.37821500	-0.38380700	-1.47968800
H	-3.10546700	0.05035100	-0.09618300
C	-3.83596900	-2.62905600	-1.36215500
H	-3.12480300	-3.17939200	-0.73514400
H	-4.54513400	-2.09781500	-0.71901200
C	-3.90041600	1.05613600	-3.11042300
H	-4.20760700	0.30111900	-3.84265300
H	-4.60457500	1.01437100	-2.27079000
O	-0.86607700	-0.68775600	-1.43556900
O	-2.56566000	0.72600300	-2.65987000
O	-3.12140100	-1.66931700	-2.17330100
C	-4.56295400	-3.57473300	-2.30286500
H	-5.27788900	-3.02493900	-2.92352900
H	-5.11217500	-4.32907000	-1.72735100
H	-3.85472800	-4.08789400	-2.96204700
C	-3.86148900	2.44234000	-3.72984700
H	-4.85294900	2.70893500	-4.11507000
H	-3.14669700	2.47403100	-4.55898000
H	-3.56007800	3.18990800	-2.98926000

7d

SCF energy: -2965.009046

SCF energy in solution: -2964.1751984000

Free energy in solution: -2963.5329434000

P	0.93437200	-1.85692800	0.60356200
C	3.21484700	0.76051300	2.42493500
H	4.19760500	0.27461400	2.44550100
H	3.33863600	1.72400000	2.92745800
C	2.41949000	-2.20870200	1.68376800
H	2.55456800	-3.29366500	1.76628900
H	3.29687200	-1.82185000	1.15195700
C	2.17561500	-0.08218700	3.19267600
H	1.16685300	0.20192900	2.86850800
H	2.24079400	0.18777900	4.25491200
C	2.35561100	-1.60592200	3.09692000
H	3.28736100	-1.88035900	3.61212900
H	1.54401300	-2.08620600	3.65643200
P	2.79171400	1.18412500	0.63509300
C	3.26329300	2.97038400	0.55655600
C	4.08541500	3.47815800	-0.45934900
C	2.72492100	3.86307000	1.49906800
C	4.38084000	4.84169700	-0.51598300
H	4.49610200	2.81321300	-1.21122600
C	3.02536700	5.22345800	1.44324400
H	2.05102400	3.50515400	2.27331100
C	3.85770800	5.71671300	0.43630200
H	5.02123400	5.21745600	-1.30945300
H	2.59953600	5.89764300	2.18123500
H	4.08987400	6.77723900	0.39055700
C	4.08424800	0.36760000	-0.39484000
C	5.43951900	0.34651000	-0.02082900
C	3.70573200	-0.21738000	-1.61282100
C	6.39048700	-0.25860800	-0.84157700
H	5.76100900	0.81660800	0.90475500
C	4.66194000	-0.81803400	-2.43653200
H	2.66157300	-0.20263500	-1.91337200
C	6.00232400	-0.84267600	-2.05133000
H	7.43464300	-0.26934000	-0.54036600
H	4.35167300	-1.27034700	-3.37392000
H	6.74523200	-1.31226100	-2.69056500

C	1.18184000	-3.03786700	-0.79458600
C	0.09012500	-3.31607300	-1.63633600
C	2.42343700	-3.63064000	-1.07524600
C	0.24212000	-4.18364200	-2.71798200
H	-0.87447700	-2.84879200	-1.46105200
C	2.56954800	-4.49353800	-2.16459700
H	3.28876400	-3.42897000	-0.45315800
C	1.47876600	-4.77586200	-2.98672600
H	-0.61315900	-4.39174400	-3.35551900
H	3.53750200	-4.94689400	-2.36323100
H	1.59148000	-5.44996100	-3.83200700
C	-0.43047600	-2.62238200	1.58199800
C	-0.37015600	-3.96579500	1.98944100
C	-1.53079800	-1.84045000	1.96196400
C	-1.38182100	-4.51164000	2.77829400
H	0.46247500	-4.59242000	1.67981100
C	-2.54206500	-2.39124500	2.75595000
H	-1.61112200	-0.82186000	1.59536200
C	-2.46774600	-3.72188800	3.16823100
H	-1.32542200	-5.55260600	3.08607700
H	-3.39257100	-1.77794100	3.04232300
H	-3.25628100	-4.14795600	3.78323300
O	0.80447700	2.73752200	-1.79173000
C	0.34074200	2.45181100	-0.70856000
C	-0.49814500	3.42743500	0.06943900
C	-1.10413000	3.08307900	1.28393600
C	-0.65042200	4.72901200	-0.43447800
C	-1.84882600	4.02808200	1.98999200
H	-1.00438000	2.06743500	1.65262400
C	-1.39264200	5.67207700	0.27164800
H	-0.17617100	4.97778900	-1.37855400
C	-1.99221000	5.32339700	1.48635100
H	-2.32515800	3.75230000	2.92729900
H	-1.50590300	6.67908500	-0.12190200
H	-2.57386700	6.05910900	2.03627800
Pd	0.64705200	0.57158400	0.00353800
P	-2.20863500	0.07727000	-1.70329700
C	-4.00274000	-1.83447200	-1.09592700
H	-3.95300800	-2.05682000	-0.02077700
H	-4.64639200	-0.94947800	-1.22036800
C	-1.21827600	-0.49007100	-4.11422800
H	-1.70197200	-1.47176600	-4.21733200
H	-1.92212500	0.26625400	-4.49398500
O	-1.42368800	0.36660600	-0.36917000
O	-0.92131500	-0.24166000	-2.74076600
O	-2.69058200	-1.56331700	-1.58187200
C	-4.59206200	-3.01860200	-1.85158600
H	-4.67271300	-2.79146200	-2.92024800
H	-5.59177600	-3.26228700	-1.47109000
H	-3.95623200	-3.90361500	-1.73725400
C	0.07822200	-0.44825100	-4.90905500
H	-0.11859900	-0.62314000	-5.97402900
H	0.76866300	-1.22093200	-4.55345000
H	0.56210100	0.52760500	-4.79704000

8d

SCF energy: -2965.030282

SCF energy in solution: -2964.2046276400

Free energy in solution: -2963.5596906400

P	0.95818500	-1.94317200	0.53958900
C	3.15104800	0.77999800	2.46486400
H	4.19636800	0.45203300	2.51058700
H	3.10342700	1.72607000	3.01196900
C	2.56036200	-2.23347100	1.46847200
H	2.76635800	-3.31042300	1.47500600
H	3.36299500	-1.76341000	0.89071400
C	2.23276000	-0.24477700	3.15638800
H	1.18934600	-0.04719800	2.88050100
H	2.29549100	-0.06824800	4.23854000
C	2.57319100	-1.72422700	2.92074600
H	3.57457800	-1.92216900	3.32953800
H	1.87656000	-2.33025400	3.51107900
P	2.72361900	1.21397500	0.68190400
C	3.07936100	3.02937200	0.65119300
C	3.87236000	3.61295000	-0.34779400
C	2.47816800	3.86548800	1.60724200
C	4.08134800	4.99313200	-0.37134100
H	4.32952500	2.99396400	-1.11205100
C	2.69261900	5.24313700	1.58505200
H	1.81998200	3.44978500	2.36551500
C	3.49928900	5.81126500	0.59718100
H	4.70146700	5.42646800	-1.15148300
H	2.21816000	5.87155700	2.33361800
H	3.66472700	6.88504200	0.57771800
C	4.09343500	0.51206900	-0.33718700
C	5.44138200	0.58993700	0.05383400
C	3.77889600	-0.09414200	-1.56312000
C	6.44612100	0.06123800	-0.75595400
H	5.71456100	1.07764000	0.98568400
C	4.78682200	-0.61951100	-2.37614900
H	2.74000500	-0.15447600	-1.87620200

C	6.12015700	-0.54564000	-1.97254500
H	7.48388900	0.12761400	-0.44028600
H	4.52459900	-1.08740200	-3.32080800
H	6.90469500	-0.95558900	-2.60288700
C	1.07807100	-3.16114300	-0.84152700
C	-0.10211800	-3.59358900	-1.47235300
C	2.31511700	-3.62568900	-1.31748400
C	-0.03660200	-4.48932500	-2.53934500
H	-1.06345000	-3.20987300	-1.14226200
C	2.37228500	-4.51750600	-2.39129400
H	3.24340400	-3.29899800	-0.86009300
C	1.19653600	-4.95525000	-3.00168800
H	-0.95684200	-4.81558100	-3.01624400
H	3.33762000	-4.87198600	-2.74403300
H	1.24085600	-5.65191700	-3.83490400
C	-0.25417900	-2.70922200	1.69915700
C	-0.14219000	-4.06036200	2.06587400
C	-1.26834600	-1.93072700	2.27046900
C	-1.02007000	-4.61602400	2.99614700
H	0.62313000	-4.68565900	1.61340400
C	-2.14412900	-2.48698800	3.20527900
H	-1.39563200	-0.90297400	1.95056600
C	-2.02041100	-3.82743500	3.57117900
H	-0.92647500	-5.66421400	3.26808700
H	-2.93366700	-1.87473800	3.63257400
H	-2.70655100	-4.26130100	4.29393600
O	0.74034500	2.66267600	-1.94610800
C	0.23514100	2.31572000	-0.89333900
C	-0.54963800	3.29944600	-0.06163900
C	-1.14970400	2.92489100	1.14565500
C	-0.66262700	4.62596500	-0.50303700
C	-1.85090300	3.85979600	1.90769900
H	-1.07201000	1.88972900	1.47113900
C	-1.36341000	5.56095000	0.25513100
H	-0.19209600	4.89977700	-1.44213200
C	-1.95757500	5.18030800	1.46313400
H	-2.32030500	3.55887200	2.84092800
H	-1.44895800	6.58758700	-0.09238100
H	-2.50649200	5.91002200	2.05331000
Pd	0.57522800	0.41975500	-0.17167100
P	-1.44158200	-0.18548100	-1.22241000
C	-3.79505100	1.05166100	-1.62117400
H	-4.15012100	0.20576200	-1.02436300
H	-4.20523900	1.97571300	-1.20000800
C	-0.44663500	0.12950700	-3.72541900
H	-1.03725000	1.03734300	-3.89686600
H	0.52949000	0.44233800	-3.33763700
O	-2.25075900	-1.28222700	-0.57776300
O	-1.11379400	-0.70314700	-2.76415200
O	-2.36534100	1.16631100	-1.47085500
C	-4.20163300	0.89671100	-3.08129200
H	-3.81904400	1.73041000	-3.68046500
H	-5.29550900	0.88373000	-3.16898900
H	-3.81074100	-0.03802800	-3.49474300
C	-0.29160500	-0.67216500	-5.00813100
H	0.22116900	-0.07281700	-5.77001800
H	-1.27025500	-0.96834900	-5.40099900
H	0.29089500	-1.58176600	-4.82624200

TS6d

SCF energy: -2964.955255

SCF energy in solution: -2964.1254632600

Free energy in solution: -2963.4827012600

P	-2.23325600	0.09502400	-1.04532000
C	0.08598400	-2.74789700	-2.53564000
H	0.16474400	-2.18680300	-3.47259700
H	0.66472300	-3.66358300	-2.68502400
C	-2.17751500	-0.62165800	-2.76753200
H	-2.89835300	-0.08225700	-3.39314900
H	-1.18923600	-0.33132700	-3.14521700
C	-1.39254700	-3.07318300	-2.23119200
H	-1.56778700	-3.05646300	-1.14816800
H	-1.61134400	-4.09676600	-2.56041500
C	-2.39108900	-2.13924600	-2.93781000
H	-2.34750200	-2.34409000	-4.01713900
H	-3.40238300	-2.41450100	-2.61785800
P	0.94455700	-1.72375000	-1.22094500
C	2.15938300	-2.87758100	-0.44799300
C	3.24245000	-2.32368100	0.25603100
C	1.99104100	-4.27022800	-0.45828600
C	4.15376900	-3.15769800	0.90343400
H	3.36363500	-1.24511700	0.32364300
C	2.90651100	-5.09879200	0.19472200
H	1.14455600	-4.72553400	-0.96408400
C	3.99381100	-4.54483000	0.87054400
H	4.98675300	-2.71557000	1.44237100
H	2.76560500	-6.17630400	0.17335100
H	4.70666800	-5.18947800	1.37768900
C	1.98645300	-0.54362100	-2.16853100
C	2.59711900	-0.91325700	-3.38131900
C	2.20775400	0.73714200	-1.64604100

C	3.39889400	-0.00205400	-4.06588700
H	2.46161100	-1.91185200	-3.78864800
C	3.02086800	1.64304000	-2.33304100
H	1.77827500	1.01953200	-0.69018000
C	3.60877700	1.27930900	-3.54337100
H	3.86559400	-0.29325500	-5.00343800
H	3.18549900	2.62279200	-1.89481200
H	4.23801400	1.98510300	-4.07989500
C	-2.00387200	1.88913000	-1.39558300
C	-0.90902800	2.56512400	-0.83978100
C	-2.89876500	2.58316400	-2.22916600
C	-0.69837000	3.91410600	-1.14346600
H	-0.22376000	2.06262400	-0.15846000
C	-2.68653000	3.92888100	-2.51983800
H	-3.77033100	2.07965000	-2.63992300
C	-1.57963500	4.59476100	-1.98176700
H	0.16643600	4.41339400	-0.71741400
H	-3.38384100	4.45891400	-3.16359500
H	-1.41340800	5.64369800	-2.21413700
C	-4.01156400	-0.00328100	-0.55233900
C	-5.03312100	-0.42348700	-1.41943300
C	-4.36256200	0.42031700	0.74060900
C	-6.36642700	-0.42963100	-1.00194200
H	-4.80603700	-0.74037800	-2.43140800
C	-5.69468100	0.42040400	1.15275600
H	-3.59397800	0.75589600	1.42877000
C	-6.70100200	-0.00869600	0.28495300
H	-7.14169400	-0.75971000	-1.68846800
H	-5.94175400	0.75186700	2.15732700
H	-7.73833700	-0.01293800	0.60865700
O	0.96377600	-1.95715300	2.84208600
C	0.27097900	-1.48566000	2.04360700
C	-1.47215800	-0.71722500	2.43921500
C	-1.42187200	0.51122000	3.11326400
C	-2.42152500	-1.68712600	2.79355900
C	-2.35613500	0.77659900	4.11808300
H	-0.64950100	1.22256500	2.83338600
C	-3.34819100	-1.41247900	3.80099800
H	-2.43478900	-2.65120700	2.29203300
C	-3.31654900	-0.18046800	4.46123900
H	-2.32701600	1.72986600	4.63988800
H	-4.08730000	-2.16103200	4.07474600
H	-4.03231100	0.02820800	5.25240700
Pd	-0.53452400	-0.83760400	0.44823700
P	2.19017200	2.01074200	1.92190200
C	2.46910500	4.62094100	1.28102400
H	1.59633900	5.18724700	0.91943700
H	2.41110700	4.61382900	2.38066300
C	4.79664000	1.55280400	1.59208900
H	5.08268600	2.23092800	0.77459400
H	4.82168600	2.14303100	2.52349300
O	0.98225900	1.21820900	1.36004600
O	3.49154800	1.04271500	1.35969200
O	2.40621400	3.29602200	0.77174500
C	3.74965300	5.31979200	0.83373700
H	4.63116400	4.80372900	1.22929600
H	3.76919700	6.35922000	1.18618800
H	3.82369400	5.32726400	-0.25988700
C	5.79068900	0.40261500	1.69314200
H	6.80582600	0.78137200	1.86601300
H	5.79940100	-0.18468900	0.76768400
H	5.52264200	-0.26208700	2.52201900

9d

SCF energy: -2965.003538

SCF energy in solution: -2964.1583639900

Free energy in solution: -2963.5222569900

P	0.61393200	-2.07819900	0.90911800
C	3.35068100	1.04364400	1.53747700
H	3.11160600	2.00400100	1.06907100
H	3.51333500	0.33787200	0.71546000
C	2.21220800	-1.96599600	1.86635900
H	2.44145000	-2.92975200	2.33460800
H	3.00065900	-1.79229300	1.12497900
C	2.17276000	0.58590600	2.41220200
H	1.22705900	0.73520000	1.84046600
H	2.06426600	1.26689800	3.26552600
C	2.22915900	-0.85829900	2.93744800
H	3.14768500	-0.97745400	3.52582700
H	1.39499600	-1.01253700	3.63292500
P	4.97018600	1.17186400	2.49953800
C	6.08608400	1.85496800	1.18716100
C	6.94719300	2.93643300	1.43635400
C	6.18449300	1.20299600	-0.05482500
C	7.85774100	3.36522200	0.46865600
H	6.90246200	3.45472400	2.38930200
C	7.08948600	1.63620400	-1.02408600
H	5.55277500	0.34634600	-0.27559900
C	7.92972400	2.72127800	-0.76714500
H	8.50963100	4.20842000	0.68295300
H	7.13790600	1.12265700	-1.98088600

H	8.63550600	3.05832300	-1.52149500
C	4.61044500	2.65534500	3.55185200
C	4.13190000	3.87624500	3.04390200
C	4.79583900	2.53356900	4.93739100
C	3.84432700	4.93954000	3.89913600
H	3.99421400	4.00128300	1.97314700
C	4.50912400	3.59831900	5.79648900
H	5.16823900	1.59659800	5.34425300
C	4.03133200	4.80176400	5.27812700
H	3.47459700	5.87648000	3.49061700
H	4.65907300	3.48577000	6.86705400
H	3.80591300	5.63122000	5.94330400
C	0.90147400	-3.44214700	-0.29898800
C	-0.09463100	-3.69016300	-1.25989500
C	2.06446200	-4.22749800	-0.30303300
C	0.07375300	-4.71118000	-2.19527300
H	-0.99648000	-3.08440300	-1.28497900
C	2.23027000	-5.24195200	-1.24862100
H	2.84955400	-4.06048400	0.42714700
C	1.23495500	-5.48728500	-2.19499200
H	-0.70405900	-4.89131000	-2.93223200
H	3.13753100	-5.84050200	-1.24022000
H	1.36463400	-6.27741600	-2.92991600
C	-0.61004000	-2.76938200	2.10624600
C	-0.23967700	-3.50444000	3.24358600
C	-1.97461100	-2.55480400	1.84474000
C	-1.21174200	-4.00666200	4.10986900
H	0.80627200	-3.69458500	3.46482400
C	-2.94229200	-3.07040000	2.70982900
H	-2.27961400	-2.00640600	0.95583800
C	-2.56553000	-3.79002000	3.84487000
H	-0.90975500	-4.56993800	4.98902800
H	-3.99412100	-2.90463700	2.49243400
H	-3.32174000	-4.18321600	4.51929900
O	1.01040300	2.62896700	-0.82300600
C	0.03132300	2.18790100	-0.24589700
C	-0.97516300	3.09811200	0.39547400
C	-2.04591000	2.59262100	1.14321900
C	-0.81371900	4.48726500	0.26634700
C	-2.94605400	3.46346700	1.75705200
H	-2.16827600	1.51627100	1.23272000
C	-1.71684700	5.35543400	0.87342500
H	0.02402500	4.86059700	-0.31449300
C	-2.78356900	4.84426800	1.62100800
H	-3.77526800	3.06627800	2.33622200
H	-1.59270100	6.43006300	0.76742600
H	-3.48770200	5.52288200	2.09572400
Pd	0.06852800	0.19550400	0.12515600
P	-1.52683600	-0.13983500	-1.46867000
C	-3.60471800	1.27074000	-2.41981900
H	-4.16868600	0.44756300	-1.97136700
H	-4.04264900	2.21793200	-2.09041100
C	0.22272900	0.25785800	-3.48105700
H	-0.26726200	1.17562400	-3.82726700
H	0.99104700	0.53946600	-2.75143900
O	-2.51943100	-1.21994400	-1.12987900
O	-0.75646800	-0.59198300	-2.85180600
O	-2.26220400	1.27192200	-1.87867700
C	-3.60076300	1.16929600	-3.93904500
H	-3.01250200	1.98111100	-4.38055700
H	-4.62647500	1.24110500	-4.32159700
H	-3.17800300	0.21402600	-4.26547500
C	0.83038200	-0.51205700	-4.64152900
H	1.57868300	0.10611600	-5.15110800
H	0.05990600	-0.79307100	-5.36721900
H	1.31606500	-1.42650100	-4.28536900

TS7d

SCF energy: -2964.977405

SCF energy in solution: -2964.1373522000

Free energy in solution: -2963.5014402000

P	0.46434000	0.74662200	0.07299700
C	-3.96678900	-0.57579800	-1.67961200
H	-4.69653900	-1.07767800	-2.32720200
H	-3.60767300	0.30396900	-2.22907900
C	-1.06169300	0.30340800	-0.90338200
H	-1.78712100	1.11820200	-0.79612000
H	-0.76515600	0.25302700	-1.95857700
C	-2.79420400	-1.53709600	-1.40663500
H	-2.34058700	-1.80075300	-2.37210100
H	-3.19102500	-2.47098700	-0.99014500
C	-1.69081500	-1.02698800	-0.46244500
H	-2.09119300	-0.90849700	0.55014300
H	-0.91689600	-1.80179400	-0.40270700
P	-4.81634800	0.07491600	-0.13077000
C	-6.35159500	0.83185900	-0.83707400
C	-7.40978600	1.12413400	0.04376700
C	-6.47934400	1.22894300	-2.17734500
C	-8.55999700	1.77082500	-0.40339200
H	-7.33459400	0.83421000	1.08917300
C	-7.62974100	1.88577600	-2.62452800

H	-5.68423200	1.02782200	-2.88849900
C	-8.67466400	2.15627600	-1.74214100
H	-9.36726200	1.97747200	0.29465200
H	-7.70675000	2.18118900	-3.66794700
H	-9.56928900	2.66486300	-2.09117800
C	-5.47554900	-1.49916500	0.59643400
C	-6.44158500	-2.30083600	-0.03520900
C	-4.96099900	-1.91650600	1.83375800
C	-6.87417800	-3.48939200	0.55209100
H	-6.86614800	-1.98631200	-0.98499100
C	-5.39082000	-3.10947800	2.42162800
H	-4.22278100	-1.30040800	2.34190300
C	-6.34752800	-3.89740300	1.78144700
H	-7.62358500	-4.09805300	0.05237200
H	-4.98155900	-3.41804400	3.38008200
H	-6.68626000	-4.82355000	2.23840800
C	0.73641600	2.53082600	-0.27182800
C	1.55737800	3.27242100	0.59630000
C	0.18305300	3.15675600	-1.40020200
C	1.79609000	4.62266500	0.34127400
H	2.02664900	2.78846100	1.44938300
C	0.43205200	4.50778700	-1.64985300
H	-0.44632700	2.60188300	-2.08879100
C	1.23514400	5.24364600	-0.77737900
H	2.43189600	5.18663000	1.01796000
H	-0.00608700	4.98261900	-2.52376400
H	1.42638200	6.29591700	-0.97088600
C	-0.12112700	0.67330600	1.81098900
C	-1.18858500	1.48697000	2.22539300
C	0.44812500	-0.22933200	2.71759100
C	-1.68505200	1.38656600	3.52431100
H	-1.63272600	2.20191800	1.53848000
C	-0.05175100	-0.32706700	4.01774400
H	1.29983300	-0.82907300	2.41802000
C	-1.11805300	0.47667000	4.42139300
H	-2.51088600	2.02041000	3.83533600
H	0.40460100	-1.02232400	4.71674200
H	-1.50257000	0.40268800	5.43527500
O	1.01012300	-2.54869800	-2.52373200
C	1.63839200	-1.92763600	-1.75142300
C	3.42380700	-2.27378600	-1.48098900
C	4.27568000	-1.94136300	-2.54649300
C	3.73962200	-3.35971000	-0.64999500
C	5.44139900	-2.67462300	-2.76363300
H	4.02216500	-1.11842200	-3.20981200
C	4.90658200	-4.09089700	-0.87010200
H	3.07583200	-3.63054800	0.16686000
C	5.75696400	-3.74750200	-1.92441800
H	6.10117900	-2.41398900	-3.58705700
H	5.15292100	-4.92676500	-0.22080600
H	6.66391600	-4.32078600	-2.09701800
Pd	2.27617400	-0.63215900	-0.48040500
P	3.83111300	0.47587400	0.96055400
C	5.93754100	-0.48742800	2.32672500
H	5.38707200	-0.02565200	3.15263900
H	6.20509200	-1.51029200	2.61444500
C	5.17677600	1.56006900	-1.10822100
H	5.97957700	0.81202700	-1.06284800
H	4.41320200	1.18755600	-1.80772200
O	3.34440500	1.03221500	2.27572100
O	4.60512700	1.73925700	0.18880200
O	5.05995900	-0.62115400	1.19018600
C	7.18579400	0.31804900	1.98624200
H	7.71742200	-0.13116900	1.13971800
H	7.86726000	0.34188900	2.84617100
H	6.92151400	1.34724900	1.72550900
C	5.71192700	2.90264500	-1.58284900
H	6.15409800	2.80794300	-2.58202100
H	6.48059500	3.27486400	-0.89734300
H	4.90527200	3.64189400	-1.62521400

10d

SCF energy: -2964.997402

SCF energy in solution: -2964.1551368300

Free energy in solution: -2963.5203168300

P	0.46880200	0.67065000	0.10419500
C	-4.00262700	-0.50841500	-1.68424500
H	-4.73198100	-0.96516400	-2.36480400
H	-3.62191200	0.39094300	-2.18501500
C	-1.07492800	0.27908400	-0.88039600
H	-1.78151700	1.10639500	-0.75063400
H	-0.78727000	0.25532400	-1.93965200
C	-2.85039900	-1.50236500	-1.44487900
H	-2.40121500	-1.73859000	-2.42020900
H	-3.26585600	-2.44351400	-1.06452100
C	-1.74086900	-1.04603700	-0.47949100
H	-2.14537900	-0.94316200	0.53277400
H	-0.99172500	-1.84668800	-0.42584700
P	-4.86226200	0.07563400	-0.11381700
C	-6.37847900	0.88663400	-0.80009700
C	-7.45096900	1.13337100	0.07729200

C	-6.47668700	1.36799300	-2.11501400
C	-8.58660600	1.81835200	-0.34978300
H	-7.39877400	0.77745700	1.10348600
C	-7.61261900	2.06284700	-2.54148000
H	-5.66948200	1.20459300	-2.82240600
C	-8.67202800	2.28819000	-1.66345100
H	-9.40533900	1.98870800	0.34463300
H	-7.66689800	2.42375500	-3.56548900
H	-9.55526700	2.82656500	-1.99650100
C	-5.54781600	-1.52601000	0.52259600
C	-6.51449200	-2.28186300	-0.16197500
C	-5.05154700	-2.01403700	1.74123300
C	-6.96602400	-3.49540600	0.35562600
H	-6.92487400	-1.91178700	-1.09795600
C	-5.50041800	-3.23206700	2.25921600
H	-4.31266100	-1.43393800	2.28926800
C	-6.45763500	-3.97408400	1.56704200
H	-7.71569000	-4.06830300	-0.18423100
H	-5.10566900	-3.59631800	3.20409500
H	-6.81091900	-4.91968400	1.96984600
C	0.69680800	2.47621100	-0.17389300
C	1.43210400	3.23051000	0.75645200
C	0.19802000	3.10623700	-1.32582200
C	1.63774000	4.59308900	0.54202300
H	1.86459300	2.74302800	1.62509200
C	0.41550000	4.46922200	-1.53688500
H	-0.36685200	2.54602400	-2.06459300
C	1.13121500	5.21650100	-0.60069900
H	2.20603100	5.16601000	1.26956900
H	0.01966900	4.94459700	-2.43043600
H	1.29670800	6.27838200	-0.76297000
C	-0.13319200	0.51964300	1.83298300
C	-1.18933800	1.32475000	2.28939200
C	0.40733300	-0.45153900	2.68523500
C	-1.70105900	1.15173600	3.57518200
H	-1.61316400	2.08989100	1.64493400
C	-0.10823200	-0.62393000	3.97113100
H	1.24920800	-1.04898500	2.35421500
C	-1.16230300	0.17449200	4.41665600
H	-2.51763400	1.78080200	3.91878300
H	0.32486400	-1.37394200	4.62717700
H	-1.55922500	0.04254000	5.41977000
O	0.92767800	-2.52522900	-2.69802400
C	1.37696400	-1.85724500	-1.88560300
C	3.96417500	-1.95657500	-1.14701400
C	4.63885500	-1.75570200	-2.35893100
C	4.30787900	-3.07051600	-0.36820300
C	5.65091500	-2.63120800	-2.77085400
H	4.38735200	-0.91088400	-2.99613900
C	5.31238900	-3.94996100	-0.78267200
H	3.80891100	-3.24999800	0.58082600
C	5.99069500	-3.73163400	-1.98408700
H	6.16713300	-2.45095200	-3.71136500
H	5.56777500	-4.80473600	-0.16013500
H	6.77362500	-4.41448500	-2.30410400
Pd	2.36017000	-0.75094200	-0.57283400
P	3.80355800	0.42040400	0.87221800
C	5.92610500	-0.24129200	2.36088400
H	5.25198800	0.04392000	3.17424800
H	6.37509500	-1.21091500	2.59905400
C	5.03390800	1.67258100	-1.18588600
H	5.83997000	0.93042300	-1.14410100
H	4.31066100	1.34437900	-1.94434200
O	3.17904800	0.90408500	2.15410200
O	4.38082400	1.75679600	0.08864900
O	5.15330600	-0.47059000	1.16200400
C	7.00278600	0.81475600	2.14713400
H	7.65543600	0.53773700	1.31196900
H	7.61991500	0.90986800	3.04932900
H	6.55413700	1.78909600	1.93129600
C	5.57249400	3.05261000	-1.52770400
H	6.05881100	3.03762600	-2.51020700
H	6.30603600	3.37727500	-0.78238900
H	4.75953800	3.78571500	-1.55080400

11d

SCF energy: -2965.001007

SCF energy in solution: -2964.1602909000

Free energy in solution: -2963.5231519000

P	-2.30557500	-1.42934200	0.06857600
C	2.33376700	-1.66620700	0.60296300
H	2.81936500	-2.57630000	0.97797200
H	1.94372400	-1.11078300	1.46098800
C	-1.25928300	-2.93417300	-0.31303400
H	-1.82489700	-3.81571900	0.01083900
H	-1.14568900	-2.99362800	-1.40327100
C	1.15524200	-2.00386900	-0.31746900
H	1.50328200	-2.47902900	-1.24590000
H	0.67496700	-1.05984300	-0.61044900
C	0.12509800	-2.91785300	0.36689200
H	0.50754200	-3.94710800	0.38296300

H	0.01256500	-2.62618700	1.41804400
P	3.58295100	-0.53958800	-0.23441500
C	4.58279900	0.00827800	1.22794200
C	3.91604300	0.63276200	2.29987700
C	5.98480500	-0.05468400	1.25893200
C	4.63513400	1.14579000	3.37995400
H	2.83221400	0.72635500	2.29328000
C	6.70078500	0.46706300	2.33921200
H	6.52552500	-0.51827000	0.43938100
C	6.02957000	1.06398400	3.40659900
H	4.10074100	1.61423900	4.20290700
H	7.78627000	0.40223600	2.34458100
H	6.58678100	1.46638300	4.24871800
C	4.68637900	-1.77225800	-1.07425800
C	4.93903500	-1.59700900	-2.44329800
C	5.25450700	-2.88521100	-0.42929400
C	5.72997400	-2.50586400	-3.15220100
H	4.51022100	-0.73976000	-2.95661400
C	6.04513100	-3.79356900	-1.13272300
H	5.08821100	-3.03550400	0.63429700
C	6.28303800	-3.60647000	-2.49790500
H	5.91270200	-2.35230500	-4.21268500
H	6.47775800	-4.64727500	-0.61688100
H	6.89859600	-4.31527700	-3.04584700
C	-3.86959900	-1.71301200	-0.86838100
C	-4.79226000	-0.65295800	-0.93085700
C	-4.17113800	-2.90633800	-1.54148000
C	-5.98604000	-0.78649700	-1.63819300
H	-4.57051400	0.28295500	-0.42359700
C	-5.36350500	-3.03484500	-2.25999500
H	-3.48301100	-3.74486800	-1.51302800
C	-6.27308600	-1.97861300	-2.30862700
H	-6.68755800	0.04252600	-1.67326300
H	-5.57870700	-3.96466500	-2.77955400
H	-7.19884200	-2.08093100	-2.86798300
C	-2.78823100	-1.73062700	1.82578200
C	-3.95770200	-2.44457000	2.13850100
C	-1.94474200	-1.30731300	2.86657300
C	-4.27579000	-2.73316900	3.46583600
H	-4.62452600	-2.77661400	1.34917000
C	-2.26723600	-1.60825100	4.19176800
H	-1.05082000	-0.72816400	2.65516400
C	-3.42939600	-2.31779900	4.49576900
H	-5.18572200	-3.28278000	3.69239700
H	-1.60780700	-1.27170100	4.98700600
H	-3.67857000	-2.54204600	5.52967400
O	-1.82651900	-0.26135900	-3.86999500
C	-1.65927400	-0.01859200	-2.76618300
C	-0.44990800	2.25073000	-1.87817800
C	-1.23152100	3.35241100	-2.25321700
C	0.90023400	2.22036800	-2.25600100
C	-0.67195000	4.40970100	-2.97876900
H	-2.28206900	3.40218700	-1.97653800
C	1.45868900	3.28148000	-2.98005300
H	1.53569300	1.38346800	-1.97478600
C	0.67588600	4.37852000	-3.34323100
H	-1.29373300	5.25741900	-3.25858200
H	2.51059500	3.24551800	-3.25474300
H	1.11056900	5.20046200	-3.90639400
Pd	-1.29354600	0.61398700	-0.91310100
P	-0.65222900	1.63091700	1.10640000
C	1.16885700	3.60455200	1.03135400
H	1.64606200	3.20347000	1.93104700
H	1.67363200	3.18574200	0.15497700
C	-3.05399900	2.70573000	1.64004500
H	-2.66732600	3.73097500	1.64497600
H	-3.37992100	2.47255800	0.61464700
O	0.36251500	0.80303500	1.85531900
O	-2.00804100	1.80463200	2.03006100
O	-0.21962600	3.21128900	1.02063900
C	1.21991000	5.12234300	1.00253200
H	0.75451900	5.50505100	0.08867900
H	2.26233500	5.46065400	1.02975300
H	0.69541300	5.54540800	1.86605500
C	-4.20681500	2.54643300	2.61801600
H	-5.02365800	3.22869500	2.35436000
H	-3.87849800	2.77593900	3.63679500
H	-4.58858400	1.52015800	2.60629700

TS8d

SCF energy: -2964.982455

SCF energy in solution: -2964.154778

Free energy in solution: -2963.5122944900

P	1.59854400	1.46185500	-0.64044100
C	-1.80343800	2.83602200	-0.30548000
H	-2.69896400	3.37096100	0.03065500
H	-1.03354500	3.04930900	0.44451200
C	1.14890900	2.61857200	-2.05887300
H	2.08740500	3.08011000	-2.38602800
H	0.80816600	1.98428900	-2.88586900
C	-1.35779800	3.33678800	-1.70222000

H	-1.95767500	4.22230700	-1.94607100
H	-1.59869900	2.60069000	-2.48019800
C	0.12015300	3.74132700	-1.83008900
H	0.20324100	4.40072700	-2.70488600
H	0.41422000	4.35195100	-0.96763000
P	-2.12886200	0.99840500	-0.17771500
C	-2.88298300	0.94641000	1.51601300
C	-2.06056000	0.63383200	2.60995600
C	-4.23012000	1.25952200	1.75429100
C	-2.56576000	0.65382700	3.91145400
H	-1.02477800	0.35189200	2.44109700
C	-4.73678200	1.27105000	3.05503500
H	-4.89047900	1.48736300	0.92298100
C	-3.90582100	0.97287100	4.13692100
H	-1.91355800	0.40672400	4.74492500
H	-5.78376100	1.51112100	3.22172400
H	-4.30286500	0.98072400	5.14855100
C	-3.57723600	0.75360300	-1.30419400
C	-3.90080900	-0.55576700	-1.70186700
C	-4.36610400	1.81209100	-1.78713100
C	-4.98527100	-0.79628500	-2.54682500
H	-3.30408900	-1.38961800	-1.34976100
C	-5.44680300	1.56951700	-2.63780000
H	-4.14660200	2.83653900	-1.50446500
C	-5.76071800	0.26411700	-3.01876000
H	-5.21774100	-1.81692400	-2.83832100
H	-6.04243500	2.40323000	-3.00080700
H	-6.60169000	0.07588500	-3.68092500
C	3.28966800	0.92699400	-1.17100300
C	4.25012300	0.58876200	-0.20329300
C	3.62151900	0.79909000	-2.53006900
C	5.51794500	0.15791500	-0.59307700
H	3.99091100	0.62794200	0.84900700
C	4.89023900	0.35959900	-2.91391200
H	2.89950700	1.03890100	-3.30397500
C	5.84400800	0.04277600	-1.94604200
H	6.24956000	-0.09935800	0.16806800
H	5.12951400	0.26928800	-3.97031300
H	6.83292700	-0.29557900	-2.24429600
C	1.95500300	2.65817700	0.71921000
C	2.80604600	3.75311600	0.48978200
C	1.36423100	2.51117800	1.97986200
C	3.04257100	4.68991800	1.49503300
H	3.29778200	3.87070500	-0.47199000
C	1.60026000	3.45201500	2.98554100
H	0.76076300	1.63700800	2.18506700
C	2.43415300	4.54362200	2.74471600
H	3.70437000	5.53061200	1.30404200
H	1.13966200	3.32081400	3.96088400
H	2.61936600	5.27317100	3.52873600
O	0.76003100	-1.14551100	-3.46689600
C	0.22559100	-0.69149100	-2.55703500
C	-1.11185400	-2.25288500	-0.26545600
C	-1.16944000	-3.18157600	-1.31771300
C	-1.93738600	-2.48626700	0.84565100
C	-2.04289800	-4.27651100	-1.27842000
H	-0.53717300	-3.07283200	-2.19251000
C	-2.81610600	-3.57242000	0.88469000
H	-1.89921500	-1.82339100	1.70096700
C	-2.87778700	-4.47400600	-0.17992500
H	-2.06183200	-4.97251300	-2.11458700
H	-3.44891700	-3.71408400	1.75828200
H	-3.55861200	-5.32092100	-0.14815900
Pd	0.02416800	-0.50419400	-0.41595000
P	1.49918700	-1.46474300	1.10258800
C	1.27235600	-2.92859900	3.33505500
H	1.76062500	-2.04618600	3.76022600
H	0.39553600	-3.17242200	3.94485800
C	2.42846900	-3.41280700	-0.52822900
H	1.79452300	-4.15613700	-0.02981700
H	1.88399500	-3.03327300	-1.40079400
O	2.17929900	-0.43822100	1.97539900
O	2.70501400	-2.33085900	0.37118200
O	0.74747800	-2.60162400	2.03126400
C	2.23157500	-4.11076800	3.27856700
H	1.74624000	-4.98055800	2.82239700
H	2.54908700	-4.38615200	4.29226700
H	3.12184300	-3.86083800	2.69364400
C	3.75657200	-4.01910000	-0.95368100
H	3.58801600	-4.84124500	-1.65936100
H	4.30014400	-4.41177700	-0.08778900
H	4.38358800	-3.26390800	-1.43879600

12d

SCF energy: -2851.681221

SCF energy in solution: -2850.8730381800

Free energy in solution: -2850.2340691800

P	-1.52964300	-1.44239800	-0.50692900
C	1.70654000	-2.91650200	0.67848700
H	2.60749400	-3.27407300	1.18956100
H	0.93413600	-2.84867200	1.45454000

C	-0.97219500	-3.00813500	-1.39744100
H	-1.88268700	-3.43903600	-1.82970000
H	-0.37317800	-2.66516000	-2.25075100
C	1.28845700	-3.91926300	-0.41628200
H	1.69612200	-4.89780300	-0.13073100
H	1.76741800	-3.67063000	-1.37216000
C	-0.21946200	-4.10965700	-0.63031500
H	-0.34569100	-5.03231500	-1.21307200
H	-0.70568400	-4.29997800	0.33484300
P	2.05110500	-1.14781200	0.16025300
C	2.86119300	-0.58111700	1.72472900
C	2.03043800	-0.13330000	2.76639800
C	4.24729200	-0.62111700	1.92959900
C	2.57749500	0.24417700	3.99352800
H	0.95879900	-0.03555500	2.60844600
C	4.79143500	-0.23373200	3.15643600
H	4.90869700	-0.94226700	1.13119300
C	3.95906500	0.19356800	4.19205100
H	1.92146300	0.59651900	4.78466400
H	5.86874100	-0.26235200	3.29842300
H	4.38530000	0.49673500	5.14472100
C	3.41631300	-1.32471100	-1.07011600
C	3.54142600	-0.35853200	-2.08175400
C	4.32849900	-2.39498300	-1.04582600
C	4.55494300	-0.45774500	-3.03745500
H	2.85266700	0.47915800	-2.11420300
C	5.33747700	-2.49437800	-2.00468900
H	4.26013100	-3.15908500	-0.27733200
C	5.45313000	-1.52490800	-3.00332000
H	4.63835900	0.30287500	-3.80892500
H	6.03214800	-3.32958000	-1.97054200
H	6.23874900	-1.60301500	-3.75016200
C	-2.75089500	-0.90074000	-1.78790500
C	-4.12872500	-1.13267200	-1.69392200
C	-2.24584000	-0.26873000	-2.93456200
C	-4.98246500	-0.74430500	-2.72922800
H	-4.54299300	-1.60266600	-0.80790300
C	-3.09872600	0.11250700	-3.97056200
H	-1.18193800	-0.05437000	-3.01004400
C	-4.47117900	-0.12453100	-3.87054500
H	-6.05067600	-0.92503700	-2.63939800
H	-2.69132300	0.60423500	-4.85002600
H	-5.13797600	0.17777300	-4.67362700
C	-2.50588600	-2.09420000	0.91459200
C	-3.24855300	-3.28622100	0.83450400
C	-2.48480200	-1.39076000	2.13053900
C	-3.95259000	-3.76321600	1.94065500
H	-3.28337900	-3.84929000	-0.09377900
C	-3.19146500	-1.87239200	3.23588500
H	-1.93817000	-0.45586300	2.21621100
C	-3.92329900	-3.05686100	3.14554400
H	-4.52129200	-4.68602100	1.86095700
H	-3.16789400	-1.31270700	4.16682700
H	-4.46967700	-3.42940600	4.00808200
C	1.33627200	1.95761300	-0.45695700
C	1.26379400	2.53068700	-1.74174400
C	2.24862000	2.51470500	0.45014400
C	2.10000300	3.58686100	-2.11775400
H	0.53217900	2.16472000	-2.45925600
C	3.08448400	3.57667500	0.07897000
H	2.31632900	2.13041100	1.46232700
C	3.02117800	4.11236800	-1.20759100
H	2.02000800	4.00697600	-3.11854700
H	3.78331800	3.98583900	0.80589600
H	3.66957800	4.93671400	-1.49435400
Pd	0.12576400	0.29485700	-0.16859800
P	-1.39445200	1.85281700	0.64723900
C	-0.78614100	4.48221300	0.65276400
H	-0.77494500	4.30988900	1.73360200
H	0.24755900	4.53749900	0.29767100
C	-4.08322100	2.14111900	0.41535100
H	-3.87200400	3.19864300	0.22691400
H	-4.80725700	1.80060600	-0.33241400
O	-1.25755900	1.90125100	2.15352600
O	-2.89483300	1.36936400	0.15524500
O	-1.43722900	3.37388000	0.00295000
C	-1.54651000	5.75241100	0.30420200
H	-1.57949800	5.89972900	-0.78072900
H	-1.05266000	6.62169000	0.75517000
H	-2.57572600	5.70882400	0.67735300
C	-4.62006800	1.92954800	1.82653400
H	-5.55569800	2.48835100	1.95822300
H	-3.89465300	2.27018500	2.57025300
H	-4.82369100	0.86857000	2.00743300

TS9d

SCF energy: -2851.656924

SCF energy in solution: -2850.8539692300

Free energy in solution: -2850.2160232300

P	-1.62252900	-1.57244000	-0.25017900
C	1.87278400	-2.88165400	1.08966900

H	2.84420100	-3.20366600	1.48416200
H	1.23753500	-2.71401100	1.96849100
C	-1.06979300	-3.28612100	-0.79374700
H	-1.97130000	-3.83334000	-1.09332400
H	-0.49229500	-3.13299800	-1.71408400
C	1.27268000	-3.99713400	0.20621200
H	1.68076700	-4.94471000	0.58227400
H	1.63834100	-3.91152000	-0.82569200
C	-0.26157000	-4.15196000	0.19646100
H	-0.46798900	-5.19609700	-0.07348000
H	-0.65076700	-4.03204700	1.21583300
P	2.10495500	-1.18831500	0.32088400
C	3.04251600	-0.39208500	1.70820800
C	2.29864700	0.27806700	2.69533300
C	4.43790400	-0.45270700	1.83710400
C	2.93774900	0.85503600	3.79451800
H	1.21935200	0.37345300	2.59169900
C	5.07523600	0.13539100	2.93210700
H	5.03308700	-0.95273700	1.07879100
C	4.32744400	0.78581900	3.91547400
H	2.34696200	1.37017000	4.54741500
H	6.15811900	0.08463300	3.01476800
H	4.82551400	1.24280200	4.76670400
C	3.38689500	-1.47643300	-0.98131400
C	3.48683800	-0.52432500	-2.01054100
C	4.24870800	-2.58584200	-1.01056600
C	4.43071600	-0.67020800	-3.02824800
H	2.82101700	0.33330600	-2.01398100
C	5.18627800	-2.73608100	-2.03471300
H	4.19763100	-3.34239100	-0.23350500
C	5.28123900	-1.77733000	-3.04503400
H	4.49454600	0.08054200	-3.81147300
H	5.84235100	-3.60284600	-2.04108100
H	6.01083400	-1.89508500	-3.84196300
C	-2.85104200	-1.26041400	-1.60347800
C	-4.23999600	-1.27604500	-1.42017900
C	-2.34578900	-0.98559000	-2.88542400
C	-5.10141900	-1.03235300	-2.49425000
H	-4.65672200	-1.47385200	-0.43794600
C	-3.20491100	-0.75437500	-3.95881100
H	-1.27008800	-0.93484000	-3.03996700
C	-4.58883500	-0.77606700	-3.76612300
H	-6.17646300	-1.04535000	-2.33229600
H	-2.79378000	-0.54773100	-4.94375500
H	-5.26035400	-0.58919000	-4.59997100
C	-2.64458600	-1.92702300	1.24662300
C	-3.43561800	-3.08296700	1.37588300
C	-2.61107500	-1.00677700	2.30798300
C	-4.17448700	-3.31455400	2.53645700
H	-3.48396500	-3.80861200	0.56862100
C	-3.35759600	-1.24086600	3.46692200
H	-2.00917600	-0.10405800	2.22874400
C	-4.13632300	-2.39231800	3.58560600
H	-4.77898000	-4.21410100	2.62116800
H	-3.32344900	-0.51765300	4.27740500
H	-4.71132700	-2.57346000	4.49019200
C	0.79457900	2.06054800	-0.67875500
C	0.66263400	2.25846800	-2.07002500
C	1.90728800	2.62534500	-0.02479000
C	1.64753500	2.93619900	-2.79135800
H	-0.22079600	1.88795100	-2.58294800
C	2.88466900	3.31187000	-0.74883400
H	2.02051200	2.50560100	1.04835400
C	2.76313500	3.46242600	-2.13357200
H	1.53606700	3.06654000	-3.86538800
H	3.74780500	3.72290900	-0.23048000
H	3.52452100	3.99991800	-2.69299500
Pd	0.08195500	0.08564800	-0.14524100
P	-1.07256000	2.10345900	0.38854500
C	-0.56074200	4.69422900	0.95295800
H	-0.71617000	4.39715200	1.99538400
H	0.51909900	4.70979800	0.75651600
C	-3.64763100	2.54328100	-0.43819800
H	-3.38222700	3.56125600	-0.73214500
H	-4.26126400	2.09432400	-1.22470700
O	-1.02444600	1.91285300	1.88762400
O	-2.45144500	1.72594900	-0.42023200
O	-1.18414900	3.73664000	0.08767200
C	-1.17228700	6.05750100	0.66731900
H	-1.02572500	6.33662000	-0.38152900
H	-0.70128100	6.82120300	1.29749300
H	-2.24762800	6.05367400	0.87564500
C	-4.37981800	2.52448300	0.89653100
H	-5.32000300	3.08446700	0.81397400
H	-3.77302200	2.97847400	1.68567400
H	-4.61281800	1.49698100	1.1947580