Supporting Information

Substrate-Controlled Mechanistic Switch Between Protodemetalation and Oxidative Addition in Rh-Catalyzed Carbometalation: A DFT Study

Chunhui Shan*, Hong Chen, Xiang Zhang and Xiaoling Luo

Chongqing Key Laboratory of Green Catalysis Materials and Technology, College of Chemistry, Chongqing Normal University, Chongqing 401331, P. R. China.

E-mail: chunhui.shan@cqnu.edu.cn

Table of Content

1. Complete reference for Gaussian 16 .....S2

2. Other potential pathways for base-assisted protodemetalation S2

3. The weak interaction analysis of 6-ts-S by IGMH S3

4. Cartesian coordinates and energies of optimized structures S3

1. Complete reference for Gaussian 16

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

2. Other potential pathways for base-assisted protodemetalation

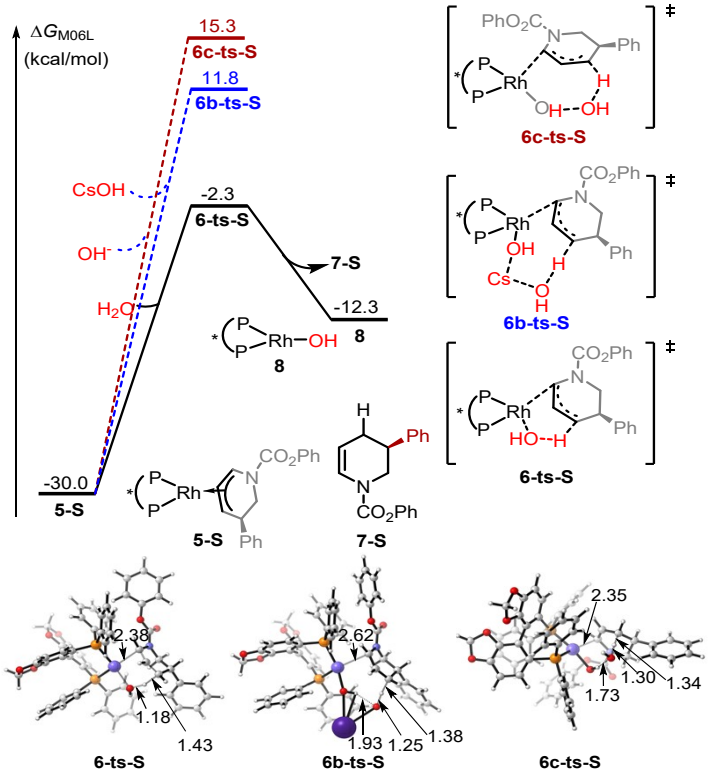

Fig. S1 Free energy profiles for the Rh(I)-catalyzed protodemetalation step.

In addition, other potential pathways for base-assisted protodemetalation were explored. The calculational results show that the energy barrier for protodemetalation assisted by CsOH is 41.8 kcal/mol, while that assisted by a hydroxide ion is 45.3 kcal/mol. Both values are relatively high and exceed the barrier for the pathway involving a single water molecule.

3. The weak interaction analysis of 6-ts-S by IGMH

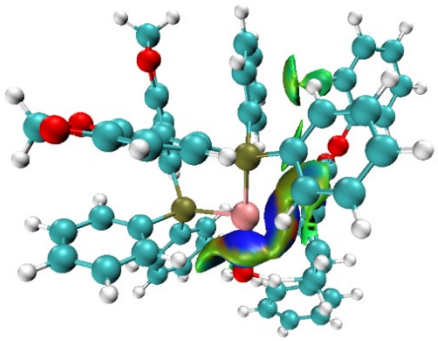

Fig.S2. The weak interaction analysis of 6-ts-S by IGMH (blue: strong attractive; green: weak attractive; and red: strong repulsive).

To further characterize the stabilizing interactions in **6-ts-S**, an Independent Gradient Model based on the Hirshfeld partition (IGMH) was employed (Fig. S2). The analysis confirms a C–H···π interaction between one phenyl ring of the NCO_2Ph group and a phenyl ring of the Segphos ligand, which contributes to the stabilization of this transition state.

4. Cartesian coordinates and energies of optimized structures

1
B3LYP-D3 SCF energy: -2789.039912 a.u.
B3LYP-D3 enthalpy: -2789.038968 a.u.
B3LYP-D3 free energy: -2789.163834 a.u.
M06 SCF energy in solution: -2789.701625 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.77584200	1.74751100	-0.19013500
P	1.20356000	-1.02528400	-0.27539500
O	-2.87833000	-1.63104600	4.25768100
O	-2.52531300	-2.62315300	2.19314500
O	-4.08384700	-1.48903900	-0.50118800
O	-4.10612200	-2.53822500	-2.56990000
C	-1.54873000	0.80957400	1.20312300
C	-1.78460500	1.39881200	2.44836600
H	-1.61652300	2.46208500	2.57603600
C	-2.22983200	0.65761000	3.55946100
H	-2.40952800	1.12419100	4.52167500
C	-2.42914600	-0.69122000	3.36359300
C	-2.77593100	-2.88825100	3.57765700
H	-3.71922600	-3.43336600	3.67719600
H	-1.93614500	-3.45903000	3.99511700
C	-2.21516700	-1.28645300	2.12188400
C	-1.76566900	-0.58936600	1.01631400
C	-0.89398700	3.51785500	0.32530400
C	0.09141400	3.98754900	1.21458300
H	0.84540200	3.29826600	1.59083700
C	0.10693500	5.32118400	1.62188500
H	0.87238700	5.66466400	2.31260600
C	-0.85339800	6.21190600	1.13499500
H	-0.83883500	7.25336400	1.44507900
C	-1.82713400	5.75934900	0.24312300
H	-2.57284400	6.44867000	-0.14449100
C	-1.85079700	4.42147000	-0.15842000
H	-2.61149000	4.08728000	-0.85588900
C	-2.03552000	1.56200500	-1.52388000
C	-3.41570900	1.63794100	-1.27978700
H	-3.77504500	1.82923500	-0.27240800
C	-4.32561600	1.44303200	-2.31913300
H	-5.39283400	1.51436400	-2.12352600
C	-3.86623400	1.14543000	-3.60622400
H	-4.57622000	0.97821900	-4.41192900
C	-2.49446200	1.05656900	-3.85299500
H	-2.13453100	0.81212800	-4.84861200
C	-1.58286600	1.26913700	-2.81729400
H	-0.51365200	1.17899900	-2.99258300
C	-0.41211600	-1.61166600	-0.96214500
C	-1.63400600	-1.29406500	-0.29301600
C	-2.79610000	-1.67741300	-0.93900400
C	-4.93245100	-1.93966600	-1.56139700
H	-5.63257300	-2.68766600	-1.17438200
H	-5.46149300	-1.08093000	-1.99179000
C	-2.81263200	-2.30608400	-2.18105400
C	-1.64483000	-2.61609200	-2.84287000
H	-1.65185800	-3.10880000	-3.80871100
C	-0.44428900	-2.25850300	-2.20383900
H	0.48778600	-2.49196400	-2.70443800
C	2.43536600	-2.03131600	-1.22441300
C	2.78932100	-3.34320000	-0.87769500

H	2.36025300	-3.81185300	0.00143700
C	3.71068100	-4.05378600	-1.64971000
H	3.98367900	-5.06633000	-1.36385000
C	4.28236800	-3.46632200	-2.78003600
H	5.00148700	-4.02041900	-3.37770900
C	3.93567300	-2.15990200	-3.13230200
H	4.38638100	-1.69022100	-4.00244700
C	3.02518000	-1.44451500	-2.35480100
H	2.78120900	-0.41479900	-2.60006400
C	1.22961200	-1.78140000	1.41043500
C	1.90203400	-1.10859000	2.44105700
H	2.37463700	-0.15422300	2.22689600
C	1.95185500	-1.65539000	3.72422500
H	2.47023900	-1.12218100	4.51658800
C	1.33478400	-2.88002000	3.99098000
H	1.37371100	-3.30425700	4.99096600
C	0.66464300	-3.55661700	2.96850500
H	0.18427000	-4.51152800	3.16723900
C	0.60517800	-3.00777900	1.68668000
H	0.05037700	-3.52232800	0.90807000
Rh	1.49371500	1.15160100	-0.36904500
C	3.49065900	1.13736400	-0.17035700
C	4.53498700	0.27132100	0.19101500
C	3.80574600	2.49559400	-0.36326200
C	5.83606500	0.75326900	0.36659000
H	4.34104300	-0.78821900	0.33745200
C	5.10335600	2.98703000	-0.19228600
H	3.01583200	3.20339700	-0.65578800
C	6.12581700	2.10766500	0.17599000
H	6.63066600	0.06719400	0.65426100
H	5.31666100	4.04232000	-0.35017000
H	7.14005200	2.47569200	0.31033100

2

B3LYP-D3 SCF energy: -668.869173 a.u.
B3LYP-D3 enthalpy: -668.868229 a.u.
B3LYP-D3 free energy: -668.924095 a.u.
M06 SCF energy in solution: -668.780175 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.10807100	1.10207400	0.48676400
C	3.39371200	1.49915800	0.49930400
C	4.43292100	0.61514800	-0.01374500
C	4.13584500	-0.64071300	-0.37815700
C	2.75176900	-1.21815400	-0.23373700
N	1.73539700	-0.16770600	0.02181200
H	5.44650600	0.99433100	-0.11231500
H	1.28931900	1.72659600	0.81403800
H	3.64151000	2.48742300	0.86913300
H	4.89264100	-1.31198200	-0.77480600
H	2.45252700	-1.75667500	-1.13890300
C	0.42805400	-0.57010400	-0.13296400
O	0.10284900	-1.69355300	-0.46197900
O	-0.43833600	0.45880300	0.12790300
C	-1.81537900	0.24707800	0.06194000
C	-2.55131500	1.24260300	-0.57714500
C	-2.43992000	-0.84276000	0.66859400
C	-3.94306800	1.14691900	-0.61195600
H	-2.02612300	2.07559600	-1.03344000
C	-3.83206700	-0.92865800	0.61965100
H	-1.84702300	-1.60960300	1.15019700
C	-4.58691800	0.06033500	-0.01609000
H	-4.52109200	1.92182000	-1.10768800
H	-4.32721100	-1.77662800	1.08461600
H	-5.67005900	-0.01589300	-0.04661600
H	2.71487600	-1.96060100	0.58096200

3

B3LYP-D3 SCF energy: -3457.959190 a.u.
B3LYP-D3 enthalpy: -3457.958246 a.u.
B3LYP-D3 free energy: -3458.107894 a.u.
M06 SCF energy in solution: -3458.522055 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.89013600	0.01304400	0.86429700
P	-2.16174300	-0.16336900	-0.80111600
O	-3.04485300	3.60868200	3.61032400
O	-2.80752100	3.79732600	1.31299900
O	0.06949200	4.56506900	-0.13855600
O	0.21914400	5.07819500	-2.39680900
C	-0.19569800	1.21149500	1.79751200
C	-0.32726900	1.13997200	3.18858500
H	0.31896000	0.48040500	3.75361500
C	-1.26738100	1.90411200	3.90710000
H	-1.35275100	1.83135200	4.98569600
C	-2.06876000	2.75052400	3.17410300
C	-3.64449900	4.14465500	2.42116900
H	-3.70136200	5.23380100	2.50497500
H	-4.63595300	3.69672300	2.27815500
C	-1.92984600	2.85708700	1.79176600
C	-1.02646200	2.11126300	1.05760200
C	2.13405700	-0.52130200	2.11951000
C	1.70886400	-1.41483400	3.11924200
H	0.67239400	-1.74191400	3.13942200
C	2.60724100	-1.92187600	4.05527100
H	2.25559200	-2.60473500	4.82434700
C	3.96155600	-1.58241500	3.98114900
H	4.66774800	-1.99408500	4.69740500
C	4.40167200	-0.72623300	2.97219800
H	5.45521200	-0.47554400	2.88217900
C	3.49361400	-0.19094000	2.05501500
H	3.86723400	0.46150000	1.27565100
C	1.82836400	1.17260200	-0.22585400
C	2.45134700	2.32537500	0.28138100
H	2.42285100	2.52781500	1.34802200
C	3.08683800	3.22042600	-0.57782500
H	3.57517500	4.10268700	-0.17188800
C	3.08403300	2.98985900	-1.95792600
H	3.56489000	3.69555400	-2.62990100
C	2.46138500	1.85011400	-2.46994500
H	2.45925400	1.65880700	-3.53828100
C	1.84372500	0.94431600	-1.60610200
H	1.34564200	0.07055000	-2.00691200
C	-1.44939300	1.43519400	-1.39891300
C	-0.96329100	2.34275400	-0.41368300
C	-0.44900200	3.53636300	-0.88342500
C	0.54056100	5.53770400	-1.07586500
H	0.03908400	6.49459000	-0.89125800
H	1.62840000	5.63379700	-0.98285600
C	-0.36353900	3.84807900	-2.23793800

C	-0.82657900	2.98337400	-3.20507100
H	-0.76691800	3.22654700	-4.26006900
C	-1.37820500	1.76884200	-2.75560200
H	-1.76184000	1.07900400	-3.49720700
C	-2.76926300	-0.94228000	-2.35631100
C	-4.12568600	-1.10421900	-2.66143000
H	-4.88421400	-0.70310300	-1.99827400
C	-4.51323400	-1.80459200	-3.80715300
H	-5.57039500	-1.93275900	-4.02412700
C	-3.55321700	-2.34392200	-4.66348300
H	-3.85799100	-2.89085700	-5.55161100
C	-2.19525700	-2.18377700	-4.36916300
H	-1.43936200	-2.60381500	-5.02748700
C	-1.80829900	-1.49777000	-3.21983900
H	-0.75426100	-1.40093000	-2.97605700
C	-3.69043100	0.47334500	0.02549300
C	-4.09231700	-0.05912800	1.25710300
H	-3.52675000	-0.86817500	1.70173700
C	-5.22335000	0.43778200	1.90775900
H	-5.52201600	0.01454300	2.86287400
C	-5.96782600	1.46945400	1.33230200
H	-6.85330700	1.85020700	1.83529000
C	-5.57015600	2.01208200	0.10614700
H	-6.14002200	2.82064300	-0.34451200
C	-4.43469400	1.52282200	-0.53876400
H	-4.11822700	1.96304700	-1.47988500
Rh	-0.72951900	-1.68374000	0.26209100
C	-2.33423100	-2.96979300	0.41696100
C	-2.72599000	-3.21306900	1.75046200
C	-3.03956600	-3.65269600	-0.58543900
C	-3.78991900	-4.06256300	2.06488700
H	-2.18878300	-2.72913100	2.56853900
C	-4.10417200	-4.50979800	-0.27915500
H	-2.77231600	-3.51539600	-1.62924600
C	-4.49089000	-4.71380000	1.04535700
H	-4.06727300	-4.22087000	3.10553000
H	-4.63375500	-5.01553900	-1.08449300
C	2.83665500	-3.21331300	0.51028100
C	1.75165100	-3.76407800	1.07960400
C	0.44003700	-3.69594000	0.45476600
C	0.33055900	-3.20462500	-0.85896500
C	1.59927100	-2.86910800	-1.61548200
N	2.73179900	-2.53993800	-0.72587500
H	-0.33926300	-4.33615300	0.85237100
H	3.81092600	-3.19682800	0.97330800
H	1.86248100	-4.25182300	2.04155600
H	-0.45529000	-3.58315500	-1.50876700
H	1.87823000	-3.74232000	-2.23134900
C	3.75513500	-1.80629300	-1.26882500
O	3.75678600	-1.32780100	-2.38770600
O	4.78681900	-1.69313000	-0.36765200
C	5.79777000	-0.75912900	-0.53013100
C	7.05516300	-1.14417200	-0.06487200
C	5.56918700	0.52941300	-1.01340900
C	8.10367100	-0.22369400	-0.08571900
H	7.19015900	-2.15329700	0.31128800
C	6.62850200	1.43738900	-1.03046300
H	4.59079800	0.81077600	-1.37238100
C	7.89509800	1.07032500	-0.56995700
H	9.08379000	-0.52108900	0.27713400
H	6.45039100	2.44200300	-1.40450300
H	8.71236200	1.78584300	-0.58595300
H	1.46530100	-2.03412600	-2.30315200
H	-5.31910700	-5.37670300	1.28348200

4-ts-S

B3LYP-D3 SCF energy: -3457.938759 a.u.
B3LYP-D3 enthalpy: -3457.937815 a.u.
B3LYP-D3 free energy: -3458.083827 a.u.
M06 SCF energy in solution: -3458.502928 a.u.
Imaginary frequency: -302.36 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.09844000	-0.54774600	-1.34975900
P	-1.33753300	-0.16748800	1.67142700
O	-1.52747100	5.22196800	-1.09429400
O	-3.09565400	3.60942600	-0.52566000
O	-4.04576800	1.32157500	-2.62546500
O	-5.87569400	-0.04615500	-2.22717300
C	-0.36715500	1.25682500	-1.39777200
C	0.55313400	2.24410500	-1.77009800
H	1.53257200	1.95819700	-2.12907300
C	0.26522200	3.62003100	-1.70313200
H	0.99429800	4.36641600	-1.99790400
C	-0.98747500	3.97114700	-1.25259300
C	-2.83247100	5.01566600	-0.53595600
H	-3.57836000	5.52084800	-1.15881800
H	-2.84918000	5.39564300	0.49300800
C	-1.92483100	3.00220300	-0.91077100
C	-1.66793000	1.64352900	-0.95649300
C	1.60273700	-0.58389400	-2.41522500
C	2.78034700	-0.06647700	-1.85426300
H	2.75651300	0.33251600	-0.84713900
C	3.98313700	-0.08142200	-2.55592500
H	4.87524300	0.31437700	-2.08193200
C	4.02783900	-0.64510000	-3.83356100
H	4.96438600	-0.67458500	-4.38449400
C	2.86851900	-1.18629500	-4.39361200
H	2.90184600	-1.64099500	-5.38054200
C	1.66044900	-1.15529800	-3.69228400
H	0.77454100	-1.59405500	-4.13758200
C	-1.22363200	-1.26779100	-2.42152300
C	-1.60749300	-0.66548900	-3.63010000
H	-1.10941200	0.24103700	-3.96188400
C	-2.63601400	-1.21342100	-4.39620400
H	-2.91864700	-0.74368400	-5.33521900
C	-3.30844700	-2.35618500	-3.95154100
H	-4.11903000	-2.77557200	-4.54200200
C	-2.93717200	-2.95541800	-2.74615300
H	-3.46206900	-3.83877100	-2.39250500
C	-1.89526900	-2.41821400	-1.98824300
H	-1.60548800	-2.87230300	-1.04677100
C	-2.83572100	-0.08825500	0.57849600
C	-2.77413100	0.71101700	-0.60128400
C	-3.86536200	0.63807500	-1.44843300
C	-5.25024900	0.80451800	-3.19871700
H	-5.92247500	1.63385900	-3.44111300
H	-5.00309300	0.21423800	-4.08964600
C	-4.96614700	-0.17906500	-1.20974800
C	-5.04987100	-0.94966500	-0.07126200
H	-5.91275700	-1.57458700	0.13055800

C	-3.96217600	-0.88346000	0.81872500
H	-4.01896500	-1.47368300	1.72431300
C	-2.02082000	-0.85805900	3.25100300
C	-2.21040800	-0.10645500	4.41828800
H	-1.99217700	0.95574600	4.42427600
C	-2.67291400	-0.71499300	5.58941900
H	-2.80657200	-0.11586900	6.48644800
C	-2.96242900	-2.07894500	5.61007700
H	-3.32391200	-2.54852700	6.52092000
C	-2.77302700	-2.84103300	4.45329700
H	-2.98439800	-3.90713400	4.46002000
C	-2.29341900	-2.23801400	3.29201000
H	-2.10826000	-2.83973300	2.40506700
C	-1.05384900	1.61516600	2.06464700
C	0.25798500	2.10826200	2.01995400
H	1.07068000	1.43236700	1.77354900
C	0.51144000	3.45733400	2.27563400
H	1.53086200	3.83045400	2.22883400
C	-0.54056100	4.32311800	2.58396900
H	-0.34195800	5.37336100	2.78104300
C	-1.85013400	3.83626600	2.63643300
H	-2.67247300	4.50491600	2.87905700
C	-2.10710200	2.49117800	2.36937200
H	-3.12942600	2.12366900	2.37670800
Rh	0.38642900	-1.43167600	0.81062600
C	1.53734600	-3.12637000	0.01687600
C	2.66477300	-3.07004800	-0.81452500
C	0.64175200	-4.20299300	-0.15868100
C	2.84712600	-4.00069400	-1.84228500
H	3.39406800	-2.27793500	-0.69108800
C	0.81050300	-5.12049700	-1.19473800
H	-0.20054800	-4.31430800	0.52252600
C	1.91577900	-5.01906100	-2.04807200
H	3.71329000	-3.90956100	-2.49269900
H	0.08779000	-5.92236900	-1.33052300
H	2.05534300	-5.73837900	-2.85105200
C	2.61466700	-0.30786500	3.26476400
C	1.44359900	-0.91169000	3.53101000
C	0.98769900	-2.09701700	2.79380100
C	1.96030200	-2.82377900	2.02033600
C	3.39673300	-2.34376800	2.15779000
N	3.47234800	-0.88783100	2.29068100
H	0.18658100	-2.66903400	3.25336900
H	2.95786100	0.60625100	3.73020300
H	0.79043500	-0.49687100	4.29249100
H	1.89137500	-3.90470600	2.08495000
H	3.79273600	-2.79184300	3.08231600
C	4.14624100	-0.17066800	1.35147600
O	4.88780300	-0.62297300	0.49605600
O	3.86623700	1.17473400	1.49675200
C	4.41416400	2.08063400	0.59407900
C	3.52412500	2.97626800	0.00322100
C	5.78281800	2.13662100	0.32895600
C	4.01481300	3.94931700	-0.86846500
H	2.46397900	2.89225300	0.21358800
C	6.25757700	3.10911700	-0.55284600
H	6.45071900	1.41965700	0.78956500
C	5.38035900	4.01717100	-1.15216600
H	3.32421300	4.65075300	-1.32825600
H	7.32118700	3.15539100	-0.77010400
H	5.75973300	4.77119100	-1.83592500
H	4.03411400	-2.64947400	1.33199800

5-S

B3LYP-D3 SCF energy: -3457.993095 a.u.
B3LYP-D3 enthalpy: -3457.992151 a.u.
B3LYP-D3 free energy: -3458.139674 a.u.
M06 SCF energy in solution: -3458.567610 a.u

Cartesian coordinates

ATOM	X	Y	Z
P	-2.17335100	-0.22304500	0.43371200
P	1.05089600	0.85389300	0.60904500
O	-0.69323100	2.06516000	-4.88568200
O	-0.33333800	3.38034100	-3.00817800
O	-2.68673900	4.32322300	-0.77779800
O	-2.18177900	5.86855500	0.87631000
C	-1.89745600	0.53087700	-1.23539500
C	-2.10025100	-0.25193100	-2.38092900
H	-2.56229800	-1.22623100	-2.27993400
C	-1.73042300	0.17002800	-3.67001700
H	-1.88912000	-0.45470600	-4.54190400
C	-1.14780300	1.41495100	-3.76749800
C	-0.09491500	3.28151700	-4.41615600
H	-0.55834800	4.13417900	-4.92426200
H	0.98575300	3.24597700	-4.59808500
C	-0.93632400	2.20307900	-2.64062200
C	-1.26506400	1.80448500	-1.35586400
C	-3.68823800	-1.26855300	0.21491200
C	-4.70176900	-1.00631900	-0.72078900
H	-4.60155000	-0.18002200	-1.41729900
C	-5.83489200	-1.81872900	-0.78600900
H	-6.60461200	-1.60863400	-1.52442000
C	-5.97920200	-2.89617000	0.09042200
H	-6.85794600	-3.53302200	0.03230100
C	-4.98583300	-3.15448000	1.03593400
H	-5.08149200	-3.99801500	1.71363800
C	-3.85025600	-2.34764200	1.09406000
H	-3.06687500	-2.56226100	1.81004800
C	-2.89730100	1.15685000	1.44016500
C	-4.03304100	1.86739600	1.02410900
H	-4.51023600	1.62729500	0.07987400
C	-4.55043300	2.89548400	1.81090900
H	-5.43607000	3.43333800	1.48105400
C	-3.93515300	3.23227500	3.02053700
H	-4.33335200	4.04051000	3.62822500
C	-2.80902200	2.52500500	3.44460900
H	-2.32264500	2.78432000	4.38111900
C	-2.29783300	1.48782000	2.66223800
H	-1.41381200	0.93888900	2.97610600
C	0.19270800	2.49412200	0.66184500
C	-0.90034200	2.71411200	-0.23047400
C	-1.60378500	3.88942000	-0.05386000
C	-3.14569700	5.51027700	-0.12321400
H	-3.22849800	6.32046200	-0.85487700
H	-4.10966000	5.30817600	0.36015200
C	-1.30139900	4.81865100	0.93881600
C	-0.23985900	4.63362700	1.79625000
H	0.00592200	5.36148200	2.56148600
C	0.50153700	3.44792000	1.63685400
H	1.33582800	3.27549100	2.30627600
C	2.51740200	1.12078500	1.70281600

C	2.31319300	0.95537100	3.08526200
H	1.32039400	0.69688900	3.44662600
C	3.36908200	1.09580900	3.98391200
H	3.19213900	0.97007900	5.04903400
C	4.65564100	1.37832700	3.51296900
H	5.48385800	1.47048200	4.21063000
C	4.87200500	1.52456100	2.14345500
H	5.87125600	1.71201000	1.76160100
C	3.80897200	1.40488200	1.24365100
H	4.00876200	1.49793300	0.18320300
C	1.73173100	0.85807100	-1.10910700
C	1.58036900	-0.29473200	-1.89038500
H	1.08080100	-1.15640300	-1.46161700
C	2.04040500	-0.32968600	-3.20757400
H	1.91648800	-1.23394500	-3.79560500
C	2.67065500	0.79002600	-3.75431000
H	3.03671300	0.76411600	-4.77722100
C	2.82581100	1.94727700	-2.98307500
H	3.31404000	2.82233900	-3.40491900
C	2.34460200	1.98769700	-1.67424400
H	2.43141300	2.90159400	-1.09362700
Rh	-0.13862600	-1.05566300	1.16941300
C	1.74545700	-2.19163600	1.71295600
C	0.63601100	-2.54608000	2.50298300
C	-0.44879400	-3.17423700	1.84249700
C	-0.09174600	-4.20070900	0.76060300
C	1.08353900	-3.75478200	-0.13810200
N	2.11051600	-2.96866500	0.57146000
H	-1.31475100	-3.44901900	2.43970700
H	2.56959800	-1.64471400	2.14478800
H	0.56966600	-2.17709500	3.52326500
H	0.23809900	-5.10634400	1.29351100
H	1.57185500	-4.62970500	-0.57279000
C	3.24101600	-2.70114300	-0.15533900
O	3.46845800	-3.13155600	-1.27041400
O	4.09916600	-1.89960700	0.56138900
C	5.21735200	-1.33687300	-0.03654800
C	6.37020600	-1.30221100	0.74537300
C	5.17421800	-0.72315300	-1.28879300
C	7.50002100	-0.63395400	0.27139000
H	6.35758000	-1.77947400	1.71978400
C	6.31105000	-0.05922000	-1.75054700
H	4.27128800	-0.75935800	-1.88119200
C	7.47430300	-0.00790000	-0.97738600
H	8.39877300	-0.60228500	0.88148600
H	6.27765800	0.42640000	-2.72211000
H	8.35327600	0.51393300	-1.34541300
H	0.71529400	-3.15508000	-0.97467000
C	-1.29868500	-4.59673300	-0.07546000
C	-1.97733400	-5.79071300	0.19689600
C	-1.79691800	-3.76784200	-1.08995400
C	-3.12323400	-6.14813200	-0.51743400
H	-1.60446600	-6.44774800	0.98008100
C	-2.93305500	-4.12500200	-1.81420800
H	-1.30605000	-2.82174000	-1.29289900
C	-3.60441100	-5.31511400	-1.52844700
H	-3.63566600	-7.07849000	-0.28578700
H	-3.31174600	-3.46303300	-2.58844700
H	-4.49709000	-5.58693200	-2.08519000

6-ts-S

B3LYP-D3 SCF energy: -3534.374272 a.u.
B3LYP-D3 enthalpy: -3534.373328 a.u.
B3LYP-D3 free energy: -3534.527334 a.u.
M06 SCF energy in solution: -3534.955733 a.u
Imaginary frequency: -1239.31 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.90700000	-1.94961500	-0.30181300
P	-0.69561700	1.09449400	0.98479500
O	-3.71076800	1.52297600	-4.26216600
O	-4.30827500	1.69482500	-2.02786400
O	-5.45676900	-0.85540300	-0.29278200
O	-6.35269000	-0.65699800	1.83641100
C	-1.81029200	-1.00332500	-1.60496500
C	-1.47997800	-1.11472000	-2.95948200
H	-0.74770000	-1.84785000	-3.27451900
C	-2.06442400	-0.30141900	-3.94793900
H	-1.79356400	-0.39238500	-4.99381200
C	-2.99503800	0.61984100	-3.52045700
C	-4.46119200	2.29816700	-3.31692400
H	-5.51892000	2.29033500	-3.59885000
H	-4.06125900	3.31917500	-3.28883800
C	-3.35208800	0.72225500	-2.17803700
C	-2.78591800	-0.05177300	-1.18266900
C	0.00441600	-3.25553000	-1.24115600
C	-0.32433500	-4.61778700	-1.19482600
H	-1.20162000	-4.94723400	-0.64840500
C	0.48344800	-5.56238400	-1.83538800
H	0.21990600	-6.61533900	-1.78211700
C	1.62404500	-5.16146200	-2.53249100
H	2.25227700	-5.89923800	-3.02409900
C	1.96037600	-3.80516800	-2.58831300
H	2.85653000	-3.48321700	-3.11071900
C	1.16150800	-2.86291100	-1.94229500
H	1.44175200	-1.81333800	-1.95847000
C	-2.27431900	-2.85024100	0.54236600
C	-3.34889000	-3.41091100	-0.16511600
H	-3.38468600	-3.32926100	-1.24788300
C	-4.38167700	-4.05120900	0.51991700
H	-5.20726600	-4.48997500	-0.03499000
C	-4.35926200	-4.11899000	1.91676500
H	-5.17095200	-4.60678000	2.45021600
C	-3.29461300	-3.55743800	2.62551400
H	-3.27838700	-3.60261800	3.71095500
C	-2.25208100	-2.92998900	1.94134300
H	-1.42377200	-2.47670600	2.47955500
C	-2.48630400	0.70164800	1.28049600
C	-3.25105300	0.12322500	0.22274600
C	-4.53353200	-0.28150300	0.54608600
C	-6.55656900	-1.23657700	0.54039700
H	-7.48707000	-0.85109400	0.11260600
H	-6.57872300	-2.32997000	0.63231700
C	-5.07317800	-0.16357400	1.82412500
C	-4.35584100	0.40310000	2.85451800
H	-4.77601600	0.50983200	3.84842100
C	-3.05057300	0.83465200	2.55379100
H	-2.46999200	1.28304700	3.35071300
C	-0.26890800	2.20502800	2.40232500
C	0.05047800	1.58099900	3.62300500
H	0.00535300	0.49645800	3.69102300

C	0.44281600	2.33406800	4.72824000
H	0.68187100	1.83481800	5.66350800
C	0.54662900	3.72450900	4.62609000
H	0.86860200	4.31227000	5.48145000
C	0.24810500	4.35118300	3.41639500
H	0.34090700	5.42973800	3.32200500
C	-0.16236300	3.59817300	2.31312000
H	-0.38077100	4.10482700	1.38172400
C	-0.79540500	2.19475900	-0.49188500
C	0.08418800	1.95436700	-1.55581700
H	0.80384700	1.14624800	-1.46868200
C	0.02136700	2.72746900	-2.71479700
H	0.71540500	2.53462800	-3.52710200
C	-0.91969600	3.75442400	-2.81851600
H	-0.96361300	4.36294400	-3.71761900
C	-1.80082700	4.00274400	-1.76129000
H	-2.53304800	4.80293400	-1.83671900
C	-1.74772600	3.21934300	-0.60702400
H	-2.45983500	3.38958200	0.19565400
Rh	0.58886200	-0.74647200	0.91982200
C	2.47747400	0.63211900	1.39431300
C	2.91907400	-0.29989400	2.34209100
C	3.81346400	-1.36110600	2.04552200
C	4.72830000	-1.12522000	0.83593400
C	3.92282800	-0.45116300	-0.30111500
N	3.23538500	0.74916200	0.18071300
H	4.27525200	-1.86250900	2.89608900
H	2.06439800	1.56687200	1.73637900
H	2.44691700	-0.24925400	3.32069900
H	5.52430200	-0.41870700	1.11627600
H	4.57652300	-0.15781900	-1.12159600
C	3.31001700	1.88226900	-0.57022200
O	3.87341700	1.98877900	-1.64644500
O	2.64762300	2.92801400	0.04729000
C	2.81514900	4.21203100	-0.45718400
C	4.08335900	4.75310400	-0.67461400
C	1.66634700	4.97366100	-0.65727200
C	4.19185200	6.07872700	-1.09457400
H	4.96278300	4.13721500	-0.52930400
C	1.78792100	6.30090800	-1.07148100
H	0.69726900	4.51935400	-0.50352800
C	3.04862700	6.85861700	-1.29171100
H	5.17723400	6.50288900	-1.26790500
H	0.89017400	6.89288500	-1.22925700
H	3.14168700	7.89097400	-1.61747500
H	3.17548800	-1.15125800	-0.68796100
C	5.40100300	-2.38576500	0.32083800
C	6.79515300	-2.51446900	0.35232800
C	4.65438300	-3.44294100	-0.22167400
C	7.42640500	-3.66133300	-0.13578100
H	7.39349100	-1.70505400	0.76504500
C	5.27782200	-4.58681300	-0.71820400
H	3.57477000	-3.36927300	-0.26209200
C	6.66959800	-4.70257400	-0.67568800
H	8.51011800	-3.73841600	-0.09632600
H	4.67172100	-5.38652700	-1.13740000
H	7.15855800	-5.59441000	-1.05906700
O	1.66862900	-2.54899000	1.26311500
H	2.75745900	-2.22823100	1.61790500
H	1.67566500	-3.23146000	0.57386600

7-S

B3LYP-D3 SCF energy: -901.048138 a.u.
B3LYP-D3 enthalpy: -901.047194 a.u.
B3LYP-D3 free energy: -901.113464 a.u.
M06 SCF energy in solution: -900.924993 a.u

Cartesian coordinates

ATOM	X	Y	Z
C	0.18863200	2.01554900	-0.31227000
C	-0.93461100	2.74484000	-0.26818100
C	-2.30523000	2.13695300	-0.13654800
C	-2.21081900	0.67062100	0.33535200
C	-1.11814300	-0.06295200	-0.46667900
N	0.17746400	0.60819700	-0.30750000
H	-2.91326000	2.70992500	0.57569100
H	1.17105300	2.46287400	-0.36989700
H	-0.84435700	3.82610500	-0.31236200
H	-1.88040500	0.68054600	1.38193600
H	-1.00882600	-1.09366700	-0.13118800
C	1.30269400	-0.17692000	-0.21050800
O	1.30594500	-1.39097900	-0.24963700
O	2.42128400	0.60367500	-0.05941600
C	3.68068900	0.01238100	0.02260900
C	4.52979200	0.52837400	0.99960900
C	4.11116300	-0.97291600	-0.86633300
C	5.83717400	0.04926700	1.09157100
H	4.15660600	1.29690300	1.66900300
C	5.41909200	-1.44765000	-0.75790300
H	3.43115500	-1.36706700	-1.61039000
C	6.28471000	-0.94155000	0.21504200
H	6.50266200	0.45047400	1.85090600
H	5.76114200	-2.21889200	-1.44252300
H	7.30125700	-1.31725000	0.28903900
H	-1.38241800	-0.08069900	-1.53243700
H	-2.84326100	2.18995900	-1.09469400
C	-3.53145900	-0.06916400	0.25501700
C	-4.19739700	-0.23472400	-0.96904600
C	-4.11129000	-0.61766800	1.40602500
C	-5.40677400	-0.92690400	-1.03881100
H	-3.76913200	0.18041200	-1.87821000
C	-5.32275900	-1.30874900	1.34186900
H	-3.60723200	-0.50139800	2.36287700
C	-5.97488600	-1.46608200	0.11777900
H	-5.90576600	-1.04499000	-1.99713700
H	-5.75534700	-1.72423700	2.24822600
H	-6.91742700	-2.00418500	0.06451800

8

B3LYP-D3 SCF energy: -2633.297838 a.u.
B3LYP-D3 enthalpy: -2633.296894 a.u.
B3LYP-D3 free energy: -2633.410271 a.u.
M06 SCF energy in solution: -2634.024263 a.u

Cartesian coordinates

ATOM	X	Y	Z
P	1.56585800	-0.92877900	-0.19610000
P	-1.66665700	-0.76556200	-0.24020100
O	0.38979000	2.99155900	4.14134500
O	-0.61322200	3.30721900	2.07450300
O	1.10889000	3.73406700	-0.68671000
O	0.30446200	4.25384600	-2.79950700

C	1.37086700	0.32190400	1.15074300
C	1.98467600	0.15559600	2.39489700
H	2.68293900	-0.66073100	2.54017600
C	1.72163300	1.00872500	3.48332100
H	2.19688500	0.86745000	4.44759400
C	0.82225000	2.02915400	3.26537000
C	-0.62214600	3.72896200	3.44247600
H	-0.39412100	4.79823200	3.49480800
H	-1.60166200	3.50630200	3.88388500
C	0.22100300	2.21877200	2.02271400
C	0.44906500	1.39183600	0.93993200
C	3.03724900	-1.92468900	0.31621300
C	2.81157200	-2.98544700	1.21268100
H	1.80242700	-3.17108900	1.57442400
C	3.86385800	-3.79814000	1.63403400
H	3.67224700	-4.61164500	2.32857200
C	5.15612200	-3.57258000	1.15398300
H	5.97618700	-4.20961500	1.47442700
C	5.38816700	-2.53136200	0.25335400
H	6.38983900	-2.35667600	-0.13065400
C	4.33784900	-1.71051800	-0.16286900
H	4.53455400	-0.91056100	-0.86825800
C	2.17418300	0.11360500	-1.59266900
C	3.08464000	1.16501000	-1.40059100
H	3.45577500	1.38237700	-0.40288900
C	3.49159500	1.94952600	-2.47975500
H	4.20449000	2.75540400	-2.32302600
C	2.97605400	1.70581500	-3.75675000
H	3.28222600	2.32662100	-4.59460300
C	2.06242200	0.66797800	-3.95194700
H	1.65019400	0.48333200	-4.94009000
C	1.66643600	-0.12854100	-2.87579800
H	0.93883600	-0.92454000	-3.01314600
C	-1.19130300	0.85049700	-0.99789700
C	-0.21152700	1.67525300	-0.36657500
C	0.18363700	2.79698400	-1.07413000
C	1.27220600	4.61402300	-1.80384300
H	1.09666400	5.64626700	-1.48305800
H	2.27982400	4.48974100	-2.21859100
C	-0.29233200	3.10719200	-2.34494600
C	-1.21879000	2.30881000	-2.98050500
H	-1.58110400	2.54010300	-3.97582500
C	-1.65678400	1.17241200	-2.27912200
H	-2.37775400	0.52136000	-2.76005600
C	-3.35163300	-1.10007800	-0.93189100
C	-3.67594900	-2.40193900	-1.34213700
H	-2.91682700	-3.18410800	-1.29157400
C	-4.96137800	-2.68432600	-1.81569100
H	-5.20052100	-3.69661600	-2.13120900
C	-5.92683800	-1.68135900	-1.89264900
H	-6.92320800	-1.90627600	-2.26480800
C	-5.60498700	-0.37935600	-1.49762300
H	-6.34659000	0.41253800	-1.56487700
C	-4.32816600	-0.09032300	-1.02104400
H	-4.08755500	0.93126100	-0.74748400
C	-2.01500200	-0.30988600	1.52473300
C	-1.47229300	-1.09666800	2.54923500
H	-0.85198800	-1.94711700	2.27847300
C	-1.69188500	-0.76937200	3.88820700
H	-1.24988300	-1.37927000	4.67141600
C	-2.46769900	0.34274800	4.21966800
H	-2.63921800	0.59852100	5.26192700
C	-3.01774800	1.13001400	3.20409200
H	-3.62293900	1.99837100	3.45281400
C	-2.78571200	0.81181400	1.86658100
H	-3.17901700	1.46297100	1.09412800
Rh	-0.16967400	-2.36640000	-0.50508100
O	-1.19210200	-4.05111400	-0.77115300
H	-1.52579000	-4.35640000	0.09000800

9

B3LYP-D3 SCF energy: -408.132470 a.u.
B3LYP-D3 enthalpy: -408.131526 a.u.
B3LYP-D3 free energy: -408.173616 a.u.
M06 SCF energy in solution: -408.110696 a.u

Cartesian coordinates

ATOM	X	Y	Z
B	1.74679100	-0.00244000	-0.00505600
O	2.38956700	-1.20172500	-0.15139900
H	3.35070200	-1.08147600	-0.11189300
O	2.52579800	1.12196900	0.14081700
H	2.00971700	1.92406300	0.29604600
C	0.17923500	0.00995800	-0.00670500
C	-0.53505500	-1.19984000	0.06926300
C	-0.56191700	1.20210000	-0.08107800
C	-1.92965200	-1.21717300	0.07893000
H	0.01894300	-2.13289000	0.12124700
C	-1.95698800	1.19601600	-0.07593600
H	-0.04970200	2.16115200	-0.15971600
C	-2.64344100	-0.01776000	0.00693500
H	-2.46176700	-2.16303600	0.14119800
H	-2.50742000	2.13120700	-0.13826600
H	-3.73044800	-0.02858600	0.01286400

10-ts

B3LYP-D3 SCF energy: -3041.470997 a.u.
B3LYP-D3 enthalpy: -3041.470053 a.u.
B3LYP-D3 free energy: -3041.600131 a.u.
M06 SCF energy in solution: -3042.158693 a.u
Imaginary frequency: -299.15 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.76213900	1.66208500	-0.33790200
P	0.84521600	-1.19472800	-0.05324200
O	-3.72791200	-1.14248000	4.02385400
O	-3.28685600	-2.30385800	2.06573700
O	-4.40493100	-1.27457300	-0.81819400
O	-4.31874900	-2.52998200	-2.76642200
C	-1.79439900	0.91492300	1.00568200
C	-2.09335400	1.60977700	2.18208200
H	-1.81946800	2.65316900	2.27352300
C	-2.74498600	1.00551600	3.27297900
H	-2.96566100	1.55623100	4.18054000
C	-3.08663100	-0.32127700	3.13197100
C	-3.74319000	-2.44077100	3.41518700
H	-4.76625900	-2.83012200	3.41522800
H	-3.06257700	-3.10481900	3.96276800
C	-2.82040900	-1.01694000	1.95582200
C	-2.17303800	-0.45420500	0.87158300
C	-0.81266000	3.47598500	0.01755300

C	-0.05285600	3.95152000	1.10732700
H	0.50448600	3.25326300	1.72742600
C	0.00971700	5.31830300	1.38631000
H	0.60166500	5.66424200	2.22927900
C	-0.67037200	6.23270700	0.57771600
H	-0.61491000	7.29693400	0.78995400
C	-1.41220200	5.77131500	-0.51040800
H	-1.93708100	6.47647400	-1.14963100
C	-1.48360900	4.40412200	-0.79092300
H	-2.06142700	4.06560200	-1.64407800
C	-1.85503700	1.45421500	-1.80932700
C	-3.23614500	1.69858500	-1.75567000
H	-3.68735300	2.04231000	-0.82898800
C	-4.03276400	1.47804800	-2.87905100
H	-5.10056800	1.67738800	-2.83194900
C	-3.46058700	0.99079500	-4.05872500
H	-4.08456600	0.80368900	-4.92871200
C	-2.08782600	0.74016700	-4.11571900
H	-1.64233900	0.35095700	-5.02707600
C	-1.28652500	0.97738900	-2.99747800
H	-0.22019900	0.76687000	-3.01974400
C	-0.73287300	-1.75836900	-0.85374300
C	-1.98108000	-1.27553500	-0.35756500
C	-3.10349400	-1.61888500	-1.09026800
C	-5.17567600	-1.74031700	-1.93005600
H	-6.00084700	-2.36124100	-1.56626500
H	-5.54485800	-0.87939700	-2.50136000
C	-3.05442100	-2.37175100	-2.25958300
C	-1.86148000	-2.85702500	-2.74776300
H	-1.81723700	-3.45416000	-3.65176500
C	-0.70294600	-2.53523400	-2.01774600
H	0.24495900	-2.90787800	-2.38534300
C	2.06590400	-2.43960600	-0.67016300
C	2.62077700	-2.21889800	-1.94029000
H	2.36156300	-1.31489200	-2.48275900
C	3.51730000	-3.13192600	-2.49407700
H	3.94014000	-2.94103300	-3.47666700
C	3.89066500	-4.26968800	-1.77665900
H	4.59817000	-4.97646400	-2.20235600
C	3.36352300	-4.48522000	-0.50241100
H	3.66108700	-5.36004200	0.07011700
C	2.45442700	-3.57957400	0.04715900
H	2.06430500	-3.75924100	1.04244800
C	0.56433000	-1.64783200	1.71542200
C	0.93545900	-0.73265800	2.71232700
H	1.38789900	0.21491700	2.42669400
C	0.69311700	-1.02554400	4.05596300
H	0.96978000	-0.30487300	4.82081700
C	0.09025400	-2.23267500	4.41712300
H	-0.09758200	-2.45686400	5.46400000
C	-0.27699000	-3.14972600	3.42808300
H	-0.74638300	-4.09143100	3.70204700
C	-0.05210100	-2.85395200	2.08346900
H	-0.38056200	-3.54955100	1.31647300
Rh	1.40811500	0.95819700	-0.34802900
O	2.37068500	2.90477400	-0.40108200
H	1.80738600	3.61010800	-0.03822500
B	3.33725900	2.44909300	0.61074000
O	2.81917300	2.40153500	1.92915600
H	3.56183700	2.51744500	2.53963400
O	4.63807400	2.97887500	0.54799000
H	4.96271900	2.96106900	-0.36163100
C	3.58978800	0.59141800	-0.15390100
C	4.23210900	0.62629500	-1.41444100
C	4.11663000	-0.30616200	0.79735400
C	5.33241000	-0.17997800	-1.70740500
H	3.86315100	1.31608400	-2.17279600
C	5.20915900	-1.12671500	0.51579000
H	3.65717300	-0.35157200	1.78215100
C	5.81797700	-1.06604000	-0.74041600
H	5.80548700	-0.13247700	-2.68645800
H	5.58355600	-1.81866200	1.26691700
H	6.66565100	-1.70850300	-0.96643000

11

B3LYP-D3 SCF energy: -252.420092 a.u.
B3LYP-D3 enthalpy: -252.419148 a.u.
B3LYP-D3 free energy: -252.450847 a.u.
M06 SCF energy in solution: -252.465316 a.u.

Cartesian coordinates

ATOM	X	Y	Z
B	-0.00028800	-0.00003400	0.00001400
O	0.26189200	-1.34695300	0.00010200
H	-0.55913600	-1.85873900	-0.00031600
O	1.03593200	0.90036600	-0.00015300
H	1.88900600	0.44385200	0.00055500
O	-1.29770400	0.44675100	-0.00015800
H	-1.32938500	1.41374600	0.00136200

12-ts-S

B3LYP-D3 SCF energy: -3457.943799 a.u.
B3LYP-D3 enthalpy: -3457.942855 a.u.
B3LYP-D3 free energy: -3458.094929 a.u.
M06 SCF energy in solution: -3458.507955 a.u.
Imaginary frequency: -750.45 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.14883300	-1.48077100	1.01928600
P	1.00211800	1.64874300	-0.44522500
O	6.77589800	0.26935300	-0.02652000
O	5.26122900	0.35576300	-1.78273200
O	3.57803000	-2.24516400	-2.92590700
O	2.29811800	-2.16141800	-4.85898600
C	2.92764700	-1.04272500	0.72967200
C	3.85959400	-1.10725200	1.77169400
H	3.55624300	-1.49941300	2.73470900
C	5.19288800	-0.68228700	1.62554400
H	5.89946500	-0.73165300	2.44653200
C	5.55722200	-0.20329800	0.38666000
C	6.59948800	0.67735700	-1.39010000
H	7.30624600	0.13376200	-2.02735200
H	6.74816000	1.76080500	-1.46450700
C	4.64705200	-0.15185400	-0.66477900
C	3.32311600	-0.53480300	-0.54534200
C	1.21827700	-2.48412700	2.57363900
C	1.22362700	-1.78330600	3.79256300
H	1.19343800	-0.69740300	3.77871700
C	1.25056700	-2.46639800	5.00788200
H	1.25780600	-1.90704400	5.93963500
C	1.24813200	-3.86348500	5.02641100

H	1.25465700	-4.39752600	5.97281200
C	1.22581100	-4.56888000	3.82263300
H	1.21360200	-5.65568600	3.82764300
C	1.21591000	-3.88590000	2.60379100
H	1.19082300	-4.45237600	1.67948300
C	0.84969300	-2.72463600	-0.31152600
C	1.80530500	-3.68768800	-0.67212100
H	2.76471200	-3.71288700	-0.16341400
C	1.53946900	-4.59561000	-1.69734200
H	2.28263500	-5.34452800	-1.95988800
C	0.32703600	-4.53520700	-2.39096900
H	0.12478500	-5.23613100	-3.19657400
C	-0.62358000	-3.57152400	-2.04676800
H	-1.56674800	-3.51771800	-2.58326600
C	-0.36547900	-2.67502900	-1.00874500
H	-1.10869200	-1.93443300	-0.73182400
C	1.41675100	0.57871300	-1.89528900
C	2.43991800	-0.40597900	-1.74036800
C	2.64136500	-1.24807100	-2.81818100
C	3.31735600	-2.90017000	-4.17193000
H	4.23091000	-2.90763600	-4.77592000
H	2.95729900	-3.91744600	-3.97790500
C	1.87618000	-1.19721500	-3.98100300
C	0.87756300	-0.26229700	-4.14329500
H	0.28736600	-0.21326300	-5.05154300
C	0.66793800	0.63089000	-3.07611700
H	-0.10149900	1.38564600	-3.18756000
C	-0.03288800	2.99703900	-1.16653500
C	-1.39187700	2.71218600	-1.38490400
H	-1.77196200	1.71885800	-1.16547100
C	-2.26218900	3.69120500	-1.85754100
H	-3.30962700	3.44952200	-2.01666400
C	-1.79192900	4.98478600	-2.09944200
H	-2.47170700	5.75586800	-2.45176000
C	-0.44799100	5.28301300	-1.87482400
H	-0.07590400	6.28872000	-2.05229600
C	0.42833300	4.29612000	-1.41548700
H	1.46674800	4.55159300	-1.23545700
C	2.61242800	2.45712300	-0.06656700
C	3.01685600	2.54995200	1.27221200
H	2.37268500	2.14813700	2.04899000
C	4.24916300	3.11894800	1.59866000
H	4.56089400	3.17107600	2.63811900
C	5.08297200	3.60920800	0.59152900
H	6.04286500	4.05053500	0.84608500
C	4.68340900	3.52547400	-0.74590900
H	5.32830900	3.90717500	-1.53356000
C	3.46021500	2.94190700	-1.07513100
H	3.16961600	2.84322100	-2.11710700
Rh	-0.20885100	0.44952600	1.24651100
C	-3.14230900	-2.08542400	1.29096700
C	-2.04182300	-1.81393500	2.02203800
C	-1.67686600	-0.47410300	2.51307200
C	-2.88699200	0.47855000	2.46811900
C	-3.64867600	0.30677200	1.13100100
N	-4.05048800	-1.08381700	0.90035000
H	-1.26006900	-0.52589400	3.52357700
H	-3.40606600	-3.07827700	0.95192200
H	-1.40223300	-2.65381700	2.27326400
H	-3.59660900	0.24602600	3.27846700
H	-4.53107000	0.94407000	1.11207900
C	-5.14039300	-1.44506300	0.14996500
O	-5.45145900	-2.58470500	-0.13960500
O	-5.83505100	-0.32342500	-0.24652900
C	-7.00427400	-0.44392800	-0.98768300
C	-7.15902300	0.47931000	-2.02144500
C	-8.01152400	-1.36107100	-0.68221000
C	-8.33935300	0.48671600	-2.76504400
H	-6.35454600	1.17962900	-2.22351700
C	-9.18403100	-1.34652700	-1.43930900
H	-7.86889700	-2.07635300	0.11694100
C	-9.35489100	-0.42820700	-2.47821700
H	-8.46185300	1.20716300	-3.56922700
H	-9.97025500	-2.06079100	-1.21022600
H	-10.27292300	-0.42552100	-3.05905200
H	-2.98375200	0.62360500	0.31456000
C	-2.42737400	1.91242000	2.54203300
C	-1.13461900	2.18606600	2.04357900
C	-3.26556000	2.95362300	2.95111800
C	-0.70158400	3.52348200	2.02167100
H	0.11334400	1.31238900	2.52936400
C	-2.82469100	4.27815100	2.90260800
H	-4.26968200	2.72720600	3.30647900
C	-1.53829900	4.56096500	2.43646400
H	0.29904300	3.76093600	1.67047700
H	-3.47728400	5.08228100	3.23349600
H	-1.18536400	5.58894900	2.39816600

13-S

B3LYP-D3 SCF energy: -3457.955716 a.u.
B3LYP-D3 enthalpy: -3457.954772 a.u.
B3LYP-D3 free energy: -3458.106590 a.u.
M06 SCF energy in solution: -3458.514681 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.84140400	0.09390800	1.86194300
P	-0.45125600	-0.92018900	-1.46795300
O	-6.29738600	0.10477400	-0.59497700
O	-4.58696700	1.20918200	-1.70699900
O	-2.83790700	3.66158300	-0.29263700
O	-1.27005500	5.00096800	-1.35761700
C	-2.58001100	0.13250600	1.21415200
C	-3.62867000	-0.50861500	1.88284900
H	-3.45080700	-0.95751800	2.85247000
C	-4.92995600	-0.58765300	1.35136600
H	-5.73182400	-1.08905400	1.88180500
C	-5.13801700	0.01425500	0.13018200
C	-5.94623200	0.77354100	-1.81457000
H	-6.59643200	1.64373800	-1.95221600
H	-6.03573200	0.06968500	-2.65065200
C	-4.10860600	0.67333000	-0.53760900
C	-2.81461800	0.74350900	-0.05657500
C	-1.04792700	-0.41455300	3.62581600
C	-1.29112100	-1.77562000	3.88490400
H	-1.39510500	-2.47234700	3.05646300
C	-1.39324000	-2.24966900	5.19181900
H	-1.58518000	-3.30440000	5.36894900
C	-1.23025000	-1.37269200	6.26737100
H	-1.29664800	-1.74144800	7.28728600
C	-0.97228100	-0.02327500	6.02345900
H	-0.83579900	0.66415500	6.85413500

C	-0.88493700	0.45479900	4.71338600
H	-0.67514900	1.50508200	4.54369300
C	-0.40636700	1.87667500	1.93575600
C	-1.30848200	2.83266000	2.43034400
H	-2.28563600	2.51970700	2.78735400
C	-0.96273800	4.18341900	2.44281400
H	-1.66283000	4.91599600	2.83697800
C	0.27375100	4.59272300	1.93366400
H	0.53581100	5.64752800	1.92442400
C	1.16952200	3.64752400	1.43011700
H	2.12310200	3.96190100	1.01933100
C	0.83613600	2.29172500	1.43946300
H	1.53165800	1.55912400	1.04826000
C	-0.70171900	0.91138300	-1.54983000
C	-1.78999800	1.49658600	-0.83443400
C	-1.88018300	2.87573700	-0.88272700
C	-2.46139400	5.01679900	-0.56028400
H	-3.26537200	5.51435300	-1.11551000
H	-2.25478100	5.52774900	0.38644700
C	-0.94158500	3.68049800	-1.52282500
C	0.13202900	3.13689000	-2.19184400
H	0.88160500	3.75667300	-2.66933500
C	0.22212500	1.73297500	-2.20451400
H	1.04418500	1.28236400	-2.74560700
C	0.75829500	-1.23569000	-2.83053400
C	2.12496300	-1.07228700	-2.54359100
H	2.44487900	-0.81301700	-1.54310600
C	3.09445600	-1.26020400	-3.52638400
H	4.13819900	-1.11409400	-3.26385400
C	2.71353700	-1.64568300	-4.81424500
H	3.46538800	-1.80678500	-5.58234500
C	1.36166400	-1.83461300	-5.10622600
H	1.05751600	-2.14656600	-6.10215600
C	0.38840800	-1.62600300	-4.12498500
H	-0.65548700	-1.78196100	-4.37436900
C	-2.05760200	-1.56872900	-2.09850800
C	-2.61967100	-2.68239300	-1.45806900
H	-2.09222300	-3.14217200	-0.62656400
C	-3.85013900	-3.19341600	-1.87346600
H	-4.27983800	-4.05039100	-1.36224000
C	-4.52758500	-2.60113700	-2.94169800
H	-5.48426600	-3.00029200	-3.26817800
C	-3.97403000	-1.49155000	-3.58743800
H	-4.49763400	-1.02607600	-4.41877900
C	-2.75300000	-0.96937000	-3.16039300
H	-2.34655600	-0.08307600	-3.63853600
Rh	0.45927200	-1.58509400	0.66239900
C	3.27128200	-0.09436300	2.52900300
C	2.24670500	-0.80758400	3.02530900
C	1.76049200	-2.01643700	2.32786900
C	2.92949800	-2.86357800	1.77974100
C	4.04668100	-1.99677500	1.11698500
N	3.88982200	-0.54577500	1.33485400
H	1.14153500	-2.63870100	2.98431000
H	3.64353000	0.83281600	2.94526900
H	1.76358600	-0.47023700	3.93779000
H	3.39424500	-3.41285300	2.61191300
H	5.02989500	-2.29980200	1.49710400
C	4.28143200	0.27368600	0.32153900
O	4.80380600	-0.07712600	-0.72333200
O	4.00289400	1.59368900	0.63252500
C	4.14414900	2.57674300	-0.33646300
C	4.65276500	3.79816900	0.10622300
C	3.70944200	2.41411000	-1.65352600
C	4.71477100	4.87851700	-0.77552300
H	4.98159600	3.88523500	1.13704900
C	3.79058900	3.49877100	-2.52763000
H	3.32918100	1.45886600	-1.98737500
C	4.28462600	4.73271800	-2.09630300
H	5.10477900	5.83136200	-0.42835200
H	3.46202200	3.37278900	-3.55614800
H	4.33796600	5.57138400	-2.78455600
H	4.05032900	-2.15088100	0.03908700
C	2.38137400	-3.81379800	0.74972700
C	2.88679200	-5.09704300	0.53247700
C	1.32494100	-3.29686900	-0.03662600
C	2.36014500	-5.89556500	-0.48756700
H	3.69249900	-5.47571700	1.15934300
C	0.82690900	-4.11133700	-1.06851200
C	1.33067900	-5.39923200	-1.28776500
H	2.75420100	-6.89481900	-0.65716400
H	0.03510100	-3.75487700	-1.72167300
H	0.92013600	-6.01002200	-2.08923200
H	1.63640100	-0.69116000	0.28691100

14

B3LYP-D3 SCF energy: -3457.959190 a.u.
B3LYP-D3 enthalpy: -3457.958246 a.u.
B3LYP-D3 free energy: -3458.107894 a.u.
M06 SCF energy in solution: -3458.523055 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.89013600	0.01304400	0.86429700
P	-2.16174300	-0.16336900	-0.80111600
O	-3.04485300	3.60868200	3.61032400
O	-2.80752100	3.79732600	1.31299900
O	0.06949200	4.56506900	-0.13855600
O	0.21914400	5.07819500	-2.39680900
C	-0.19569800	1.21149500	1.79751200
C	-0.32726900	1.13997200	3.18858500
H	0.31896000	0.48040500	3.75361500
C	-1.26738100	1.90411200	3.90710000
H	-1.35275100	1.83135200	4.98569600
C	-2.06876000	2.75052400	3.17410300
C	-3.64449900	4.14465500	2.42116900
H	-3.70136200	5.23380100	2.50497500
H	-4.63595300	3.69672300	2.27815500
C	-1.92984600	2.85708700	1.79176600
C	-1.02646200	2.11126300	1.05760200
C	2.13405700	-0.52130200	2.11951000
C	1.70886400	-1.41483400	3.11924200
H	0.67239400	-1.74191400	3.13942200
C	2.60724100	-1.92187600	4.05527100
H	2.25559200	-2.60473500	4.82434700
C	3.96155600	-1.58241500	3.98114900
H	4.66774800	-1.99408500	4.69740500
C	4.40167200	-0.72623300	2.97219800
H	5.45521200	-0.47554400	2.88217900
C	3.49361400	-0.19094000	2.05501500
H	3.86723400	0.46150000	1.27565100
C	1.82836400	1.17260200	-0.22585400

C	2.45134700	2.32537500	0.28138100
H	2.42285100	2.52781500	1.34802200
C	3.08683800	3.22042600	-0.57782500
H	3.57517500	4.10268700	-0.17188800
C	3.08403300	2.98985900	-1.95792600
H	3.56489000	3.69555400	-2.62990100
C	2.46138500	1.85011400	-2.46994500
H	2.45925400	1.65880700	-3.53828100
C	1.84372500	0.94431600	-1.60610200
H	1.34564200	0.07055000	-2.00691200
C	-1.44939300	1.43519400	-1.39891300
C	-0.96329100	2.34275400	-0.41368300
C	-0.44900200	3.53636300	-0.88342500
C	0.54056100	5.53770400	-1.07586500
H	0.03908400	6.49459000	-0.89125800
H	1.62840000	5.63379700	-0.98285600
C	-0.36353900	3.84807900	-2.23793800
C	-0.82657900	2.98337400	-3.20507100
H	-0.76691800	3.22654700	-4.26006900
C	-1.37820500	1.76884200	-2.75560200
H	-1.76184000	1.07900400	-3.49720700
C	-2.76926300	-0.94228000	-2.35631100
C	-4.12568600	-1.10421900	-2.66143000
H	-4.88421400	-0.70310300	-1.99827400
C	-4.51323400	-1.80459200	-3.80715300
H	-5.57039500	-1.93275900	-4.02412700
C	-3.55321700	-2.34392200	-4.66348300
H	-3.85799100	-2.89085700	-5.55161100
C	-2.19525700	-2.18377700	-4.36916300
H	-1.43936200	-2.60381500	-5.02748700
C	-1.80829900	-1.49777000	-3.21983900
H	-0.75426100	-1.40093000	-2.97605700
C	-3.69043100	0.47334500	0.02549300
C	-4.09231700	-0.05912800	1.25710300
H	-3.52675000	-0.86817500	1.70173700
C	-5.22335000	0.43778200	1.90775900
H	-5.52201600	0.01454300	2.86287400
C	-5.96782600	1.46945400	1.33230200
H	-6.85330700	1.85020700	1.83529000
C	-5.57015600	2.01208200	0.10614700
H	-6.14002200	2.82064300	-0.34451200
C	-4.43469400	1.52282200	-0.53876400
H	-4.11822700	1.96304700	-1.47988500
Rh	-0.72951900	-1.68374000	0.26209100
C	-2.33423100	-2.96979300	0.41696100
C	-2.72599000	-3.21306900	1.75046200
C	-3.03956600	-3.65269600	-0.58543900
C	-3.78991900	-4.06256300	2.06488700
H	-2.18878300	-2.72913100	2.56853900
C	-4.10417200	-4.50979800	-0.27915500
H	-2.77231600	-3.51539600	-1.62924600
C	-4.49089000	-4.71380000	1.04535700
H	-4.06727300	-4.22087000	3.10553000
H	-4.63375500	-5.01553900	-1.08449300
C	2.83665500	-3.21331300	0.51028100
C	1.75165100	-3.76407800	1.07960400
C	0.44003700	-3.69594000	0.45476600
C	0.33055900	-3.20462500	-0.85896500
C	1.59927100	-2.86910800	-1.61548200
N	2.73179900	-2.53993800	-0.72587500
H	-0.33926300	-4.33615300	0.85237100
H	3.81092600	-3.19682800	0.97330800
H	1.86248100	-4.25182300	2.04155600
H	-0.45529000	-3.58315500	-1.50876700
H	1.87823000	-3.74232000	-2.23134900
C	3.75513500	-1.80629300	-1.26882500
O	3.75678600	-1.32780100	-2.38770600
O	4.78681900	-1.69313000	-0.36765200
C	5.79777000	-0.75912900	-0.53013100
C	7.05516300	-1.14417200	-0.06487200
C	5.56918700	0.52941300	-1.01340900
C	8.10367100	-0.22369400	-0.08571900
H	7.19015900	-2.15329700	0.31128800
C	6.62850200	1.43738900	-1.03046300
H	4.59079800	0.81077600	-1.37238100
C	7.89509800	1.07032500	-0.56995700
H	9.08379000	-0.52108900	0.27713400
H	6.45039100	2.44200300	-1.40450300
H	8.71236200	1.78584300	-0.58595300
H	1.46530100	-2.03412600	-2.30315200
H	-5.31910700	-5.37670300	1.28348200

15-ts-R

B3LYP-D3 SCF energy: -3457.924093 a.u.
B3LYP-D3 enthalpy: -3457.923148 a.u.
B3LYP-D3 free energy: -3458.074317 a.u.
M06 SCF energy in solution: -3458.492437 a.u.
Imaginary frequency: -308.94 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.73127200	-1.71604800	-0.35824200
P	1.27033300	1.64311200	-0.33535300
O	2.77108500	-0.32226200	5.09050600
O	3.93743800	0.46011200	3.24838700
O	5.20144500	-1.64374300	0.94198800
O	6.63791500	-0.95454100	-0.74496600
C	1.38063500	-1.44700000	1.36054000
C	0.70877000	-1.93828000	2.48488400
H	-0.14178000	-2.59558200	2.35523400
C	1.09147000	-1.61237100	3.79992000
H	0.55739300	-2.00023200	4.66027800
C	2.17825600	-0.77829600	3.94061100
C	3.75791100	0.62522200	4.65891000
H	4.70278800	0.42255900	5.17063100
H	3.39710400	1.64242100	4.86048000
C	2.87587700	-0.30545700	2.83099500
C	2.51877100	-0.60092300	1.52892800
C	-0.46831900	-3.10714600	-0.15642100
C	-1.70852800	-2.81161600	0.43779600
H	-1.89650100	-1.80547000	0.79969100
C	-2.70509000	-3.77963500	0.54014600
H	-3.66011700	-3.52218000	0.99015100
C	-2.49054900	-5.05904400	0.02140800
H	-3.27171700	-5.81198200	0.08285800
C	-1.27191900	-5.35938800	-0.58998900
H	-1.09966800	-6.34982500	-1.00345600
C	-0.26451400	-4.39390300	-0.67434200
H	0.67402000	-4.64675500	-1.15577100
C	2.18299100	-2.48281700	-1.19988300
C	2.95785100	-3.48716000	-0.59939700
H	2.69607400	-3.84984300	0.39069200

C	4.07213600	-4.00470500	-1.25980100
H	4.66215600	-4.78840000	-0.79093200
C	4.43635600	-3.50798700	-2.51556000
H	5.31371500	-3.90108600	-3.02241900
C	3.67479100	-2.50197800	-3.11433300
H	3.96261000	-2.10446200	-4.08373300
C	2.54959400	-1.99610900	-2.46131900
H	1.96313400	-1.19511900	-2.90382200
C	2.99169100	0.97443800	-0.46484800
C	3.36484100	-0.08210500	0.41705300
C	4.61892800	-0.63013900	0.22240900
C	6.44281300	-1.92886800	0.28969300
H	7.25997900	-1.85684000	1.01545700
H	6.39411500	-2.92791400	-0.15993400
C	5.48271000	-0.21667300	-0.78830700
C	5.14361700	0.80560200	-1.64699100
H	5.81859400	1.13898700	-2.42752000
C	3.87990500	1.39728400	-1.45981200
H	3.59645800	2.20876100	-2.11888600
C	1.30922200	3.10504000	-1.46749300
C	1.19205700	2.86040100	-2.84820600
H	1.14119700	1.83238900	-3.20007900
C	1.11367900	3.91477500	-3.75640500
H	1.02496600	3.70699000	-4.81968700
C	1.13268100	5.23588800	-3.29742600
H	1.05683100	6.05989500	-4.00185900
C	1.24289200	5.48874400	-1.92984600
H	1.25222800	6.51245900	-1.56462500
C	1.33557700	4.43152800	-1.01995200
H	1.40897500	4.64550200	0.04084200
C	1.27312800	2.40502700	1.34487600
C	0.07376800	2.39840000	2.07074400
H	-0.81272400	1.94969500	1.63622600
C	0.02057700	2.96149200	3.34687600
H	-0.91508700	2.94965300	3.89933800
C	1.16272900	3.53698500	3.90825700
H	1.12052900	3.97597600	4.90190600
C	2.36152100	3.54998800	3.18772500
H	3.25278700	4.00035900	3.61820900
C	2.41879800	2.98266500	1.91407900
H	3.35630700	2.97718800	1.36576500
Rh	-0.33125600	0.16368100	-1.12840100
C	-3.65598000	-1.70366500	-2.14096800
C	-2.37863300	-1.87227800	-2.52276800
C	-1.47352900	-0.74637700	-2.75695600
C	-2.03919900	0.58246300	-2.73329800
C	-3.56302400	0.64031700	-2.87126900
N	-4.21602300	-0.40472600	-2.08063100
H	-4.31480100	-2.51756400	-1.87341800
H	-1.99001800	-2.88212300	-2.59720700
H	-3.98032200	1.60101700	-2.57618700
C	-5.21424400	-0.04831400	-1.21836400
O	-5.80179500	1.01345300	-1.20063200
O	-5.44703800	-1.08306400	-0.32881000
C	-6.28454000	-0.85672800	0.75524700
C	-5.75714600	-1.15092900	2.01249200
C	-7.60099100	-0.42076600	0.60734800
C	-6.56344600	-1.01344100	3.14357700
H	-4.72460500	-1.47936700	2.08572800
C	-8.39475900	-0.28084800	1.74656900
H	-7.97933100	-0.18197900	-0.37859800
C	-7.88372800	-0.57676400	3.01334100
H	-6.15669400	-1.24424000	4.12438400
H	-9.42003900	0.06311000	1.64088200
H	-8.51095100	-0.46613400	3.89341000
H	-3.78672500	0.46975200	-3.93660200
C	-1.93387400	1.59905800	-0.93862400
C	-2.75213000	1.10711300	0.10064500
C	-1.91658700	2.98561100	-1.15980700
C	-3.45778000	1.97336800	0.93614100
H	-2.84928000	0.03618300	0.24647000
C	-2.61724900	3.85429300	-0.31880500
H	-1.33300600	3.39464500	-1.97845700
C	-3.38196000	3.35565100	0.73827500
H	-4.08381500	1.56463600	1.72565800
H	-2.56181400	4.92641800	-0.49349000
H	-3.93748100	4.03250000	1.38157100
H	-1.55734300	1.32929700	-3.36286200
H	-0.63887600	-0.92929200	-3.43148900

16-R

B3LYP-D3 SCF energy: -3457.994143 a.u.
B3LYP-D3 enthalpy: -3457.993198 a.u.
B3LYP-D3 free energy: -3458.140730 a.u.
M06 SCF energy in solution: -3458.562870 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.72976800	0.94838900	0.13203300
P	-2.07897900	-0.91234700	-0.59087100
O	-3.47727200	2.63943000	4.02896300
O	-4.01631300	2.60610600	1.77209700
O	-2.23319400	4.37388900	-0.54963800
O	-3.12691800	4.59383800	-2.67227400
C	-0.48570500	1.56443300	1.38697100
C	-0.17060700	1.60792200	2.75050500
H	0.82965200	1.35204700	3.07566600
C	-1.11177100	1.96197500	3.73429600
H	-0.85577500	1.97793700	4.78782700
C	-2.37848400	2.27527000	3.29410500
C	-4.54952600	2.78626500	3.08753500
H	-4.97415800	3.79270700	3.17403600
H	-5.30684300	2.01720600	3.28042300
C	-2.69935300	2.25514500	1.93999400
C	-1.80014800	1.89679500	0.95234900
C	2.23771300	0.78531400	1.17989400
C	2.47537200	-0.47617300	1.74525000
H	1.82284000	-1.30403300	1.48809900
C	3.54234800	-0.67268600	2.62060100
H	3.72938000	-1.66292700	3.02577200
C	4.37997600	0.39568900	2.94958300
H	5.22289100	0.24279200	3.61761000
C	4.14839700	1.65546600	2.39584100
H	4.81535800	2.48145100	2.62480700
C	3.08591600	1.85056600	1.51173600
H	2.92747200	2.83142500	1.07587900
C	1.03592900	2.46786000	-0.87409600
C	0.91764100	3.76127400	-0.34305300
H	0.60273600	3.89463100	0.68722000
C	1.18153100	4.87874100	-1.13754700
H	1.08926200	5.87505700	-0.71224300
C	1.55768500	4.71812300	-2.47376900

H	1.76120800	5.58889800	-3.09171500
C	1.66376000	3.43397000	-3.01479700
H	1.94215500	3.30252400	-4.05712300
C	1.39986800	2.31701600	-2.22040000
H	1.44925500	1.31795600	-2.64148200
C	-2.64616200	0.74731800	-1.21322700
C	-2.27500000	1.90597500	-0.46167500
C	-2.48463000	3.12708900	-1.07375500
C	-2.39145200	5.27715100	-1.64779300
H	-2.95686800	6.15257500	-1.31894200
H	-1.39981600	5.55498100	-2.03263800
C	-3.03367500	3.26279200	-2.34735400
C	-3.44989700	2.16280900	-3.06414000
H	-3.91381600	2.26136100	-4.03944400
C	-3.24043400	0.90342200	-2.47025900
H	-3.55762300	0.02961600	-3.02477200
C	-3.07044400	-2.14985000	-1.54728800
C	-2.81526800	-2.29551400	-2.92422100
H	-2.08733200	-1.64555300	-3.40202600
C	-3.45945900	-3.27717100	-3.67577500
H	-3.25290300	-3.36298100	-4.73942800
C	-4.35135900	-4.15923700	-3.05923000
H	-4.84607900	-4.93266000	-3.64046400
C	-4.59144100	-4.04532900	-1.68991300
H	-5.27398200	-4.73310900	-1.19727800
C	-3.96122700	-3.04777300	-0.94035500
H	-4.16230300	-2.97811600	0.12276600
C	-2.84992700	-0.97968100	1.08430100
C	-2.05073400	-1.34884400	2.17177900
H	-1.00923100	-1.60281800	2.00391000
C	-2.58502600	-1.37687400	3.46139200
H	-1.95043800	-1.65518900	4.29794600
C	-3.92451600	-1.04636800	3.67196800
H	-4.33942300	-1.06515500	4.67631400
C	-4.73245300	-0.68523300	2.58796800
H	-5.77840600	-0.43379900	2.74668000
C	-4.19575700	-0.64234700	1.30178700
H	-4.81609400	-0.33485000	0.46436400
Rh	0.17943100	-1.01759300	-0.99748000
C	2.10714500	-1.41731000	-2.08553900
C	0.97786100	-1.99058700	-2.72949700
C	0.27803600	-2.99232600	-2.01444700
C	1.07758900	-3.97325200	-1.14372400
C	2.58044000	-3.71453400	-1.34807100
N	2.91857100	-2.29182700	-1.28812200
H	2.65060600	-0.60500900	-2.54818800
H	0.57575600	-1.53524300	-3.63071400
H	3.19951000	-4.24620400	-0.62791800
C	4.04884400	-1.89395900	-0.63767900
O	4.72134500	-2.60200000	0.09826300
O	4.31375700	-0.59085400	-0.95795700
C	5.37003200	0.16512900	-0.47871200
C	6.43118500	-0.30402000	0.29895700
C	5.29977200	1.50753100	-0.86489100
C	7.41407700	0.60497900	0.70093600
H	6.47081400	-1.34231200	0.59089700
C	6.29045200	2.39636200	-0.45756500
H	4.45353200	1.83595200	-1.46047400
C	7.35267700	1.94985300	0.33397000
H	8.23881300	0.24643500	1.31158300
H	6.22690000	3.43985600	-0.75450800
H	8.12605300	2.64194200	0.65560500
H	2.84196300	-4.07414700	-2.35321400
C	0.60641400	-4.03363600	0.30774000
C	1.45631900	-3.82139700	1.39961500
C	-0.73342600	-4.37110400	0.56144000
C	0.97641400	-3.93634200	2.70970000
H	2.49765200	-3.55612200	1.24317100
C	-1.20852900	-4.50008800	1.86372800
H	-1.41281900	-4.52392000	-0.27333700
C	-0.35282400	-4.28201100	2.94829600
H	1.65223100	-3.75757100	3.54247000
H	-2.25136100	-4.75367100	2.03439600
H	-0.72343100	-4.37514400	3.96565500
H	0.90301900	-4.97865600	-1.56003700
H	-0.64277400	-3.37911600	-2.43756000

17-ts-R

B3LYP-D3 SCF energy: -3534.365525 a.u.
B3LYP-D3 enthalpy: -3534.364581 a.u.
B3LYP-D3 free energy: -3534.517948 a.u.
M06 SCF energy in solution: -3534.943082 a.u.
Imaginary frequency: -1360.33 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.50795600	0.17952900	-1.19787700
C	2.69730300	-0.92346700	-2.03367900
C	3.56990500	-2.00183800	-1.73048400
C	4.69520700	-1.68787000	-0.73566200
C	4.15828800	-0.74030500	0.37025100
N	3.52374500	0.43675000	-0.22205700
H	3.84182700	-2.65869000	-2.55776900
H	2.03775100	1.06745400	-1.58431200
H	2.02104200	-1.01263800	-2.88251500
H	5.49076900	-1.13337100	-1.25571000
H	4.96307300	-0.40224800	1.02178500
C	3.98997600	1.68222000	0.07912600
O	4.83439900	1.94060900	0.91947900
O	3.36853100	2.61170700	-0.72872100
C	3.40565700	3.97906300	-0.52576500
C	2.33028700	4.66031200	-1.10674200
C	4.40647500	4.67173300	0.16013200
C	2.23936100	6.04409400	-0.98095800
H	1.57054500	4.09062000	-1.63161900
C	4.29637100	6.06064000	0.27785900
H	5.22862700	4.13133900	0.60491300
C	3.22087600	6.75295500	-0.28152000
H	1.39475700	6.56337900	-1.42618800
H	5.06915700	6.60316400	0.81650900
H	3.15054700	7.83231300	-0.17875100
H	3.41379800	-1.26841300	0.97760700
C	5.33021900	-2.91822300	-0.11158100
C	6.71276300	-3.12289400	-0.20659700
C	4.56427100	-3.85611700	0.60004700
C	7.32083600	-4.23318200	0.38348000
H	7.32009700	-2.40259800	-0.75094600
C	5.17022400	-4.96413500	1.19385400
H	3.48982000	-3.71923100	0.67905500
C	6.54989400	-5.15902500	1.08802000
H	8.39525300	-4.37285900	0.29244500
H	4.56089200	-5.67939400	1.74145100

H	7.01880400	-6.02425800	1.54988500
O	1.54933700	-2.86026400	-0.35751100
H	2.54157800	-2.66931500	-1.03375200
P	-1.50234700	-1.97479300	-0.33083300
P	-0.25031400	1.01941000	0.36594000
O	-4.84947600	1.97283300	-3.31133300
O	-4.46758400	2.34201200	-1.05670600
O	-5.37972800	0.13309400	1.31313500
O	-5.25833300	0.54231900	3.59434500
C	-2.68394400	-0.89860600	-1.27131100
C	-2.95234900	-1.12421500	-2.62560800
H	-2.58682000	-2.02651000	-3.10094600
C	-3.67883400	-0.21229000	-3.41467500
H	-3.87578700	-0.39945400	-4.46448700
C	-4.12398100	0.93221100	-2.78963100
C	-4.89054200	2.96423200	-2.27466000
H	-5.91581300	3.32624600	-2.16058000
H	-4.19719000	3.77901300	-2.52269700
C	-3.89100700	1.15452900	-1.43385900
C	-3.17903800	0.28021300	-0.63506100
C	-1.44313700	-3.54697300	-1.30953900
C	-0.66145300	-3.55839200	-2.48222200
H	-0.14371800	-2.65093000	-2.78171000
C	-0.53350100	-4.71857400	-3.24511100
H	0.07149400	-4.70526300	-4.14773800
C	-1.16924200	-5.89590400	-2.84094100
H	-1.06224600	-6.80372500	-3.42830700
C	-1.93261800	-5.90059500	-1.67319100
H	-2.42207900	-6.81419300	-1.34622000
C	-2.07137300	-4.73627900	-0.91274400
H	-2.66405900	-4.76314500	-0.00524900
C	-2.47375300	-2.42303800	1.17042200
C	-3.83678600	-2.75431400	1.11143200
H	-4.35145200	-2.75541300	0.15456200
C	-4.53748400	-3.05556200	2.27903200
H	-5.59065500	-3.31994200	2.22407400
C	-3.88893400	-3.00777600	3.51726200
H	-4.43968000	-3.22669200	4.42813400
C	-2.53516600	-2.67153500	3.58228000
H	-2.03128300	-2.62228700	4.54354700
C	-1.82826400	-2.38562600	2.41272200
H	-0.77931100	-2.10329000	2.45147000
C	-1.77904100	0.98581100	1.41259000
C	-3.00856300	0.59283000	0.81062200
C	-4.10131600	0.50027700	1.65189700
C	-6.11752000	0.08911700	2.53921300
H	-6.98571400	0.75342900	2.46594400
H	-6.42343100	-0.94429700	2.74128300
C	-4.02955400	0.74307000	3.02086100
C	-2.85061100	1.12685600	3.62139100
H	-2.79264900	1.32045600	4.68666400
C	-1.72462000	1.24694300	2.78605800
H	-0.78590300	1.54621400	3.23551900
C	0.96236400	1.79626300	1.51845500
C	1.70086000	0.91933900	2.33384700
H	1.56583400	-0.15370000	2.21611600
C	2.60739800	1.41310700	3.26913800
H	3.18452700	0.72217700	3.87689200
C	2.79756100	2.79089700	3.39788000
H	3.52448500	3.17586200	4.10726400
C	2.07324300	3.66840800	2.59218500
H	2.23858400	4.73956900	2.66025200
C	1.15670300	3.17551600	1.66079100
H	0.62878900	3.87585700	1.02596700
C	-0.69643800	2.31856800	-0.87093800
C	-0.40481100	2.08451900	-2.22239900
H	0.04091200	1.13552100	-2.50609900
C	-0.71688000	3.03885400	-3.19217100
H	-0.48743900	2.84396700	-4.23608500
C	-1.32754700	4.23937700	-2.82009300
H	-1.56133100	4.98800900	-3.57256500
C	-1.65170700	4.46795000	-1.47900800
H	-2.14543000	5.39110600	-1.18651400
C	-1.35164400	3.50695600	-0.51275500
H	-1.64079900	3.67358800	0.52065800
Rh	0.53201400	-0.99804100	-0.28948800
H	1.07167800	-3.61850100	-0.73235200

18-R

B3LYP-D3 SCF energy: -901.048964 a.u.
B3LYP-D3 enthalpy: -901.048020 a.u.
B3LYP-D3 free energy: -901.113240 a.u.
M06 SCF energy in solution: -900.927892 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.17555500	2.04256200	0.88671200
C	-3.42153600	1.56127200	0.78996100
C	-3.83884600	0.54333800	-0.24415600
C	-2.64819300	0.01001600	-1.07608500
C	-1.67469700	1.18532800	-1.33513000
N	-1.18487400	1.71183500	-0.06025000
H	-4.35090200	-0.29432100	0.24813600
H	-1.84361900	2.70031300	1.68084100
H	-4.16556500	1.89610500	1.50711100
H	-0.82738500	0.86976300	-1.93902600
C	0.11669400	1.60363200	0.37677200
O	0.48971700	1.83023200	1.50780300
O	0.94551700	1.23819800	-0.65573000
C	2.19758200	0.72349200	-0.31849700
C	3.32813300	1.40112800	-0.76153100
C	2.28915100	-0.48607900	0.36765300
C	4.58757500	0.85122900	-0.51082300
H	3.21047600	2.34023900	-1.29241600
C	3.55228200	-1.02096300	0.61783800
H	1.38477700	-0.99174900	0.68866700
C	4.70231400	-0.35693900	0.18003800
H	5.47771100	1.37166900	-0.85335000
H	3.63620800	-1.96297400	1.15292700
H	5.68336900	-0.78060100	0.37581500
H	-2.20208900	1.99304800	-1.85832500
H	-4.58025600	0.98865000	-0.92337100
H	-3.02687300	-0.31402200	-2.05349300
C	-1.88389200	-1.15696300	-0.46686700
C	-1.22960500	-2.05843800	-1.32047400
C	-1.73816100	-1.33060100	0.91641100
C	-0.45577000	-3.10216900	-0.81435600
H	-1.32597300	-1.93654400	-2.39769700
C	-0.96696900	-2.37797300	1.42822600
H	-2.21757800	-0.63928800	1.60126800
C	-0.32269100	-3.26735200	0.56674100
H	0.04133700	-3.78638900	-1.49678300

H	-0.86677400	-2.49143400	2.50441600
H	0.27849100	-4.07986700	0.96584200

19

B3LYP-D3 SCF energy: -822.477625 a.u.
B3LYP-D3 enthalpy: -822.476681 a.u.
B3LYP-D3 free energy: -822.536272 a.u.
M06 SCF energy in solution: -822.346305 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.76845700	0.19043900	-0.35489900
C	-2.95838300	0.21014300	0.41028200
C	-3.39852600	-1.01696000	1.07256800
C	-2.88775000	-2.20277100	0.71368900
C	-1.85017700	-2.27166900	-0.37907400
N	-1.04725400	-1.03917100	-0.40663500
H	-4.16726100	-0.93910700	1.83771400
H	-3.22085500	-3.13202000	1.16749900
H	-1.15905000	-3.10136700	-0.23166000
C	0.31597100	-1.17738900	-0.24383700
O	0.90533000	-2.24030300	-0.24805000
O	0.91236500	0.03939300	-0.07116900
C	2.29539500	0.14090700	0.06260800
C	2.73798700	1.04796900	1.02373700
C	3.19204200	-0.53811600	-0.76302800
C	4.10652200	1.27884600	1.16642700
H	2.00513500	1.55951900	1.63935000
C	4.55843500	-0.30131700	-0.60395700
H	2.82748100	-1.24558400	-1.49627900
C	5.02084300	0.60325700	0.35502500
H	4.45531900	1.98600100	1.91389600
H	5.26452200	-0.82996500	-1.23843700
H	6.08657000	0.78024400	0.46860800
H	-2.33175400	-2.41189600	-1.36035900
C	-1.35858700	1.33696500	-1.04073600
H	-0.45599700	1.30887800	-1.63829100
C	-3.68736100	1.40443500	0.49661500
C	-2.10239700	2.51277800	-0.94232400
C	-3.26609800	2.55233200	-0.17003000
H	-1.77147400	3.39794500	-1.47818800
H	-3.84307100	3.46951200	-0.09424100
H	-4.59709300	1.42021900	1.09219300

20

B3LYP-D3 SCF energy: -3611.572557 a.u.
B3LYP-D3 enthalpy: -3611.571612 a.u.
B3LYP-D3 free energy: -3611.725235 a.u.
M06 SCF energy in solution: -3612.091846 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.14864300	1.64873900	0.01530100
P	0.31616300	-1.67577700	-0.46863900
O	5.88990900	-1.61122500	1.66426900
O	3.82361800	-2.11872300	2.59000100
O	1.98381000	-0.01308600	4.28062400
O	0.07141000	-0.64661900	5.42926900
C	2.68103900	0.73289500	0.52241000
C	3.93750000	1.04002800	-0.01041700
H	4.04188500	1.88026200	-0.68574400
C	5.09389500	0.30081100	0.30313700
H	6.05963200	0.54738400	-0.12388500
C	4.94090600	-0.74575700	1.18530800
C	5.18859900	-2.53994000	2.50336000
H	5.63472500	-2.53408700	3.50394600
H	5.23080700	-3.53775700	2.05147100
C	3.69997500	-1.05086200	1.73765600
C	2.54151800	-0.36468400	1.42323600
C	1.84034300	3.17597700	-0.76052900
C	2.29438200	3.07963500	-2.08732700
H	2.24597000	2.12204100	-2.59807900
C	2.78717600	4.19712700	-2.75963600
H	3.13275400	4.10056900	-3.78549500
C	2.82157500	5.43900900	-2.11806700
H	3.19436400	6.31471300	-2.64252900
C	2.36695400	5.54716200	-0.80351200
H	2.37874100	6.51038200	-0.30020800
C	1.88067600	4.42500800	-0.12802000
H	1.50701000	4.53629500	0.88313200
C	0.49075600	2.20433900	1.64054100
C	1.30141200	2.72428300	2.66241900
H	2.37423800	2.80965700	2.51386100
C	0.73176500	3.11153200	3.87536700
H	1.36285300	3.52261900	4.65977000
C	-0.64440400	2.96341600	4.08616300
H	-1.08237100	3.26222800	5.03525400
C	-1.45224700	2.43113900	3.07949800
H	-2.52135100	2.30760800	3.21678300
C	-0.88169300	2.05442600	1.86374100
H	-1.50027000	1.62532800	1.08846000
C	0.19412500	-1.45217400	1.37283800
C	1.26188900	-0.79204500	2.05476300
C	1.09452700	-0.59569600	3.41304600
C	1.30312400	0.08248200	5.53590500
H	1.92253900	-0.36523800	6.31952800
H	1.08194300	1.13530800	5.74832800
C	-0.05104000	-0.97852100	4.10592300
C	-1.08763100	-1.62313900	3.46880600
H	-1.97430600	-1.94366600	4.00421500
C	-0.93783000	-1.85679100	2.08860100
H	-1.73833500	-2.37931200	1.58198200
C	-0.99099400	-2.92469500	-0.83505700
C	-0.72051400	-4.22760500	-1.27108600
H	0.30257900	-4.57624400	-1.35249400
C	-1.76597300	-5.08253500	-1.63100600
H	-1.53890100	-6.08724300	-1.97789500
C	-3.09068200	-4.65219800	-1.55235000
H	-3.90055000	-5.32159500	-1.82997500
C	-3.37084600	-3.35220600	-1.12129600
H	-4.39625700	-3.00284200	-1.04871900
C	-2.32704400	-2.49410500	-0.78190600
H	-2.54667900	-1.47554500	-0.48484100
C	1.88765700	-2.63694700	-0.59618000
C	2.85212600	-2.26998300	-1.54269800
H	2.65296900	-1.44432700	-2.21444800
C	4.06434000	-2.95813000	-1.61690800
H	4.80957800	-2.65626400	-2.34755000
C	4.31951800	-4.02640100	-0.75507100
H	5.26299900	-4.56271800	-0.81594700
C	3.35801900	-4.40384800	0.18763300
H	3.54965100	-5.23486600	0.86196300

C	2.15393000	-3.70617400	0.27451600
H	1.42220000	-3.98309500	1.02809800
Rh	-0.02447000	0.28587700	-1.64722900
C	0.16674800	-0.85521300	-3.35120000
C	1.28218300	-0.48862300	-4.13085700
C	-0.64595700	-1.88621100	-3.85380800
C	1.59278400	-1.14055200	-5.32855700
H	1.93899000	0.31367700	-3.79566300
C	-0.34007900	-2.54370200	-5.05041700
H	-1.53671400	-2.18555600	-3.31085900
C	0.78471300	-2.18094200	-5.79277300
H	2.46866800	-0.83344900	-5.89727000
H	-0.98874500	-3.34445100	-5.40071600
C	-0.95356300	2.17122900	-2.60267000
C	-1.73540100	1.04850200	-2.87380500
C	-3.10168200	0.93335200	-2.24869100
N	-3.19154000	1.65091100	-0.96045500
H	-0.18127600	2.47324100	-3.30553200
H	-1.66084400	0.55621900	-3.83588700
H	-3.84557800	1.36354400	-2.94115800
C	-3.87787900	1.14340700	0.10892800
O	-3.97281800	1.63943500	1.21678800
O	-4.48490900	-0.05103200	-0.22531900
C	-5.04380700	-0.84185600	0.77357000
C	-4.39304300	-1.10118100	1.98056400
C	-6.25133000	-1.45928400	0.45419700
C	-4.97395000	-2.00135300	2.87387400
H	-3.46020500	-0.60587600	2.21403400
C	-6.81656300	-2.36357600	1.35530200
H	-6.72486200	-1.22926600	-0.49506800
C	-6.17998200	-2.63738100	2.56748300
H	-4.47692200	-2.20609200	3.81850200
H	-7.75559600	-2.85045900	1.10740300
H	-6.62061800	-3.33946500	3.26937300
H	-3.36602000	-0.10845900	-2.09342600
C	-3.19177100	3.99922400	-0.15797400
C	-2.63523500	2.97234500	-0.92648100
C	-1.49589000	3.22058300	-1.72909400
C	-0.95073600	4.51270000	-1.72944800
C	-1.49018900	5.52817200	-0.94519000
C	-2.61229600	5.26845500	-0.15819600
H	-4.05933100	3.80174000	0.45575900
H	-0.08035200	4.70834200	-2.34807800
H	-1.03435100	6.51439900	-0.95039300
H	-3.04993400	6.05202600	0.45398600
H	1.02358300	-2.69252500	-6.72180300

21-ts-S

B3LYP-D3 SCF energy: -3611.555322 a.u.
B3LYP-D3 enthalpy: -3611.554378 a.u.
B3LYP-D3 free energy: -3611.704850 a.u.
M06 SCF energy in solution: -3612.074856 a.u.
Imaginary frequency: -295.16 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.08633000	1.65608800	-0.38867800
P	0.31766900	-1.61388200	-0.34039500
O	6.29710900	-1.18026000	0.42328700
O	4.52507900	-1.72306900	1.81815700
O	3.05232400	0.40411800	3.73961400
O	1.57511800	-0.30173900	5.38193900
C	2.75946000	0.89814800	-0.11211700
C	3.84816900	1.23038900	-0.92794700
H	3.74595300	2.01661700	-1.66458100
C	5.09427800	0.58505900	-0.83464200
H	5.92317300	0.85265600	-1.48048000
C	5.20982800	-0.40309400	0.11783500
C	5.84798000	-2.10199700	1.42702000
H	6.51370400	-2.04663400	2.29470900
H	5.82510000	-3.11344200	1.00356400
C	4.14519500	-0.72760700	0.95217900
C	2.90259600	-0.12394000	0.87009800
C	1.54868500	3.20019300	-1.30500700
C	1.75928100	3.09215900	-2.69045300
H	1.65344000	2.11981300	-3.16584900
C	2.08433500	4.21102300	-3.45654700
H	2.24303500	4.10566500	-4.52657100
C	2.19103600	5.46573300	-2.84963400
H	2.43064700	6.34235100	-3.44547400
C	1.98324200	5.58530100	-1.47497900
H	2.05818600	6.55778600	-0.99529600
C	1.66903800	4.46108200	-0.70665300
H	1.49036100	4.57924500	0.35579800
C	0.63592700	2.26446200	1.29461200
C	1.57449200	2.82736500	2.17357700
H	2.61795100	2.89531800	1.87939000
C	1.17855300	3.27319300	3.43502400
H	1.91200800	3.71522900	4.10507300
C	-0.15540800	3.15000700	3.83606900
H	-0.46142800	3.49351300	4.82085800
C	-1.09196000	2.58402700	2.96845400
H	-2.13128300	2.48489300	3.26851000
C	-0.69860200	2.14135700	1.70443400
H	-1.42479300	1.69134700	1.03635900
C	0.68927600	-1.32761100	1.46576100
C	1.84495300	-0.56785200	1.81852000
C	2.01961700	-0.29687600	3.16360300
C	2.71026000	0.53550900	5.12267800
H	3.55294200	0.20583700	5.73845300
H	2.44504500	1.57947100	5.33382800
C	1.13626000	-0.71969800	4.15105900
C	0.03149100	-1.47854000	3.83710400
H	-0.64854300	-1.83983200	4.59988400
C	-0.17244800	-1.77134700	2.47581600
H	-1.03639800	-2.37035800	2.22320800
C	-0.89356200	-3.00337000	-0.27175800
C	-0.63020800	-4.30584300	-0.71471800
H	0.34891300	-4.56744100	-1.09941800
C	-1.63660000	-5.27435600	-0.68821000
H	-1.42023800	-6.27903400	-1.04270700
C	-2.91339900	-4.95805000	-0.21891600
H	-3.69220000	-5.71618300	-0.20348200
C	-3.18938800	-3.65896500	0.21410400
H	-4.18072800	-3.37533600	0.55188300
C	-2.18680600	-2.69323100	0.17431400
H	-2.41625500	-1.67848200	0.47358400
C	1.88069600	-2.43871100	-0.88243300
C	2.50195500	-2.01302300	-2.06310300
H	2.04161500	-1.22036800	-2.64290900
C	3.70861900	-2.58408000	-2.47162300
H	4.19079700	-2.23382300	-3.38028700

C	4.29836200	-3.59594400	-1.71161700
H	5.23782200	-4.04014500	-2.03024500
C	3.67838100	-4.03442700	-0.53715600
H	4.13019100	-4.82507400	0.05702300
C	2.48251900	-3.45174900	-0.11905600
H	2.01913500	-3.77293900	0.80937800
Rh	-0.39865700	0.30258000	-1.52903700
C	-1.24435800	-0.95707500	-3.11546200
C	-0.27744800	-1.05626200	-4.13936000
C	-2.15121500	-2.01589800	-2.96644000
C	-0.15792100	-2.21168000	-4.90976500
H	0.39149800	-0.21757100	-4.32638500
C	-2.04569300	-3.16821100	-3.75203600
H	-2.92538500	-1.96834300	-2.20942500
C	-1.04271000	-3.27930500	-4.71526400
H	0.61669100	-2.27634600	-5.67100300
H	-2.74201800	-3.98657100	-3.58820800
C	-1.37428500	1.98414700	-2.51506500
C	-2.12515800	0.90469600	-3.10599200
C	-3.56354000	0.78156700	-2.63677200
N	-3.69143000	1.11695000	-1.21654200
H	-0.66528000	2.49505800	-3.16161500
H	-2.04557800	0.81942400	-4.18478700
H	-4.15755700	1.50505700	-3.21503900
C	-4.10864900	0.14264800	-0.35753200
O	-4.60389500	-0.92159400	-0.68617000
O	-3.87730600	0.50982900	0.94687200
C	-4.26318300	-0.32474400	1.99025000
C	-5.51722400	-0.93503400	2.05077200
C	-3.33936400	-0.46019400	3.02558100
C	-5.83545200	-1.70372000	3.17195400
H	-6.21456300	-0.82445500	1.23055300
C	-3.67814800	-1.22223500	4.14423000
H	-2.37029700	0.01802800	2.93914100
C	-4.92328600	-1.84984800	4.22023600
H	-6.80683700	-2.18783800	3.22395700
H	-2.96353300	-1.32296400	4.95614200
H	-5.18239200	-2.44764300	5.08940900
H	-3.98416600	-0.20707100	-2.79846400
C	-3.84725500	3.21677000	0.08209500
C	-3.19870100	2.40681400	-0.85142600
C	-2.05703400	2.86132100	-1.54597600
C	-1.62268300	4.17435600	-1.29839200
C	-2.24670100	4.97328100	-0.34371000
C	-3.35332900	4.49124000	0.36034100
H	-4.72667900	2.84208800	0.59335800
H	-0.77651200	4.55909200	-1.85635800
H	-1.87242800	5.97593800	-0.15473500
H	-3.84918800	5.11120300	1.10168100
H	-0.95836200	-4.17781600	-5.32120000

22-S

B3LYP-D3 SCF energy: -3611.576865 a.u.
B3LYP-D3 enthalpy: -3611.575921 a.u.
B3LYP-D3 free energy: -3611.732155 a.u.
M06 SCF energy in solution: -3612.098640 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.04718200	-1.47696300	0.29692500
P	-1.77835400	1.36531400	-0.25867900
O	-4.35911800	-3.14050000	-3.46271500
O	-4.94875400	-1.92002300	-1.58044800
O	-4.28143300	-2.98456900	1.47149200
O	-5.11156400	-1.99846900	3.39950000
C	-1.33112000	-2.15250200	-0.83912500
C	-0.99103400	-2.90605600	-1.96594200
H	0.04103700	-3.20208200	-2.11700300
C	-1.94464900	-3.29190700	-2.92683700
H	-1.67152500	-3.87139900	-3.80167400
C	-3.24453500	-2.89538300	-2.70111300
C	-5.43328900	-2.43874300	-2.82295500
H	-6.25760800	-3.13340800	-2.62981000
H	-5.75336100	-1.60709900	-3.46252500
C	-3.59726100	-2.16027600	-1.57132000
C	-2.68211500	-1.74623300	-0.62169800
C	1.49194600	-2.40900900	-0.12313800
C	2.26350500	-1.91092800	-1.19118800
H	1.92411700	-1.03271300	-1.73714800
C	3.46432800	-2.52258800	-1.55170800
H	4.06139200	-2.10118300	-2.35418600
C	3.91912400	-3.63695300	-0.84269700
H	4.86731300	-4.09729300	-1.10422300
C	3.16723200	-4.13441800	0.22340300
H	3.52207500	-4.99529000	0.78460500
C	1.96243600	-3.52574800	0.58389900
H	1.39709300	-3.91789100	1.42263500
C	-0.59213800	-2.13980600	1.93061800
C	-1.05919900	-3.45214900	2.10179300
H	-1.09366600	-4.12742500	1.25126600
C	-1.50749700	-3.88304500	3.35096900
H	-1.85861000	-4.90446200	3.47600600
C	-1.51920500	-2.99945100	4.43492900
H	-1.88292400	-3.33170800	5.40372500
C	-1.07405500	-1.68619200	4.26679900
H	-1.10222900	-0.98985200	5.10068800
C	-0.60876600	-1.25958800	3.02206100
H	-0.29710400	-0.22919500	2.87301200
C	-2.92701000	0.40451200	0.83636300
C	-3.16126100	-0.98147200	0.56871600
C	-3.91919000	-1.65997800	1.50667100
C	-4.93350700	-3.24767600	2.71740100
H	-5.91218500	-3.70029100	2.52728000
H	-4.29984100	-3.90462800	3.32620200
C	-4.41917400	-1.07056200	2.66414900
C	-4.21033800	0.26386800	2.93453000
H	-4.60699100	0.73239800	3.82838500
C	-3.45585200	0.98787000	1.99379700
H	-3.28307300	2.03970600	2.18638600
C	-2.17968600	3.13487100	0.10146100
C	-1.62300000	3.69562800	1.26547300
H	-0.98513100	3.08930600	1.90238400
C	-1.85190100	5.03135700	1.59084100
H	-1.41115600	5.43927200	2.49531900
C	-2.61238800	5.84046200	0.74230100
H	-2.77913700	6.88599800	0.98810400
C	-3.13991900	5.30315900	-0.43215800
H	-3.71779400	5.92900200	-1.10746700
C	-2.92885300	3.95880500	-0.75078000
H	-3.34390100	3.56221700	-1.67050400
C	-2.51974800	1.05263600	-1.92210600
C	-1.68644400	0.66942000	-2.98132700

H	-0.61901000	0.58206600	-2.80932700
C	-2.22739600	0.38109700	-4.23521300
H	-1.57078800	0.07378100	-5.04434900
C	-3.60420100	0.48227200	-4.44543200
H	-4.02474500	0.25749100	-5.42219700
C	-4.44210000	0.86758100	-3.39423200
H	-5.51510200	0.94669600	-3.55088100
C	-3.90501300	1.13893300	-2.13596900
H	-4.56437000	1.39799200	-1.31234000
Rh	0.34786200	0.79377000	0.00598700
C	1.18391500	2.69452100	-0.44093500
C	2.34389500	2.75874600	0.55449300
C	3.08003800	1.41875600	0.42139400
N	3.65761800	1.24170800	-0.91819500
H	0.53413300	3.56936200	-0.39737800
H	3.06078500	3.54813000	0.26717800
H	3.86846500	1.33617000	1.16411200
C	4.77135100	0.43737800	-1.04703100
O	5.36142100	0.15031900	-2.07078800
O	5.15858100	-0.03458100	0.18719700
C	6.25654300	-0.88158500	0.30041200
C	7.49247600	-0.60066300	-0.28182900
C	6.07359100	-2.00045200	1.11106400
C	8.55724300	-1.47266900	-0.04777300
H	7.60858800	0.27037300	-0.91370600
C	7.14840900	-2.85949300	1.34142400
H	5.09299800	-2.18719000	1.53485500
C	8.39220900	-2.60015400	0.76066900
H	9.52236600	-1.26471500	-0.50153500
H	7.00946300	-3.73314600	1.97247100
H	9.22810600	-3.27119900	0.93739800
H	2.40163700	0.55316300	0.62075500
C	3.23688200	1.38145000	-3.37692700
C	2.87241700	1.67288600	-2.04818700
C	1.66992100	2.40072500	-1.80074500
C	0.91100000	2.82536300	-2.91260500
C	1.27499000	2.52982600	-4.21601600
C	2.44449600	1.79776600	-4.44343900
H	4.14752200	0.83947100	-3.57260000
H	-0.00117200	3.38192200	-2.71139100
H	0.65890900	2.86591300	-5.04591200
H	2.75712400	1.55673300	-5.45577000
C	1.87445100	3.05946200	1.96730500
C	1.66843700	4.39592500	2.33306800
C	1.56274800	2.06324400	2.90509600
C	1.14900900	4.73207400	3.58470700
H	1.90301700	5.18110500	1.61804200
C	1.04035600	2.39335100	4.15783800
H	1.71236200	1.01641100	2.66248000
C	0.82373100	3.72959500	4.50132100
H	0.99766600	5.77740400	3.84237900
H	0.80342700	1.60154400	4.86433800
H	0.41567700	3.98708200	5.47503300

23-ts-S

B3LYP-D3 SCF energy: -3611.565821 a.u.
B3LYP-D3 enthalpy: -3611.564876 a.u.
B3LYP-D3 free energy: -3611.715698 a.u.
M06 SCF energy in solution: -3612.079718 a.u.
Imaginary frequency: -722.41 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.45208300	-1.53636400	-0.83660500
P	1.00648000	1.76208600	-0.07184600
O	2.38045000	-1.66881600	4.82092700
O	3.58576600	-0.42456700	3.27981200
O	4.85966000	-1.82945800	0.65308800
O	6.35693600	-0.84117100	-0.81880900
C	1.02668400	-1.68407000	0.91646800
C	0.32153300	-2.44641900	1.85342200
H	-0.54796700	-3.01153200	1.54130100
C	0.69604900	-2.50918200	3.20892400
H	0.14169800	-3.10996300	3.92021100
C	1.79803900	-1.77342100	3.58401300
C	3.42969100	-0.70163000	4.67507700
H	4.36273100	-1.11572400	5.06951300
H	3.14659100	0.22021200	5.19874600
C	2.51832700	-1.02329300	2.65739100
C	2.17285200	-0.93616000	1.32203400
C	-0.76683900	-2.90791800	-0.99292700
C	-2.06303800	-2.63784600	-0.52829900
H	-2.28003300	-1.67351400	-0.08557300
C	-3.07812900	-3.58495200	-0.63580200
H	-4.06945700	-3.33257900	-0.27523100
C	-2.80848100	-4.81896300	-1.23291300
H	-3.59822700	-5.55865500	-1.33511800
C	-1.52580000	-5.09549000	-1.71035700
H	-1.31508800	-6.05064900	-2.18482500
C	-0.50615600	-4.14799500	-1.59003500
H	0.48025100	-4.37436000	-1.98020200
C	1.93646300	-2.10586000	-1.76927900
C	2.68818400	-3.21695000	-1.35435300
H	2.39407100	-3.76445000	-0.46361100
C	3.82431200	-3.60428500	-2.06449800
H	4.39273800	-4.47246800	-1.74023300
C	4.23622900	-2.87199500	-3.18218200
H	5.12973200	-3.16559100	-3.72665100
C	3.50101900	-1.75809600	-3.59231200
H	3.82445200	-1.17719400	-4.45155400
C	2.35420300	-1.37915600	-2.89244200
H	1.79201400	-0.50112500	-3.19540500
C	2.71052600	1.04168800	-0.27385500
C	3.05034200	-0.17385400	0.39137200
C	4.31141100	-0.68296900	0.13335500
C	6.13130100	-1.98611000	0.01551200
H	6.91632600	-2.04105600	0.77794300
H	6.11562300	-2.88847900	-0.60684200
C	5.21033300	-0.09329200	-0.74895500
C	4.90028500	1.07666100	-1.40598000
H	5.59730700	1.54715600	-2.09046100
C	3.63535300	1.63294900	-1.14352300
H	3.38385900	2.56118200	-1.64015900
C	1.28207600	3.50061800	-0.63820100
C	1.20514400	3.74722100	-2.01943300
H	1.00609800	2.91987100	-2.69478800
C	1.35423700	5.03937400	-2.52311500
H	1.28794800	5.21124500	-3.59415900
C	1.56862200	6.10980800	-1.65077300
H	1.66953000	7.11966800	-2.03928700
C	1.64672600	5.87454400	-0.27690700
H	1.80685000	6.70219400	0.40924800

C	1.50953500	4.57922900	0.22648300
H	1.54594400	4.42094400	1.29808200
C	0.86908800	1.88775400	1.76335600
C	-0.35115700	1.53503600	2.35428100
H	-1.18231600	1.22114100	1.73240900
C	-0.50482300	1.57901500	3.74101500
H	-1.45750700	1.29971400	4.18177300
C	0.56004700	1.97849500	4.55090600
H	0.44069400	2.01383900	5.63070700
C	1.78162900	2.33246200	3.96908100
H	2.61469500	2.64474300	4.59411500
C	1.93942100	2.27772100	2.58427000
H	2.90190300	2.51611700	2.14084700
Rh	-0.59622900	0.57391600	-1.38459900
C	-1.90851100	2.25002100	-1.81378500
C	-3.14176800	1.69023800	-2.58711200
C	-4.33700100	1.40215600	-1.62868700
N	-3.88137600	1.14812100	-0.25749700
H	-1.36544700	2.95301700	-2.44954300
H	-3.50927000	2.45939300	-3.28460300
H	-5.00003800	2.27455700	-1.58873300
C	-4.15345400	-0.03900300	0.34538900
O	-4.84225400	-0.93269600	-0.11430900
O	-3.49574100	-0.11210000	1.55652600
C	-3.73794200	-1.13634400	2.46188100
C	-2.65451600	-1.45716200	3.28089400
C	-4.97905300	-1.75501100	2.63231300
C	-2.81309500	-2.41164200	4.28496600
H	-1.70547800	-0.95963400	3.12019500
C	-5.11567800	-2.71726600	3.63528600
H	-5.80856100	-1.50266900	1.98639800
C	-4.04242200	-3.04969700	4.46452700
H	-1.97188500	-2.65103400	4.92954500
H	-6.07702000	-3.20630400	3.76783800
H	-4.16397600	-3.79668600	5.24377600
H	-4.91436000	0.53921100	-1.95771100
C	-3.54523200	2.78525000	1.57069800
C	-3.20982300	2.26654600	0.31957000
C	-2.28019100	2.90330600	-0.53107800
C	-1.75356900	4.13155800	-0.09194900
C	-2.05550700	4.64070500	1.16918200
C	-2.93623000	3.95894000	2.01437700
H	-4.26920600	2.26546400	2.18904300
H	-1.09336100	4.68375500	-0.75026200
H	-1.60751800	5.57791900	1.48891000
H	-3.17451700	4.35372500	2.99788400
C	-2.78725700	0.45400700	-3.37712000
C	-3.65486600	-0.05286900	-4.35363500
C	-1.59465500	-0.22622800	-3.06584800
C	-3.34129400	-1.21775900	-5.05171300
H	-4.58511500	0.47148100	-4.56783300
C	-1.27785800	-1.38231400	-3.80677800
H	-0.26475000	0.64239100	-2.92501400
C	-2.14236800	-1.88246000	-4.77815300
H	-4.01849700	-1.59683800	-5.81307700
H	-0.34553900	-1.90585500	-3.62135600
H	-1.88062500	-2.78687000	-5.32217300

24-S

B3LYP-D3 SCF energy: -3611.573861 a.u.
B3LYP-D3 enthalpy:V a.u.
B3LYP-D3 free energy: -3611.723699 a.u.
M06 SCF energy in solution: -3612.087757 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.42453100	-1.74616900	-0.54209600
P	0.87778400	1.70896700	-0.56024100
O	2.01145800	-0.07620800	4.96580100
O	3.39330700	0.54346300	3.20761600
O	4.83641400	-1.44670700	1.03203000
O	6.31214100	-0.81734300	-0.64463500
C	0.93458300	-1.34321300	1.18627400
C	0.12542600	-1.72958600	2.25999600
H	-0.74098300	-2.35146200	2.07831900
C	0.38659800	-1.33852600	3.58537900
H	-0.27727200	-1.61732000	4.39599400
C	1.51852000	-0.57956600	3.78923400
C	3.19648800	0.65313000	4.62104900
H	4.05744700	0.21777200	5.14245500
H	3.06095300	1.70757700	4.88527700
C	2.34456000	-0.20257700	2.73248300
C	2.07533900	-0.51465100	1.41235000
C	-0.68230000	-3.21003200	-0.31071000
C	-2.06331600	-2.97190700	-0.26230100
H	-2.44752200	-1.97351100	-0.42188500
C	-2.96755400	-4.01088900	-0.04324100
H	-4.02814800	-3.78189800	-0.00170100
C	-2.49898700	-5.31642400	0.11319500
H	-3.19796900	-6.13293100	0.27445400
C	-1.12668700	-5.57093100	0.04881200
H	-0.75501700	-6.58658600	0.15769000
C	-0.22321800	-4.52682300	-0.15782200
H	0.83621000	-4.74941800	-0.21385100
C	1.95578400	-2.44065400	-1.29455200
C	2.83795800	-3.26091700	-0.57282900
H	2.64576100	-3.47167700	0.47479000
C	3.98871900	-3.76504200	-1.17801000
H	4.65877300	-4.40537200	-0.60982900
C	4.28503900	-3.43787100	-2.50389400
H	5.18905100	-3.81970000	-2.97054400
C	3.42118200	-2.60987000	-3.22314000
H	3.65223700	-2.34110500	-4.25021600
C	2.26117500	-2.11587600	-2.62376600
H	1.59590400	-1.46273400	-3.17959500
C	2.59384400	0.99285700	-0.62274100
C	2.96609300	0.00131800	0.33593800
C	4.25328700	-0.49339500	0.23415100
C	6.16101200	-1.63421700	0.52361800
H	6.89033500	-1.32493700	1.28324400
H	6.29815000	-2.68519900	0.24836500
C	5.13954500	-0.11793900	-0.77057000
C	4.79162000	0.81841200	-1.71878700
H	5.47874900	1.11610800	-2.50292700
C	3.50304700	1.37424600	-1.61535500
H	3.22247900	2.13449200	-2.33374600
C	1.05226200	3.23826000	-1.59129200
C	0.96377100	3.10630900	-2.98803100
H	0.82634100	2.12298900	-3.42566800
C	1.02195200	4.22498700	-3.81936800
H	0.94788300	4.09794800	-4.89608900
C	1.15614700	5.50168800	-3.26859700

H	1.18811000	6.37566600	-3.91362200
C	1.24201500	5.64555100	-1.88311300
H	1.33776200	6.63449400	-1.44234300
C	1.19314200	4.52491200	-1.05172500
H	1.22939500	4.66580500	0.02160200
C	0.84231200	2.33578800	1.17362200
C	-0.28069400	2.07046400	1.96540400
H	-1.11747700	1.52011200	1.55368900
C	-0.31663200	2.49114400	3.29603600
H	-1.18068600	2.25633600	3.90787600
C	0.75894500	3.19139300	3.84288100
H	0.72528100	3.51995700	4.87854600
C	1.88559900	3.45845100	3.05861400
H	2.73287200	3.99332300	3.48054700
C	1.93411100	3.01777300	1.73736400
H	2.82828200	3.18785900	1.14463700
Rh	-0.73975500	0.13343800	-1.55726900
C	-2.12757500	1.61249600	-2.29145900
C	-3.39550000	0.83053000	-2.74478400
C	-4.37849700	0.57990700	-1.55589100
N	-3.71568500	0.77608500	-0.25428000
H	-1.68689100	2.13003200	-3.14624500
H	-3.95292100	1.43475000	-3.47662700
H	-5.22041700	1.28154000	-1.60318100
C	-3.89383000	-0.14818600	0.73593700
O	-4.57676300	-1.15269600	0.65626100
O	-3.13973400	0.18807100	1.83886600
C	-3.20447200	-0.53913400	3.02110700
C	-3.19750400	-1.93360400	3.07623300
C	-3.17608500	0.22644600	4.18682900
C	-3.13689500	-2.55476700	4.32551500
H	-3.23038100	-2.51532100	2.16694900
C	-3.10969800	-0.40677900	5.42773500
H	-3.20320400	1.30784000	4.10255900
C	-3.08584400	-1.80183500	5.50164100
H	-3.12455700	-3.64028400	4.37230600
H	-3.07858500	0.19128300	6.33419000
H	-3.03386700	-2.29759000	6.46676600
H	-4.77420800	-0.43430600	-1.58000100
C	-3.51022200	2.92496300	0.98073200
C	-3.19162500	2.09935800	-0.09721300
C	-2.42933200	2.56389700	-1.19114100
C	-2.01149800	3.90460700	-1.16235400
C	-2.28460500	4.72336100	-0.06757900
C	-3.02639400	4.23370400	1.01067700
H	-4.11796700	2.54022800	1.79235200
H	-1.45766900	4.29867200	-2.00764300
H	-1.92542200	5.74905900	-0.06227400
H	-3.24943800	4.87173200	1.86112100
C	-2.98109400	-0.47498100	-3.36552600
C	-1.77950700	-1.03622000	-2.89072700
C	-3.76594000	-1.13535200	-4.31822500
C	-1.38075900	-2.26774300	-3.44165600
C	-3.35826300	-2.36464600	-4.83702400
C	-2.15820500	-2.92779800	-4.39657900
H	-0.45599100	-2.73961700	-3.12269400
H	-3.96391800	-2.87262400	-5.58372400
H	-1.82479100	-3.88293000	-4.79715300
H	0.12300400	0.23985100	-2.81261100
H	-4.69428900	-0.68081800	-4.66179300

25-ts-S

B3LYP-D3 SCF energy: -3611.554028 a.u.
B3LYP-D3 enthalpy: -3611.553084 a.u.
B3LYP-D3 free energy: -3611.703535 a.u.
M06 SCF energy in solution: -3612.069958 a.u.
Imaginary frequency: -882.54 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.27160200	-1.02417800	1.48151600
P	-1.04480800	1.63614400	-0.57388700
O	-1.88541900	-3.30488000	-3.79185700
O	-3.34890500	-1.82486400	-2.76658200
O	-4.67023400	-2.15829000	0.20320100
O	-6.27066200	-0.75592500	1.12853300
C	-0.79381800	-1.83519800	-0.09182900
C	0.06631200	-2.74738700	-0.71193700
H	0.97771900	-3.04546900	-0.21119400
C	-0.19698200	-3.29803500	-1.97842900
H	0.50350600	-3.97447800	-2.45522000
C	-1.37933800	-2.91967900	-2.57688700
C	-3.11705900	-2.58886000	-3.95405700
H	-3.93750900	-3.30250200	-4.09299200
H	-3.02948600	-1.90897000	-4.80902000
C	-2.25480700	-2.02657900	-1.96315600
C	-1.99442600	-1.42401400	-0.74536700
C	0.92441200	-2.23915300	2.19585600
C	2.28904900	-1.98320800	2.00556800
H	2.60017000	-1.06921500	1.51877300
C	3.25918400	-2.87248400	2.46743500
H	4.30570100	-2.64350700	2.29054700
C	2.87304900	-4.02969800	3.14562500
H	3.62367400	-4.72238400	3.51728300
C	1.51605800	-4.28829700	3.35615600
H	1.20818700	-5.18153500	3.89363500
C	0.54666100	-3.40259200	2.88240000
H	-0.49910600	-3.61854600	3.06735400
C	-1.76768100	-1.13559900	2.54957600
C	-2.58203900	-2.27888500	2.57597400
H	-2.36244900	-3.11665300	1.92126200
C	-3.71100200	-2.32169700	3.39343700
H	-4.33024800	-3.21503100	3.40935100
C	-4.05254200	-1.21553100	4.17592100
H	-4.94039400	-1.24458500	4.80177200
C	-3.25857000	-0.06760100	4.13868500
H	-3.52881000	0.80182100	4.73166000
C	-2.12026000	-0.02669300	3.33178400
H	-1.50790300	0.86966100	3.28520900
C	-2.71230600	0.97263300	-0.07935800
C	-2.96135800	-0.42830300	-0.20297300
C	-4.20678700	-0.86543800	0.20903100
C	-5.99824700	-2.10657800	0.73352900
H	-6.71306300	-2.41261200	-0.04125100
H	-6.06388500	-2.75903600	1.61072400
C	-5.16731000	-0.02672000	0.76520500
C	-4.94275200	1.32486200	0.90356900
H	-5.68884500	1.98454400	1.33235800
C	-3.69739200	1.80681500	0.46026200
H	-3.51252300	2.87077800	0.53951500
C	-1.37537200	3.45477600	-0.71521700
C	-1.37288200	4.21358300	0.46881700

H	-1.23143600	3.71355500	1.42287100
C	-1.53482200	5.59874700	0.43456600
H	-1.52801400	6.16389500	1.36285200
C	-1.69275000	6.25565900	-0.78841800
H	-1.80662900	7.33594700	-0.81891400
C	-1.69984700	5.51321800	-1.97015900
H	-1.81613100	6.01409800	-2.92785500
C	-1.54622300	4.12555000	-1.93462900
H	-1.52281300	3.57496900	-2.86725300
C	-0.97912100	1.04927900	-2.32337000
C	0.17579400	0.39455300	-2.76567300
H	1.01361800	0.26501600	-2.09161400
C	0.23812800	-0.12153700	-4.06126700
H	1.12678500	-0.65368400	-4.38251900
C	-0.84364900	0.02435800	-4.93008400
H	-0.79015400	-0.37661100	-5.93914100
C	-2.00313100	0.67411300	-4.49429400
H	-2.85530000	0.77997500	-5.16119700
C	-2.07689300	1.16705100	-3.19265100
H	-2.99536900	1.62924000	-2.84206400
Rh	0.63812100	1.16120900	1.11821700
C	2.03069800	2.91561000	0.75174100
C	3.29563200	2.54752400	1.57858500
C	4.32856200	1.72297200	0.74782100
N	3.71461000	1.01827400	-0.38512200
H	1.72833200	3.93345000	1.01897900
H	3.81309600	3.48455500	1.83130100
H	5.09342500	2.39438100	0.33742400
C	3.95475100	-0.31384400	-0.56073700
O	4.69976900	-0.99569400	0.11917600
O	3.19967000	-0.79927800	-1.60463900
C	3.34210300	-2.09954400	-2.07202900
C	3.43090500	-3.21743100	-1.24149100
C	3.28944800	-2.23748300	-3.45927800
C	3.44072600	-4.48655500	-1.82412800
H	3.48073100	-3.09662000	-0.16956800
C	3.29493500	-3.51108400	-4.02784600
H	3.24041000	-1.34350400	-4.07226700
C	3.36648100	-4.64228200	-3.21086200
H	3.50190100	-5.35954400	-1.18006000
H	3.24466600	-3.61660200	-5.10797700
H	3.37002200	-5.63542400	-3.65088100
H	4.82234100	0.98278700	1.37544400
C	3.28900900	1.85637400	-2.67641600
C	3.04966600	1.88440500	-1.30106200
C	2.23107100	2.87790300	-0.72511200
C	1.67784200	3.84549800	-1.57795100
C	1.87123200	3.79123800	-2.95648500
C	2.67299700	2.79022100	-3.50915800
H	3.94543300	1.09826300	-3.08796500
H	1.07760400	4.64014200	-1.14763700
H	1.40606900	4.53753300	-3.59443100
H	2.84033000	2.74793300	-4.58159100
C	2.92199700	1.83822100	2.85687400
C	1.73754100	1.07312600	2.85961100
C	3.74849200	1.91644100	3.98477600
C	1.40863200	0.42436800	4.06571800
C	3.40679100	1.24699200	5.15950500
C	2.22475100	0.50461100	5.19673200
H	0.50487100	-0.17330800	4.13863700
H	4.04624600	1.31454600	6.03630800
H	1.93698900	-0.01756800	6.10707600
H	0.64267000	2.66978700	1.56022700
H	4.65900100	2.51386300	3.94635300

26-S

B3LYP-D3 SCF energy: -3611.578593 a.u.
B3LYP-D3 enthalpy: -3611.577649 a.u.
B3LYP-D3 free energy: -3611.730454 a.u.
M06 SCF energy in solution: -3612.100332 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.57422100	-0.28548200	-1.74135200
P	0.74356000	1.26707900	1.25501700
O	2.14545400	-4.31895800	2.37553700
O	3.42002600	-2.38606400	2.23405600
O	5.06336400	-1.26823300	-0.39480100
O	6.45696200	0.58715400	-0.34560900
C	1.13239800	-1.60251200	-0.56888000
C	0.39052000	-2.78547800	-0.48373600
H	-0.41949100	-2.95401700	-1.18028100
C	0.63742700	-3.77264200	0.48578600
H	0.02172000	-4.66239900	0.55356600
C	1.68448700	-3.53411400	1.34934500
C	3.18493200	-3.56375800	3.01230100
H	4.10039200	-4.16425800	3.04780900
H	2.85688100	-3.27258400	4.01742100
C	2.44785800	-2.37219300	1.26423700
C	2.19993400	-1.36297200	0.35043600
C	-0.31119200	-1.25218500	-3.05367300
C	-1.71140800	-1.27517400	-3.00563000
H	-2.22785500	-0.68151900	-2.26381400
C	-2.44922700	-2.03309900	-3.91545800
H	-3.53266800	-2.03595900	-3.83944100
C	-1.79210700	-2.76920100	-4.90263600
H	-2.36145000	-3.35532200	-5.61951800
C	-0.39684200	-2.73948700	-4.97261600
H	0.12255300	-3.29988500	-5.74585300
C	0.34005400	-1.98959000	-4.05426400
H	1.42053400	-1.97500700	-4.13546700
C	2.15291000	0.24145600	-2.54812400
C	3.16353800	-0.67435100	-2.88161700
H	3.05007400	-1.72409000	-2.62880100
C	4.34473300	-0.23763900	-3.48126700
H	5.11529500	-0.95964600	-3.73984700
C	4.54198500	1.12220500	-3.73385500
H	5.46812400	1.46358900	-4.18863400
C	3.55008600	2.04195300	-3.38695200
H	3.70339700	3.10268000	-3.56644100
C	2.36152200	1.60489500	-2.79985800
H	1.59235600	2.31616300	-2.51197600
C	2.54591900	1.13945600	0.85585800
C	3.03041900	-0.12625400	0.40981000
C	4.36670100	-0.17675600	0.06155600
C	6.38957400	-0.80695200	-0.67159100
H	7.10482900	-1.36184700	-0.05250400
H	6.60457900	-0.93910400	-1.73816200
C	5.20358300	0.93565000	0.08992600
C	4.75086800	2.16698500	0.51007200
H	5.40375800	3.03226100	0.53852900
C	3.40063700	2.24427000	0.90098700

H	3.02300900	3.19890000	1.24822800
C	0.59827200	2.92488700	2.06652100
C	0.51955100	4.04910300	1.22318400
H	0.59225700	3.91293800	0.14610100
C	0.33566200	5.32723000	1.75064700
H	0.27607600	6.18222800	1.08238700
C	0.22267800	5.50422000	3.13273600
H	0.07341300	6.49831200	3.54578200
C	0.30121500	4.39636900	3.97831900
H	0.20953500	4.52438600	5.05390400
C	0.48678900	3.11615200	3.45072600
H	0.52031100	2.26526000	4.12140800
C	0.61665700	0.06968200	2.65265700
C	-0.46366800	-0.82006600	2.67074200
H	-1.20480200	-0.78115200	1.88051500
C	-0.56833900	-1.77322900	3.68562400
H	-1.39476000	-2.47548300	3.67781500
C	0.39556200	-1.83902600	4.69253200
H	0.30994100	-2.58249900	5.48109800
C	1.47876500	-0.95377700	4.67911300
H	2.23748600	-1.00533100	5.45623100
C	1.59597000	-0.01371000	3.65625600
H	2.45704700	0.64821700	3.62549300
Rh	-0.60820000	1.29722500	-0.70336300
C	-2.70650500	2.87228500	0.40196900
C	-3.62769400	2.59426200	-0.81503800
C	-4.51123800	1.33566100	-0.58499500
N	-3.88487700	0.33963100	0.29563400
H	-2.66236500	3.94835900	0.60335100
H	-4.34266100	3.42489900	-0.85687800
H	-5.45717000	1.63374900	-0.11473500
C	-3.83718700	-0.96238000	-0.12942700
O	-4.33649200	-1.37827800	-1.15831600
O	-3.12532600	-1.73771700	0.75031400
C	-3.04909400	-3.12023900	0.61522400
C	-2.86335800	-3.77744200	-0.60182800
C	-3.08019000	-3.82876100	1.81659300
C	-2.68680500	-5.16277100	-0.59490400
H	-2.84815700	-3.22074600	-1.52661100
C	-2.89674900	-5.21124300	1.80924400
H	-3.24501300	-3.28571600	2.74125400
C	-2.69589800	-5.88436300	0.60155700
H	-2.53448100	-5.67606700	-1.54039700
H	-2.91270300	-5.75926500	2.74715400
H	-2.55245400	-6.96106600	0.59260300
H	-4.73776400	0.85122000	-1.53236500
C	-3.85222400	0.11571700	2.76907300
C	-3.56886300	0.82520600	1.59593400
C	-3.04238000	2.12734900	1.66679400
C	-2.77709600	2.68154100	2.92249400
C	-3.01292600	1.95979700	4.09128100
C	-3.55368500	0.67511900	4.00979800
H	-4.29208600	-0.87168200	2.70544800
H	-2.35381700	3.68049700	2.97623900
H	-2.78076800	2.39922700	5.05713600
H	-3.75731300	0.10784200	4.91369400
C	-2.90657200	2.56193900	-2.15873800
C	-1.65153400	1.91605200	-2.35737700
C	-3.57639100	3.16600900	-3.23593400
C	-1.15505900	1.92585100	-3.67920100
C	-3.05034500	3.15642700	-4.52603000
C	-1.82422700	2.52989900	-4.74433600
H	-0.21024500	1.43810000	-3.89987400
H	-3.58733300	3.63441000	-5.34168000
H	-1.38767400	2.50717200	-5.74091600
H	-1.63739000	2.68029000	0.14795600
H	-4.53302000	3.65662400	-3.05767200

27-ts-S

B3LYP-D3 SCF energy: -3687.972591 a.u.
B3LYP-D3 enthalpy: -3687.971647 a.u.
B3LYP-D3 free energy: -3688.128336 a.u.
M06 SCF energy in solution: -3688.508231 a.u.
Imaginary frequency: -1359.56 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-2.17022100	1.16118600	-0.15775500
P	-0.05676100	-1.27057600	-0.87130900
O	-1.18939400	-1.53331700	5.08884500
O	-1.73330100	-2.86285000	3.26799300
O	-4.51257300	-2.61404600	1.63901500
O	-5.18925900	-4.17184900	0.05880900
C	-2.02198600	0.39135400	1.52463600
C	-1.72020400	1.17897300	2.64106400
H	-1.72437300	2.25826400	2.54797100
C	-1.41575100	0.62955900	3.89981300
H	-1.17945100	1.25508900	4.75342800
C	-1.43557100	-0.74442600	3.99405300
C	-1.27145400	-2.88665900	4.62166700
H	-1.98494900	-3.44208300	5.23960000
H	-0.27404300	-3.34208000	4.65653900
C	-1.75950600	-1.54019800	2.89910900
C	-2.04448100	-1.03300400	1.64294200
C	-2.72500500	2.89928800	0.17292400
C	-1.76582400	3.82160200	0.61734700
H	-0.73967500	3.50262300	0.73738100
C	-2.10199500	5.15081400	0.86298000
H	-1.33420400	5.84335000	1.19515600
C	-3.40854800	5.59193000	0.64556800
H	-3.67307000	6.63090100	0.82386600
C	-4.36718400	4.69267400	0.17803600
H	-5.38372600	5.02839100	-0.01057500
C	-4.03174400	3.35678000	-0.05554700
H	-4.79354300	2.68089700	-0.42522700
C	-3.71270100	0.36938800	-0.80049100
C	-4.84686300	0.20655600	0.01119500
H	-4.82216500	0.53821800	1.04532800
C	-5.99534600	-0.40092900	-0.49469500
H	-6.87051400	-0.51386100	0.14047100
C	-6.01718000	-0.87050100	-1.81153700
H	-6.90695700	-1.35807500	-2.20101000
C	-4.89097500	-0.71690300	-2.62230400
H	-4.89936100	-1.08943400	-3.64301100
C	-3.74620500	-0.09309900	-2.12185400
H	-2.85740000	0.01552500	-2.73853000
C	-1.56892100	-2.29136500	-0.57918900
C	-2.38283500	-2.00069200	0.55655900
C	-3.56190100	-2.71696700	0.65311900
C	-5.58984100	-3.46763800	1.24129400
H	-5.79874200	-4.18722600	2.04066000
H	-6.47323000	-2.85708800	1.01714300

C	-3.97049800	-3.65066500	-0.29513400
C	-3.19309800	-3.94867300	-1.39251900
H	-3.50487100	-4.68161800	-2.12822200
C	-1.97941800	-3.24795800	-1.51328500
H	-1.34837000	-3.45944100	-2.36840100
C	0.85204900	-2.20219300	-2.17223900
C	0.50073400	-1.93248600	-3.50692400
H	-0.22603600	-1.15713800	-3.72017800
C	1.10134100	-2.63495700	-4.55046200
H	0.82003300	-2.41577700	-5.57696100
C	2.07678900	-3.59666800	-4.27741000
H	2.55256900	-4.13736700	-5.09179900
C	2.45056000	-3.84935600	-2.95723000
H	3.22407800	-4.57683000	-2.73442500
C	1.84406700	-3.15597300	-1.90809500
H	2.16465700	-3.35540000	-0.89285100
C	0.86794600	-1.58510900	0.70523900
C	1.48995100	-0.52346600	1.37485300
H	1.44854100	0.46862800	0.94196300
C	2.11429300	-0.72068300	2.60786800
H	2.58317400	0.11818100	3.11244400
C	2.12848500	-1.99307100	3.18386800
H	2.60872500	-2.14936700	4.14642300
C	1.52593600	-3.06511300	2.51705000
H	1.53747700	-4.05925900	2.95726700
C	0.89150600	-2.86134400	1.29167400
H	0.38655700	-3.68950300	0.80364700
Rh	-0.33516500	0.90182000	-1.45285500
C	2.00623200	3.33327300	1.19949400
C	1.98207000	2.97894600	-0.29593700
C	3.42488100	2.94215600	-0.82000500
N	4.14575100	1.86870700	-0.11340500
H	1.06658500	3.01447300	1.66796600
H	1.61495000	1.94877400	-0.38723500
H	3.45173000	2.72918300	-1.88700000
C	4.20326200	0.64994000	-0.75481000
O	3.86360600	0.45942600	-1.91111300
O	4.70612400	-0.31725500	0.05798500
C	4.90959100	-1.61694700	-0.40191500
C	5.52605200	-1.90282100	-1.61972900
C	4.55373700	-2.62491100	0.49053100
C	5.79157300	-3.23601000	-1.93520700
H	5.77528600	-1.10374600	-2.30550600
C	4.82697300	-3.95267100	0.16103800
H	4.06770300	-2.35562300	1.42019800
C	5.45100700	-4.26233200	-1.04994100
H	6.26710400	-3.47057300	-2.88340800
H	4.54864600	-4.74189200	0.85410900
H	5.66712300	-5.29617800	-1.30508200
H	3.94814300	3.88701700	-0.63262100
C	5.28180900	1.51056300	2.05195200
C	4.20290000	2.01458700	1.31113100
C	3.16690500	2.71435500	1.95640300
C	3.22551200	2.85256600	3.35021600
C	4.27519100	2.32013400	4.09379200
C	5.31090100	1.65012800	3.43541200
H	6.08463100	0.99997500	1.53571200
H	2.41948100	3.38365200	3.85233200
H	4.29190400	2.43378600	5.17412000
H	6.14754600	1.24449500	3.99725400
H	2.05670300	4.42225200	1.33208400
C	1.03532400	3.81678700	-1.13965300
C	0.19990200	3.14189500	-2.06686300
C	0.97563500	5.20915200	-1.02396300
C	-0.71355100	3.90562800	-2.81274400
C	0.05127400	5.94243900	-1.77499500
C	-0.80819800	5.29131700	-2.66106500
H	-1.35578000	3.40137100	-3.53184100
H	0.00285300	7.02313800	-1.66312800
H	-1.53535400	5.86214200	-3.23362700
H	1.63374400	5.73654000	-0.33587000
O	1.15254200	0.88824000	-2.98621300
H	0.77178300	2.07397200	-2.64364000
H	2.04338000	0.70794900	-2.62972000

28-S

B3LYP-D3 SCF energy: -1054.652591 a.u.
B3LYP-D3 enthalpy: -1054.651647 a.u.
B3LYP-D3 free energy: -1054.723931 a.u.
M06 SCF energy in solution: -1054.487442 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.91265200	1.34047300	1.00168400
C	1.45653700	1.47349700	1.48731800
C	1.00261800	0.07645300	1.96476400
N	1.00984400	-0.85527800	0.83214000
H	3.18299900	2.19885100	0.37495800
H	0.00530200	0.10614100	2.39439400
C	-0.15169400	-1.22357600	0.18077300
O	-0.22315700	-1.76053900	-0.90294700
O	-1.24426200	-0.93154900	0.96363700
C	-2.51301900	-1.02505700	0.39675800
C	-2.83881600	-0.32469200	-0.76356100
C	-3.46291300	-1.76935100	1.09003500
C	-4.14978900	-0.38263200	-1.23504700
H	-2.07805100	0.25141300	-1.27553200
C	-4.77395400	-1.81346800	0.61081300
H	-3.16701900	-2.29807700	1.99052600
C	-5.11967700	-1.12323600	-0.55274100
H	-4.41384500	0.15865500	-2.13953900
H	-5.52179400	-2.39076400	1.14752400
H	-6.13926100	-1.16085300	-0.92600400
H	1.69863600	-0.30217700	2.72351300
C	2.59087800	-2.18180200	-0.51227800
C	2.26926000	-1.00119200	0.17409000
C	3.20385400	0.04813100	0.25579400
C	4.44992000	-0.11921000	-0.36353200
C	4.77004200	-1.28456200	-1.05311000
C	3.83101600	-2.31770800	-1.12648600
H	1.85792200	-2.97562400	-0.57150300
H	5.17303400	0.69172300	-0.30326000
H	5.74071600	-1.38758400	-1.53001300
H	4.06573900	-3.23538800	-1.65850000
H	3.57174700	1.38581700	1.87953400
H	1.44350200	2.13906900	2.35977800
C	0.47604300	2.02864300	0.46432200
C	-0.68762000	2.67080400	0.91339600
C	0.65943600	1.87764800	-0.91681900
C	-1.63652300	3.15688000	0.01527100
H	-0.85125400	2.78802200	1.98290100
C	-0.28713200	2.36759100	-1.82131900

H	1.53919000	1.36825200	-1.29661500
C	-1.43615900	3.01096200	-1.35994400
H	-2.53059100	3.64955200	0.38760900
H	-0.12367200	2.23918000	-2.88796700
H	-2.17261500	3.38986500	-2.06340800

29-ts-S

B3LYP-D3 SCF energy: -3687.962905 a.u.
B3LYP-D3 enthalpy: -3687.961961 a.u.
B3LYP-D3 free energy: -3688.121289 a.u.
M06 SCF energy in solution: -3688.496971 a.u.
Imaginary frequency: -1310.02 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.57042500	-1.61767500	-0.29178400
P	1.47851700	1.49857300	0.15468400
O	5.05957000	-1.93548200	3.61620500
O	5.38714400	-0.71449600	1.67221900
O	5.15528700	-1.99744000	-1.34549300
O	5.75135100	-0.86754200	-3.28065600
C	1.96188500	-1.87673500	0.88936100
C	1.78549500	-2.62677000	2.05632600
H	0.85386800	-3.15811200	2.21231600
C	2.77595900	-2.71323100	3.05190400
H	2.62613100	-3.29157000	3.95667900
C	3.94493000	-2.02089000	2.82270100
C	5.93401700	-1.00535600	2.96269500
H	6.92346300	-1.45830500	2.84457900
H	5.98379100	-0.08100500	3.55159500
C	4.14049700	-1.28816100	1.65398200
C	3.18245300	-1.17157600	0.66433900
C	-0.66115000	-2.92662500	0.12444800
C	-1.54054200	-2.68176100	1.19700400
H	-1.44918800	-1.76460000	1.77467600
C	-2.55650200	-3.58495400	1.50942500
H	-3.25722200	-3.34060800	2.29948200
C	-2.70026500	-4.75422900	0.76010300
H	-3.50946100	-5.44335600	0.98094500
C	-1.82974800	-5.01103200	-0.29974600
H	-1.94699100	-5.91374800	-0.89396600
C	-0.81933400	-4.10226500	-0.62279400
H	-0.16833500	-4.30683000	-1.46586000
C	1.31090400	-2.13689000	-1.89697000
C	2.15779900	-3.25132400	-1.99942000
H	2.38343900	-3.84182500	-1.11592000
C	2.73258200	-3.58650900	-3.22555000
H	3.38084200	-4.45630600	-3.29788300
C	2.48371200	-2.79983900	-4.35442800
H	2.94362000	-3.05322200	-5.30601300
C	1.64692200	-1.68562200	-4.25646200
H	1.45925100	-1.06667000	-5.12954200
C	1.05751900	-1.35796800	-3.03439500
H	0.41918900	-0.48300300	-2.94046000
C	2.88979900	0.89265500	-0.87743000
C	3.48944100	-0.36143800	-0.54995700
C	4.44073100	-0.82910800	-1.43788700
C	5.89091100	-2.10474600	-2.56869400
H	6.94801100	-2.27697800	-2.34329700
H	5.47187900	-2.91900000	-3.17316900
C	4.79921600	-0.15229200	-2.60124100
C	4.23818000	1.06287700	-2.92718600
H	4.52308200	1.59770700	-3.82631700
C	3.27453400	1.57244000	-2.03734300
H	2.81698600	2.52584200	-2.27340500
C	1.29719200	3.27450900	-0.32007300
C	0.57426800	3.55091000	-1.49559600
H	0.15583400	2.73256100	-2.07575200
C	0.34715000	4.86544800	-1.89955200
H	-0.22980100	5.05246000	-2.79958900
C	0.82438600	5.92521900	-1.12383900
H	0.63674000	6.95143900	-1.42861300
C	1.52720200	5.66229500	0.05302800
H	1.88874500	6.48286600	0.66729400
C	1.76490700	4.34515800	0.45452000
H	2.30339900	4.15907700	1.37735300
C	2.22173400	1.51796300	1.84144400
C	1.48521700	0.98557900	2.90824400
H	0.48943000	0.59589400	2.72173400
C	2.03542600	0.94125100	4.19017000
H	1.45854500	0.51737400	5.00726900
C	3.32192100	1.43455200	4.41808100
H	3.74983100	1.39929200	5.41655100
C	4.06158900	1.96966000	3.35845800
H	5.06363200	2.35460800	3.53086600
C	3.51933600	2.00114200	2.07372300
H	4.11170800	2.38033100	1.24561400
Rh	-0.44561200	0.38629400	-0.17017300
C	-2.09143500	2.14283900	0.37031800
C	-3.36285200	2.75309700	-0.29652800
C	-4.59331300	1.84237700	-0.04651400
N	-4.45145300	1.05063500	1.20391800
H	-1.26658800	2.82187500	0.15477700
H	-3.55505000	3.70760100	0.21483800
H	-5.50671000	2.44650500	0.00428500
C	-4.77002500	-0.27967600	1.23942800
O	-4.40204900	-1.08306400	2.07960600
O	-5.57798400	-0.62344900	0.17979300
C	-5.63996600	-1.97935500	-0.14487800
C	-6.47035200	-2.83816700	0.56978800
C	-4.88813500	-2.42230300	-1.23095300
C	-6.56208900	-4.17308200	0.17152700
H	-7.02481200	-2.45690800	1.42013200
C	-4.99024600	-3.75835900	-1.62088100
H	-4.22229900	-1.72638000	-1.73031100
C	-5.82814900	-4.63366000	-0.92542900
H	-7.20921400	-4.85284500	0.71938600
H	-4.40237200	-4.11594500	-2.46135500
H	-5.90531300	-5.67315100	-1.23289000
H	-4.70467000	1.13559200	-0.86489100
C	-3.93186800	1.44970500	3.58644100
C	-3.58475600	1.53881800	2.23864800
C	-2.35334100	2.08223100	1.83258200
C	-1.48723000	2.56569200	2.82346900
C	-1.81687800	2.46342100	4.17440100
C	-3.03919800	1.90147100	4.55916900
H	-4.88288800	1.00731700	3.86401900
H	-0.54163500	3.00890600	2.52230000
H	-1.12244100	2.82820300	4.92740400
H	-3.30121900	1.82301300	5.61069900
C	-3.15251000	3.06960800	-1.76554000
C	-3.23639700	4.39359100	-2.21397200

C	-2.80642800	2.07230900	-2.69363500
C	-2.97860100	4.72491800	-3.54682700
H	-3.49587500	5.17790100	-1.50630000
C	-2.53838300	2.40199200	-4.02296400
H	-2.73713800	1.03901500	-2.37142100
C	-2.62044000	3.72880600	-4.45671100
H	-3.05362600	5.76037000	-3.87032800
H	-2.26705900	1.61657500	-4.72452000
H	-2.41410700	3.98106800	-5.49377400
O	-2.43688300	-0.31700300	-0.63285500
H	-2.67060900	-0.95649300	0.06142100
H	-2.36578300	0.77846200	-0.15829100

30

B3LYP-D3 SCF energy: -3611.560376 a.u.
B3LYP-D3 enthalpy: -3611.559431 a.u.
B3LYP-D3 free energy: -3611.714494 a.u.
M06 SCF energy in solution: -3612.086193 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.56914000	-1.61748000	0.13026000
P	1.36490700	1.57156400	-0.74071000
O	3.20723400	0.89602700	4.87145900
O	4.32030700	0.95817800	2.83739700
O	5.16892600	-1.64631200	1.05754300
O	6.45179300	-1.59187600	-0.87578600
C	1.36667400	-0.93946500	1.65965200
C	0.71437900	-0.98495300	2.89581900
H	-0.23615100	-1.49901200	2.97820900
C	1.24772400	-0.38170800	4.05116300
H	0.72876800	-0.41682500	5.00263700
C	2.46492400	0.24946400	3.91686500
C	4.33401100	1.45383500	4.18038000
H	5.25705200	1.13466700	4.67529200
H	4.24357300	2.54651300	4.16201300
C	3.13176700	0.28864100	2.69441900
C	2.61775900	-0.26394600	1.53666800
C	-0.71197200	-2.74955800	0.82770000
C	-1.99230900	-2.21510600	1.04811400
H	-2.21275500	-1.19614500	0.74499100
C	-3.00242900	-2.99293600	1.61206000
H	-3.99044200	-2.56515700	1.74352700
C	-2.74990600	-4.32047300	1.96103900
H	-3.53937700	-4.93037400	2.39213100
C	-1.48718400	-4.86766000	1.73002800
H	-1.28731500	-5.90598300	1.98232300
C	-0.47525600	-4.09001300	1.16492500
H	0.49211000	-4.54086000	0.97710500
C	1.89183300	-2.73603300	-0.51479100
C	2.68257300	-3.54223900	0.31969100
H	2.53406100	-3.51464900	1.39507400
C	3.68642600	-4.34689700	-0.21930100
H	4.28532800	-4.97280100	0.43763000
C	3.93355600	-4.33469900	-1.59511800
H	4.72541200	-4.95093800	-2.01243700
C	3.16940700	-3.51635500	-2.42960900
H	3.37184800	-3.48452200	-3.49664500
C	2.15345100	-2.72486900	-1.89168200
H	1.58462900	-2.05829900	-2.53187500
C	2.98002800	0.65590300	-0.84808600
C	3.38235500	-0.14303700	0.26512900
C	4.57635100	-0.82606000	0.13037300
C	6.33919900	-2.17801700	0.42871300
H	7.22235000	-1.91657300	1.02278100
H	6.23435200	-3.26442300	0.32773200
C	5.34772200	-0.79425100	-1.02797100
C	4.97556200	-0.03446600	-2.11461200
H	5.57842500	0.00327800	-3.01513200
C	3.77861800	0.69724600	-1.99603200
H	3.48573400	1.32141500	-2.83055400
C	1.45329400	2.75690900	-2.15613600
C	1.56712700	4.14306300	-1.99436400
H	1.67989000	4.56883700	-1.00396100
C	1.50639200	4.99354600	-3.10176100
H	1.58360600	6.06767200	-2.95544500
C	1.33696800	4.47304600	-4.38445500
H	1.28647900	5.13749400	-5.24281700
C	1.22075100	3.09040700	-4.55798000
H	1.07986200	2.67359100	-5.55183900
C	1.26683300	2.24320200	-3.45252200
H	1.13910600	1.17248500	-3.58578000
C	1.69344700	2.62807900	0.74081300
C	0.72257500	2.74532100	1.74243600
H	-0.22791800	2.24146200	1.62561100
C	0.97623200	3.50645500	2.88486100
H	0.21614600	3.58395700	3.65723800
C	2.19863800	4.16419600	3.03369700
H	2.39206200	4.76210200	3.92081900
C	3.17491200	4.05039700	2.03851000
H	4.13156700	4.55459600	2.15031300
C	2.92775000	3.27885700	0.90371100
H	3.69805600	3.17313600	0.14496600
Rh	-0.43087700	0.20022900	-1.06930100
C	-1.55281600	1.91848000	-0.80018000
C	-2.28629100	1.87952200	0.40197100
C	-1.70651500	3.05596200	-1.60632900
C	-3.12691600	2.92695700	0.78581100
H	-2.20433600	1.01665700	1.06113000
C	-2.54242500	4.11222300	-1.22372700
H	-1.17765200	3.12525300	-2.55245100
C	-3.25335100	4.05624000	-0.02523000
H	-3.69370000	2.84674500	1.71025800
H	-2.63918100	4.97942200	-1.87435000
C	-1.35064000	-1.27171400	-2.59767100
C	-1.74186600	0.03569000	-2.90622600
C	-3.22052000	0.35786600	-2.86122500
N	-3.87642700	-0.40689200	-1.79276200
H	-0.44674900	-1.68476700	-3.03369700
H	-1.17224400	0.62324200	-3.62238500
H	-3.40669600	1.41337100	-2.67569700
C	-4.66164400	0.29015900	-0.90711000
O	-5.14436700	1.38254900	-1.10700700
O	-4.79638700	-0.41111200	0.27736700
C	-5.43197000	0.19866800	1.35163700
C	-6.70275900	0.76535500	1.25211200
C	-4.75318400	0.15748000	2.56968900
C	-7.29065900	1.30468500	2.39702700
H	-7.20321400	0.80030500	0.29299200
C	-5.35595600	0.69390700	3.70840200
H	-3.76492800	-0.28832200	2.60899100
C	-6.62459700	1.27216900	3.62510000

H	-8.27711200	1.75466000	2.32527200
H	-4.82892400	0.66285700	4.65814600
H	-7.09163100	1.69464800	4.51028200
H	-3.67432700	0.09554700	-3.83152500
C	-4.61478500	-2.72701400	-1.39176500
C	-3.63002900	-1.80496700	-1.75512600
C	-2.35107500	-2.24844700	-2.15543200
C	-2.08227000	-3.62403900	-2.13179200
C	-3.05094300	-4.54078200	-1.73290500
C	-4.32203700	-4.08970600	-1.36765600
H	-5.59914100	-2.37241900	-1.10734400
H	-1.08837100	-3.96524500	-2.41246500
H	-2.81635200	-5.60093000	-1.70470200
H	-5.08928500	-4.79713000	-1.06583400
H	-3.91049700	4.87142800	0.26601100

31-ts-R

B3LYP-D3 SCF energy: -3611.540658 a.u.
B3LYP-D3 enthalpy: -3611.539714 a.u.
B3LYP-D3 free energy: -3611.695211 a.u.
M06 SCF energy in solution: -3612.062231 a.u.
Imaginary frequency: -309.34 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.98411800	1.60533000	0.27475800
P	-1.26808800	-1.60650700	-0.78837000
O	-3.33531600	-1.59596000	4.74845900
O	-4.33828600	-1.74335900	2.66380600
O	-5.58148300	0.86469000	0.99395600
O	-6.80136500	0.65129900	-0.96886700
C	-1.75370500	0.74035300	1.72499400
C	-1.17128900	0.83148900	2.99413900
H	-0.33413600	1.50145900	3.14899700
C	-1.62432600	0.07486800	4.09096300
H	-1.15810400	0.15279600	5.06685200
C	-2.68980800	-0.76859900	3.86476500
C	-4.27095900	-2.34529300	3.96097000
H	-5.25748900	-2.30213700	4.43216300
H	-3.91555000	-3.37889500	3.86142000
C	-3.29099200	-0.85616300	2.61150100
C	-2.85647400	-0.14049100	1.51116400
C	0.01689600	2.92582100	1.09369000
C	1.33732600	2.60010300	1.44190700
H	1.73017500	1.62413300	1.17830700
C	2.15944600	3.51828900	2.09091800
H	3.18611100	3.24133000	2.30824700
C	1.66860400	4.78853500	2.39877800
H	2.30816200	5.51497300	2.89337800
C	0.36137200	5.13088000	2.04778000
H	-0.02112000	6.12352600	2.27221900
C	-0.46035600	4.20876000	1.39673500
H	-1.46572300	4.50207700	1.11637700
C	-2.41437800	2.50717400	-0.46498500
C	-3.41031200	3.12197000	0.30996800
H	-3.36800900	3.05749100	1.39323700
C	-4.47365600	3.78372400	-0.30435200
H	-5.23336400	4.26543000	0.30630800
C	-4.56769800	3.81889500	-1.69870900
H	-5.40380500	4.32337000	-2.17566700
C	-3.58955800	3.19545500	-2.47650500
H	-3.66610900	3.20687500	-3.56046000
C	-2.51737400	2.54627100	-1.86198100
H	-1.76521900	2.03622600	-2.45762100
C	-3.01905000	-1.01464200	-0.90791700
C	-3.56366200	-0.32031000	0.21248300
C	-4.84608100	0.17276600	0.06362300
C	-6.79932000	1.23616300	0.34050900
H	-7.65111500	0.85149900	0.91245300
H	-6.84291000	2.32785900	0.24803400
C	-5.57907800	0.04632900	-1.11321500
C	-5.07139900	-0.62057200	-2.20636100
H	-5.64416600	-0.73089800	-3.12050400
C	-3.77578900	-1.15545400	-2.07619100
H	-3.36332300	-1.69608000	-2.91918200
C	-1.07732500	-2.64232200	-2.30788600
C	-0.99309800	-4.03974900	-2.28785300
H	-1.12203500	-4.57823400	-1.35530800
C	-0.71667500	-4.75071300	-3.45942500
H	-0.64296600	-5.83459300	-3.42348800
C	-0.53074300	-4.07751600	-4.66707800
H	-0.31319000	-4.63282700	-5.57552400
C	-0.62019100	-2.68196600	-4.70047300
H	-0.47424000	-2.14724100	-5.63555700
C	-0.88122900	-1.97213100	-3.52975300
H	-0.91362100	-0.88517900	-3.54804000
C	-1.38583300	-2.84603500	0.57330700
C	-0.31339100	-2.94079000	1.46994300
H	0.55010400	-2.29868800	1.33642900
C	-0.35941600	-3.84810600	2.52981700
H	0.47641900	-3.90937600	3.22143600
C	-1.47534400	-4.67024400	2.70035200
H	-1.51095900	-5.37720100	3.52543000
C	-2.54856500	-4.58258600	1.80715400
H	-3.41935200	-5.22104600	1.93551500
C	-2.50808000	-3.67009700	0.75268200
H	-3.35278100	-3.58737100	0.07466800
Rh	0.29476200	0.11492200	-0.91718100
C	1.97894000	-1.25700500	-1.02851300
C	2.63122000	-1.15540000	0.21993500
C	2.07101800	-2.48081000	-1.71285300
C	3.24847400	-2.26165100	0.80361900
H	2.64033100	-0.21130600	0.75402600
C	2.69296500	-3.58879900	-1.13134100
H	1.62438700	-2.58362700	-2.69690700
C	3.27137500	-3.49114900	0.13608300
H	3.72868200	-2.15755900	1.77293000
H	2.71328100	-4.53296200	-1.67095800
C	1.42954200	1.49392700	-2.14177100
C	2.19652400	0.28366800	-2.34252200
C	3.70814100	0.46238600	-2.21275000
N	4.04581900	1.36193000	-1.10402800
H	0.63613600	1.69026100	-2.86338700
H	1.93980600	-0.29838400	-3.22670100
H	4.22560100	-0.48231000	-2.08037300
C	4.85277400	1.00656000	-0.05374200
O	4.90375400	1.57819900	1.02121900
O	5.62288000	-0.07480300	-0.39486200
C	6.43844000	-0.72528800	0.52500400
C	7.18502400	-0.07055900	1.50685900
C	6.53773600	-2.10595600	0.34379000
C	8.02554500	-0.82943400	2.32515400

H	7.09710100	0.99902100	1.63334600
C	7.38535300	-2.84707200	1.16559600
H	5.93740900	-2.57673600	-0.42636800
C	8.13039800	-2.21208700	2.16266800
H	8.60544000	-0.32685000	3.09465200
H	7.45968600	-3.92220700	1.02597100
H	8.78884300	-2.78963400	2.80550700
H	4.05548800	0.92232000	-3.15104400
C	4.06705200	3.79603300	-0.70011800
C	3.40894700	2.64072800	-1.12803000
C	2.10837300	2.70500700	-1.66350700
C	1.48559700	3.96200900	-1.73180800
C	2.12497800	5.11141000	-1.28137200
C	3.42178900	5.02878200	-0.76492500
H	5.06795900	3.72043300	-0.29196900
H	0.47123800	4.01772400	-2.12069900
H	1.61267100	6.06841000	-1.32412600
H	3.93104500	5.92119200	-0.41250800
H	3.75763400	-4.35114200	0.58883800

32-R

B3LYP-D3 SCF energy: -3611.578691 a.u.
B3LYP-D3 enthalpy: -3611.577747 a.u.
B3LYP-D3 free energy: -3611.731756 a.u.
M06 SCF energy in solution: -3612.102279 a.u.
Imaginary frequency: -35.57 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.81319000	1.56110300	0.21280000
P	-1.15626600	-1.69594700	-0.61838000
O	-3.91288600	-1.10537200	4.59433100
O	-4.68077600	-1.34971600	2.41890300
O	-5.53950000	1.07708600	0.40565700
O	-6.55788700	0.67233500	-1.63820100
C	-1.79240700	0.82558100	1.61154000
C	-1.35131400	0.97335300	2.93273100
H	-0.47936700	1.58220200	3.13714000
C	-1.99479200	0.35802200	4.02189400
H	-1.63247700	0.47649600	5.03702500
C	-3.10664600	-0.40323600	3.73542000
C	-4.85673800	-1.79888700	3.76595200
H	-5.87329800	-1.56310300	4.09824300
H	-4.65832900	-2.87645800	3.81691100
C	-3.56594800	-0.54766900	2.43001700
C	-2.94143100	0.02537600	1.33652000
C	0.16742400	2.84190200	1.12016000
C	1.46096200	2.48766100	1.52901000
H	1.86508900	1.52521200	1.23875500
C	2.24525900	3.36554500	2.27524300
H	3.25798800	3.07267300	2.53251300
C	1.73671500	4.61532000	2.63193800
H	2.34570600	5.30808800	3.20704200
C	0.45161700	4.98300600	2.22680700
H	0.05579500	5.96101200	2.48933000
C	-0.32739600	4.10610800	1.47115500
H	-1.31242700	4.42112400	1.14665100
C	-2.11823600	2.51939000	-0.68486300
C	-3.15849100	3.19014400	-0.02256600
H	-3.23471700	3.13595000	1.05905900
C	-4.12140000	3.89367100	-0.74678000
H	-4.91530600	4.41629900	-0.21892900
C	-4.07346200	3.91558200	-2.14327900
H	-4.82998700	4.45530900	-2.70687000
C	-3.05529000	3.23216800	-2.81194500
H	-3.02112400	3.23104000	-3.89812200
C	-2.08414900	2.54046300	-2.08627600
H	-1.30414500	1.98716100	-2.60111000
C	-2.87458500	-1.09070700	-0.98355800
C	-3.50024200	-0.24831400	-0.01627400
C	-4.73497100	0.26897800	-0.36005000
C	-6.63137400	1.45480000	-0.43895100
H	-7.57566900	1.24625900	0.07382000
H	-6.54078400	2.51804200	-0.69486600
C	-5.34873700	0.02590400	-1.58613400
C	-4.76417500	-0.78800200	-2.53091100
H	-5.24688100	-0.99449600	-3.47977800
C	-3.51412500	-1.34567300	-2.20097700
H	-3.04572500	-1.99916500	-2.92639800
C	-0.88744200	-2.98758900	-1.91178800
C	-0.83905800	-4.36270500	-1.64982400
H	-1.01253600	-4.73167700	-0.64511800
C	-0.54984500	-5.27099900	-2.67220100
H	-0.51035200	-6.33409700	-2.44873800
C	-0.31114900	-4.82014900	-3.97077000
H	-0.08955500	-5.52882300	-4.76433900
C	-0.35467500	-3.44960100	-4.24379700
H	-0.16422000	-3.08635400	-5.25044200
C	-0.62847800	-2.54330700	-3.22138300
H	-0.62844900	-1.47620800	-3.43107000
C	-1.44065000	-2.65736600	0.93272800
C	-0.57350100	-2.44421300	2.01148600
H	0.23759500	-1.73314100	1.89896300
C	-0.77928400	-3.10214800	3.22504800
H	-0.11202400	-2.91359500	4.06157700
C	-1.85053500	-3.98650700	3.36805100
H	-2.01187000	-4.49818900	4.31328600
C	-2.72268500	-4.20373300	2.29618700
H	-3.56137500	-4.88714700	2.40472700
C	-2.52621900	-3.53355700	1.08852500
H	-3.22434300	-3.67730400	0.26843000
Rh	0.41029300	0.02475000	-0.92103300
C	1.70569200	1.33986200	-2.04260400
C	2.73708200	0.26996300	-2.47084700
C	4.19145500	0.77731000	-2.36531700
N	4.38158000	1.53042900	-1.11839900
H	0.99156400	1.53370000	-2.85297200
H	2.57311900	0.00980400	-3.52515400
H	4.90379000	-0.04437400	-2.40929600
C	4.96862900	1.02691700	0.00650900
O	4.87324000	1.49127500	1.12936700
O	5.70477700	-0.09467600	-0.30374100
C	6.17315600	-0.92484800	0.70873000
C	5.92535900	-2.28667400	0.53795300
C	6.90952800	-0.45116500	1.79493600
C	6.42180000	-3.19310900	1.47495200
H	5.34013400	-2.61274100	-0.31492400
C	7.39469200	-1.37011000	2.72756100
H	7.07918900	0.61139000	1.90781400
C	7.15550700	-2.73794700	2.57332300
H	6.22867500	-4.25473300	1.34622500
H	7.96549300	-1.01017600	3.57936400

H	7.53940200	-3.44425300	3.30429300
H	4.39911100	1.46725100	-3.19108500
C	4.09541100	3.90570500	-0.55384700
C	3.57231300	2.70873700	-1.04369500
C	2.26773300	2.62395300	-1.56890500
C	1.52073400	3.81649200	-1.60936800
C	2.02718300	5.01120500	-1.11120300
C	3.31667000	5.05930800	-0.56935700
H	5.10253400	3.91475300	-0.15047400
H	0.50958400	3.78356200	-2.00824400
H	1.41212500	5.90677700	-1.13307900
H	3.71293900	5.98864700	-0.17054300
C	2.53259900	-1.01823800	-1.66602000
C	2.56212400	-1.01314700	-0.24818400
C	2.46811500	-2.26632200	-2.32136800
C	2.53266700	-2.22755700	0.46495900
H	2.76386900	-0.09934900	0.29461400
C	2.42471000	-3.45865400	-1.61088200
H	2.44096400	-2.28807900	-3.40757400
C	2.44949400	-3.43911200	-0.20770000
H	2.60173500	-2.20584400	1.54818500
H	2.34458600	-4.40120800	-2.14320200
H	2.41465800	-4.37084100	0.35053600

33-ts-R

B3LYP-D3 SCF energy: -3611.551312 a.u.
B3LYP-D3 enthalpy: -3611.550368 a.u.
B3LYP-D3 free energy: -3611.703644 a.u.
M06 SCF energy in solution: -3612.068317 a.u.
Imaginary frequency: -732.54 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.80525200	1.61102500	0.09975100
P	-0.98584100	-1.78962200	-0.48427800
O	-3.85871200	-0.94710000	4.59215200
O	-4.58218800	-1.34866900	2.42332600
O	-5.49974600	0.88140800	0.21151100
O	-6.39993500	0.33894700	-1.85774100
C	-1.76910900	0.89127000	1.52577800
C	-1.35654400	1.13172200	2.84281000
H	-0.51436600	1.78610100	3.02687100
C	-1.99151000	0.55609300	3.95772800
H	-1.64469900	0.74428000	4.96761900
C	-3.07348600	-0.25749800	3.70418900
C	-4.82749700	-1.64804600	3.80151900
H	-5.83484100	-1.31016300	4.07420500
H	-4.71375600	-2.72569200	3.96359900
C	-3.50656400	-0.49419300	2.40455300
C	-2.88007400	0.02812400	1.28690100
C	0.02205800	3.01965500	0.96025500
C	1.27875400	2.75843900	1.52187300
H	1.77760800	1.81582400	1.32596200
C	1.91049000	3.70921600	2.32539900
H	2.89429700	3.48106400	2.72064100
C	1.29520800	4.93629800	2.56966800
H	1.78568900	5.67952700	3.19336000
C	0.05581500	5.21788000	1.98822500
H	-0.41976800	6.18132400	2.15493100
C	-0.57729400	4.26811200	1.18792400
H	-1.53110800	4.51184000	0.73499000
C	-2.15703800	2.37686200	-0.90418800
C	-3.24697700	3.05371800	-0.33446300
H	-3.33255100	3.12615000	0.74519600
C	-4.24584800	3.59678100	-1.14286300
H	-5.07672600	4.12850400	-0.68586500
C	-4.18824600	3.44372100	-2.53061200
H	-4.97395500	3.85521100	-3.15856300
C	-3.12218200	2.74920500	-3.10648200
H	-3.07905700	2.61005800	-4.18323000
C	-2.11338300	2.22434900	-2.29751700
H	-1.29359000	1.67041900	-2.74650100
C	-2.69331700	-1.24016600	-0.94241000
C	-3.38935400	-0.36770100	-0.05370600
C	-4.63252200	0.06728200	-0.47282000
C	-6.61103000	1.10340000	-0.66254800
H	-7.53190800	0.76682900	-0.17265800
H	-6.66322300	2.16738000	-0.92010400
C	-5.17591100	-0.25977700	-1.71222300
C	-4.51077700	-1.08467300	-2.59292700
H	-4.93591300	-1.34937400	-3.55464700
C	-3.25945600	-1.57630400	-2.17791200
H	-2.73049400	-2.24612700	-2.84489100
C	-0.69424300	-3.20191900	-1.64362400
C	-0.82053000	-4.54900100	-1.28209500
H	-1.13611700	-4.81962300	-0.28072300
C	-0.51305700	-5.56047200	-2.19589400
H	-0.60477400	-6.60059700	-1.89391300
C	-0.08520900	-5.24086200	-3.48424900
H	0.15915200	-6.02942300	-4.19090800
C	0.03967300	-3.90004300	-3.85745300
H	0.38694900	-3.63870400	-4.85323300
C	-0.25287300	-2.89208000	-2.94206300
H	-0.10440500	-1.85372100	-3.22499800
C	-1.21240700	-2.57898400	1.16163400
C	-0.25999000	-2.30857700	2.15400200
H	0.56976000	-1.64461000	1.92724100
C	-0.39767900	-2.85795800	3.43014200
H	0.33794300	-2.63010700	4.19630000
C	-1.48409700	-3.68464800	3.72276100
H	-1.59343500	-4.10818800	4.71747900
C	-2.43741100	-3.95896300	2.73700600
H	-3.28514300	-4.60174300	2.96112700
C	-2.30900500	-3.40146000	1.46519200
H	-3.07172400	-3.58369900	0.71357600
Rh	0.64024800	-0.04343800	-0.89536100
C	1.86763600	1.21059100	-2.11963700
C	3.12318800	0.43814400	-2.61964000
C	4.44051100	1.11595000	-2.15088100
N	4.25535500	1.81509000	-0.87418300
H	1.10038000	1.20066400	-2.91488400
H	3.14097300	0.48886800	-3.71988700
H	5.24702300	0.39173300	-2.05799900
C	4.56313100	1.29186100	0.34909300
O	4.23691900	1.75826300	1.42611300
O	5.33856900	0.16673200	0.20100500
C	5.56942200	-0.66018800	1.29596400
C	5.30979100	-2.01441700	1.09463400
C	6.09355300	-0.18868200	2.49961500
C	5.57690500	-2.91771000	2.12384800
H	4.90396000	-2.33675100	0.14283200
C	6.35068300	-1.10448000	3.52181400

H	6.27583100	0.87003100	2.63007200
C	6.09505500	-2.46623200	3.34039900
H	5.37431900	-3.97451600	1.97127900
H	6.75490400	-0.74750800	4.46540800
H	6.30014700	-3.17047200	4.14218100
H	4.74473300	1.88015300	-2.87365100
C	3.60850300	4.16812900	-0.51347200
C	3.32578400	2.89332100	-0.99340400
C	2.14800800	2.60798400	-1.71223200
C	1.27882100	3.68005200	-1.97157800
C	1.54766400	4.95886400	-1.48854500
C	2.70571800	5.20565000	-0.74591800
H	4.52171300	4.33059300	0.04975500
H	0.36537000	3.49695100	-2.53125100
H	0.84492500	5.76486200	-1.68221500
H	2.90683400	6.19850000	-0.35480200
C	3.08947200	-1.01592700	-2.21975000
C	2.16920900	-1.43103500	-1.24076900
C	3.96754400	-1.94541100	-2.79821500
C	2.25172100	-2.75780600	-0.77183500
H	1.86464300	-0.42134600	0.02525000
C	3.99108500	-3.27051700	-2.36721100
H	4.64660000	-1.62196500	-3.58591900
C	3.13859500	-3.67305400	-1.33251300
H	1.59780300	-3.08720900	0.02961800
H	4.68045000	-3.97944300	-2.81884000
H	3.16181600	-4.69781400	-0.96996300

34-R

B3LYP-D3 SCF energy: -3611.557485 a.u.
B3LYP-D3 enthalpy: -3611.556540 a.u.
B3LYP-D3 free energy: -3611.710186 a.u.
M06 SCF energy in solution: -3612.073969 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.51944900	1.71887100	0.01301800
P	-1.05943900	-1.62894400	-0.66838200
O	-3.42585400	-0.74003500	4.66399800
O	-4.35553800	-1.01064200	2.55411200
O	-5.26959300	1.35787500	0.50110500
O	-6.37981800	0.97074700	-1.49715800
C	-1.46085100	1.04230200	1.47898300
C	-0.92493000	1.20283800	2.76423500
H	-0.02705600	1.79094600	2.89978200
C	-1.50357700	0.63552800	3.91218900
H	-1.05946500	0.76490100	4.89270600
C	-2.66159800	-0.08809100	3.73068300
C	-4.48820800	-1.36766800	3.93464900
H	-5.45236300	-1.00748800	4.31220100
H	-4.40279500	-2.45555900	4.03702800
C	-3.21655700	-0.24620900	2.46719900
C	-2.64715900	0.26680400	1.31384200
C	0.29048300	3.18291400	0.79147200
C	1.49590000	2.94491900	1.46314000
H	1.96414900	1.96975300	1.41696200
C	2.11798800	3.95702300	2.19337100
H	3.05937300	3.73571500	2.68483000
C	1.54864800	5.22909600	2.24678100
H	2.03274400	6.02250800	2.81068200
C	0.36496700	5.48617500	1.55077600
H	-0.07425300	6.48062300	1.56909400
C	-0.26264700	4.47203700	0.82706100
H	-1.17500300	4.69691900	0.28720100
C	-1.83022800	2.46524900	-1.04841700
C	-2.93323900	3.16212000	-0.52985000
H	-3.06499800	3.23832900	0.54493400
C	-3.88616200	3.71580000	-1.38397100
H	-4.73463800	4.25285300	-0.96766100
C	-3.75714600	3.57244500	-2.76816100
H	-4.50651800	3.99475400	-3.43203700
C	-2.66842200	2.87496000	-3.29411700
H	-2.56713300	2.75060400	-4.36885200
C	-1.71115600	2.32673700	-2.43799600
H	-0.87034200	1.77415900	-2.85003500
C	-2.74519200	-0.92070700	-0.96081300
C	-3.30144300	-0.04789200	0.01750200
C	-4.54416500	0.48351900	-0.27065700
C	-6.49432600	1.57995000	-0.20457900
H	-7.32401100	1.11672000	0.34669700
H	-6.65343600	2.65581200	-0.32558400
C	-5.21188500	0.25300700	-1.46924800
C	-4.68235200	-0.57157500	-2.43810500
H	-5.20056400	-0.75688400	-3.37228200
C	-3.43879600	-1.16332700	-2.15405700
H	-3.01773000	-1.83494900	-2.89148400
C	-1.00500000	-2.94345300	-1.96855900
C	-1.38470600	-4.27283600	-1.74717800
H	-1.73005400	-4.58601100	-0.76790000
C	-1.29615900	-5.21466800	-2.77498000
H	-1.58229600	-6.24559800	-2.58358800
C	-0.83917400	-4.83815000	-4.03835800
H	-0.76688800	-5.57360000	-4.83502100
C	-0.46430600	-3.51256300	-4.27139600
H	-0.09487000	-3.21139900	-5.24776100
C	-0.53827200	-2.57716600	-3.24146300
H	-0.20751200	-1.55789600	-3.42273900
C	-1.23439800	-2.53072400	0.92602800
C	-0.15328500	-2.51085900	1.82035900
H	0.75532400	-1.97836800	1.55739300
C	-0.24430200	-3.16467200	3.05019300
H	0.60240800	-3.13344100	3.72950400
C	-1.41282800	-3.84595400	3.39624700
H	-1.48480200	-4.35305600	4.35484700
C	-2.49358700	-3.87160200	2.50904900
H	-3.40441100	-4.40372200	2.77244100
C	-2.41015400	-3.20967400	1.28398900
H	-3.26665100	-3.19765300	0.61628000
Rh	0.85984700	-0.09397700	-0.95398900
C	2.34450400	1.01041800	-1.98687200
C	3.56547600	0.13806400	-2.37639200
C	4.86241900	0.56872200	-1.61904000
N	4.57390900	1.38206100	-0.43326500
H	1.65508200	1.05779000	-2.85631400
H	3.77943600	0.30857500	-3.44382500
H	5.44661100	-0.29933900	-1.32320300
C	4.53964800	0.90777200	0.84768800
O	4.15597700	1.53579600	1.81929900
O	5.04191600	-0.37038700	0.91475500
C	4.53539900	-1.25099500	1.86986500
C	4.16061000	-2.49939500	1.37491200
C	4.42751800	-0.94416200	3.22765400

C	3.64463700	-3.45456800	2.24919800
H	4.25798800	-2.69541400	0.31458800
C	3.90673000	-1.91212300	4.09099700
H	4.72519800	0.03099600	3.58635300
C	3.51248200	-3.16349300	3.61031300
H	3.33600600	-4.41977200	1.85767400
H	3.81370400	-1.68155100	5.14907300
H	3.11332000	-3.90959200	4.29267300
H	5.48360300	1.19401400	-2.26884700
C	4.25425500	3.83138900	-0.33674200
C	3.84792500	2.57072700	-0.75937900
C	2.72087700	2.38648900	-1.58497600
C	2.01124700	3.53228700	-1.97507400
C	2.39914100	4.79951900	-1.54345400
C	3.51947300	4.95338400	-0.72254000
H	5.12401500	3.91991600	0.30609100
H	1.13072900	3.41981400	-2.60403300
H	1.82133700	5.66998600	-1.84164500
H	3.81603400	5.94010400	-0.37942300
C	3.26439000	-1.32016200	-2.16398500
C	2.11573400	-1.65617400	-1.42174300
C	4.13787200	-2.31072900	-2.64164400
C	1.95108500	-3.01797600	-1.09507100
C	3.91933500	-3.65483100	-2.34802600
H	5.00491500	-2.02099100	-3.23422900
C	2.82284800	-4.00472300	-1.55395700
H	1.12946400	-3.33558300	-0.46427100
H	4.60024900	-4.41679100	-2.71935600
H	2.64671900	-5.04531000	-1.28987600
H	1.59322100	-0.19745500	0.38944100

35-ts-R

B3LYP-D3 SCF energy: -3611.546639 a.u.
B3LYP-D3 enthalpy: -3611.545695 a.u.
B3LYP-D3 free energy: -3611.698285 a.u.
M06 SCF energy in solution: -3612.063472 a.u.
Imaginary frequency: -747.35 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.44273300	1.67495600	0.05327300
P	-1.16684300	-1.60411000	-0.70048400
O	-3.53510900	-0.55211700	4.68602400
O	-4.43282700	-0.82740100	2.56336600
O	-5.19997900	1.60257600	0.51861000
O	-6.33508900	1.28597700	-1.47912500
C	-1.44710400	1.10194800	1.51491200
C	-0.93048300	1.26984300	2.80637600
H	-0.01214800	1.82618500	2.94497200
C	-1.55285800	0.74514200	3.95211400
H	-1.12781800	0.87908100	4.94049600
C	-2.72847600	0.05418300	3.75679500
C	-4.59804300	-1.16448200	3.94511700
H	-5.56026200	-0.77842900	4.30092000
H	-4.53945800	-2.25297100	4.06186500
C	-3.26435400	-0.10797900	2.48471800
C	-2.65844000	0.36884200	1.33475500
C	0.47528400	3.10278700	0.78600800
C	1.68021700	2.81513100	1.44182500
H	2.07726100	1.80637100	1.43555500
C	2.39097100	3.81695400	2.10349000
H	3.33019900	3.55826000	2.57915000
C	1.91144800	5.12646400	2.10747700
H	2.46567500	5.91033100	2.61763400
C	0.72785000	5.43073800	1.43151400
H	0.35734200	6.45276100	1.41090200
C	0.01424300	4.42866400	0.77428700
H	-0.89328700	4.69197100	0.24440200
C	-1.69841400	2.48547600	-1.03164900
C	-2.74184600	3.28214600	-0.53331300
H	-2.85922500	3.40710500	0.53880200
C	-3.65676100	3.87555700	-1.40234000
H	-4.45779700	4.49223800	-1.00238100
C	-3.55142000	3.66963300	-2.78080300
H	-4.27214000	4.12284800	-3.45604000
C	-2.52632900	2.86756000	-3.28524500
H	-2.44880200	2.68973600	-4.35451800
C	-1.60539200	2.28032700	-2.41492200
H	-0.82220600	1.63358900	-2.80172800
C	-2.81456400	-0.80891900	-0.95752000
C	-3.31819600	0.08615400	0.03045800
C	-4.52691700	0.69185500	-0.25818600
C	-6.39453400	1.92780200	-0.19847300
H	-7.26707000	1.55791800	0.35617000
H	-6.44874400	3.01202800	-0.34050100
C	-5.20907700	0.50455600	-1.45633900
C	-4.73129800	-0.34636400	-2.42905800
H	-5.26079700	-0.49719500	-3.36305600
C	-3.52163000	-1.00639000	-2.15043500
H	-3.13391500	-1.69208600	-2.89366200
C	-1.18642100	-2.93013400	-1.98551500
C	-1.71434400	-4.20991200	-1.77531800
H	-2.12150300	-4.48211500	-0.80772000
C	-1.69555800	-5.15797100	-2.80066200
H	-2.09623500	-6.15203400	-2.62004000
C	-1.16098200	-4.83431800	-4.04855900
H	-1.14421500	-5.57497500	-4.84363500
C	-0.63545600	-3.55846800	-4.26736900
H	-0.20266200	-3.30296100	-5.23071500
C	-0.63901000	-2.61703800	-3.23970100
H	-0.18621000	-1.64186900	-3.39448200
C	-1.35072000	-2.45711900	0.92116200
C	-0.26996100	-2.42560900	1.81687500
H	0.64810000	-1.91651300	1.53485300
C	-0.37511700	-3.03253400	3.06894200
H	0.47016200	-2.99085300	3.74972300
C	-1.55645400	-3.68037100	3.43642400
H	-1.63917800	-4.15177100	4.41223300
C	-2.63685500	-3.71527400	2.54967900
H	-3.55889600	-4.21793300	2.83106100
C	-2.54052000	-3.09675400	1.30282400
H	-3.40092100	-3.08208800	0.64023500
Rh	0.80260300	-0.20034300	-0.82563900
C	2.35983800	0.83713800	-1.99596500
C	3.49783900	-0.13057000	-2.38843100
C	4.85245600	0.27479300	-1.72174800
N	4.67268900	1.18143700	-0.58070100
H	1.59111200	0.85043000	-2.77706800
H	3.65277500	-0.01609100	-3.47231000
H	5.39949000	-0.60413300	-1.39103200
C	4.71377600	0.79595800	0.73425200
O	4.44193700	1.51188900	1.68036300

O	5.13566400	-0.50558400	0.85487200
C	4.58242300	-1.29404100	1.86791200
C	4.03488600	-2.50337900	1.44408800
C	4.58811200	-0.92551900	3.21374500
C	3.45701900	-3.35546800	2.38442100
H	4.04831000	-2.74995400	0.39018700
C	4.00401300	-1.78992900	4.14363300
H	5.01883300	0.02016800	3.51257800
C	3.43616100	-3.00013600	3.73638600
H	3.01282000	-4.28861500	2.04998800
H	3.99687900	-1.51126100	5.19410200
H	2.98801100	-3.66606900	4.46946500
H	5.47510900	0.81595500	-2.44188900
C	4.46067700	3.64963800	-0.57776700
C	3.99543500	2.38915700	-0.93608900
C	2.82476200	2.22255000	-1.69960600
C	2.13308600	3.36837400	-2.10675100
C	2.58541400	4.63720300	-1.74502100
C	3.74430700	4.77870900	-0.97773900
H	5.35616000	3.73429400	0.02842500
H	1.21498900	3.25934300	-2.67909800
H	2.02451500	5.51641000	-2.04877700
H	4.08764500	5.76668300	-0.68530200
C	3.12736300	-1.56442500	-2.09404500
C	1.96942200	-1.83298400	-1.33093500
C	3.97018000	-2.59701000	-2.53665300
C	1.75663700	-3.18557400	-0.98683000
C	3.71438200	-3.92400600	-2.19920700
H	4.84464600	-2.35518800	-3.14034200
C	2.60151200	-4.21356000	-1.40499300
H	0.91224900	-3.46473200	-0.36662500
H	4.37457200	-4.71668500	-2.54235400
H	2.38813000	-5.24009300	-1.11396500
H	2.20638600	0.38863000	-0.38053400

36-R

B3LYP-D3 SCF energy: -3611.570077 a.u.
B3LYP-D3 enthalpy: -3611.569133 a.u.
B3LYP-D3 free energy: -3611.725998 a.u.
M06 SCF energy in solution: -3612.096168 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.69674800	1.77556300	0.04393900
P	1.01938400	-1.53969600	-0.24691000
O	6.52972100	-0.40063800	-2.67356100
O	5.72556900	-1.50127700	-0.79998600
O	5.47385300	0.13446500	2.11472300
O	4.99752000	-0.84989000	4.15991400
C	3.27262400	1.27203500	-0.76988200
C	3.78143800	1.93950000	-1.88684100
H	3.31529000	2.86138600	-2.21618700
C	4.88358100	1.45134300	-2.61485300
H	5.27334000	1.97521800	-3.48059700
C	5.44566400	0.27444800	-2.17120700
C	6.59974200	-1.62249900	-1.92724100
H	7.62431800	-1.77572900	-1.57650800
H	6.26122100	-2.45359600	-2.55969800
C	4.95932600	-0.38822200	-1.04480200
C	3.87366700	0.05846700	-0.31630900
C	1.29390800	3.44675800	-0.62950100
C	0.74075400	3.49872900	-1.92445600
H	0.65747600	2.58320400	-2.50687700
C	0.28832500	4.70465600	-2.45878800
H	-0.13513500	4.72524800	-3.45939800
C	0.37004900	5.87843700	-1.70391300
H	0.00970400	6.81772300	-2.11472200
C	0.91238000	5.83717800	-0.41845700
H	0.97589600	6.74569300	0.17476500
C	1.37334900	4.63127000	0.11654700
H	1.78463600	4.61460700	1.12041400
C	2.21999000	2.08348800	1.78256900
C	3.41210100	2.74858900	2.10833700
H	4.05644800	3.11911500	1.31567500
C	3.78131100	2.91394000	3.44349000
H	4.70131900	3.43879600	3.68917400
C	2.97467900	2.39693500	4.46285200
H	3.27093600	2.51341000	5.50198400
C	1.79232300	1.72533800	4.14415200
H	1.17079200	1.31028400	4.93264400
C	1.41375200	1.57331800	2.80910800
H	0.50965800	1.02890000	2.54796200
C	2.28394700	-1.44817300	1.10026000
C	3.46585200	-0.66396900	0.92554500
C	4.29205200	-0.55985100	2.03045900
C	5.87781700	0.06008400	3.48559300
H	6.90381300	-0.31775100	3.54269800
H	5.78984900	1.05309200	3.94322200
C	4.00744100	-1.14800300	3.26018600
C	2.87348100	-1.90768600	3.44631400
H	2.64861900	-2.37037700	4.40074700
C	2.01921900	-2.04719000	2.33780400
H	1.11796500	-2.63645000	2.45856100
C	-0.06002500	-2.94594700	0.27645600
C	0.19534700	-4.28679400	-0.04536000
H	1.06614800	-4.55539700	-0.63408000
C	-0.68672000	-5.28810300	0.36825100
H	-0.48579300	-6.32279400	0.10180900
C	-1.82460500	-4.96298200	1.11092200
H	-2.51404800	-5.74383200	1.42225400
C	-2.08257400	-3.63010900	1.43987500
H	-2.97484500	-3.34884800	1.98889100
C	-1.20890100	-2.62906400	1.01765400
H	-1.44778100	-1.59420000	1.23274700
C	1.99446500	-2.20298500	-1.66692600
C	1.69027700	-1.76094900	-2.96266300
H	0.89501500	-1.03282500	-3.09659500
C	2.41034700	-2.24035600	-4.05787500
H	2.17121000	-1.88585900	-5.05687600
C	3.43682800	-3.16955400	-3.87100400
H	3.99646500	-3.54286700	-4.72478800
C	3.74408400	-3.61576700	-2.58279300
H	4.54121000	-4.33913300	-2.42987000
C	3.03349400	-3.12886400	-1.48484900
H	3.30335800	-3.45139600	-0.48368000
Rh	-0.05746800	0.35642900	-0.59407300
C	-3.29601900	3.00946000	-1.24595900
C	-2.47836400	1.80825100	-0.73413800
C	-2.74943900	1.69041100	0.78336000
N	-4.15876300	1.34046700	0.97929100
H	-2.75579600	3.93348800	-0.99748200
H	-1.41329400	2.09855300	-0.85411800

H	-2.13526700	0.91650100	1.23877400
C	-4.40860000	0.01842300	1.28558800
O	-3.59773900	-0.72873500	1.79949000
O	-5.68061900	-0.35713400	0.95469800
C	-5.97229800	-1.72159800	0.94069500
C	-7.13911700	-2.12678900	1.58138800
C	-5.17027900	-2.62394000	0.24166600
C	-7.51386800	-3.47129400	1.52456300
H	-7.73676500	-1.39112100	2.11033800
C	-5.55068200	-3.96491000	0.20299800
H	-4.26763500	-2.28508500	-0.25079200
C	-6.71915500	-4.39347600	0.84018400
H	-8.42487800	-3.79501200	2.02057100
H	-4.92303200	-4.67364600	-0.33016600
H	-7.00944600	-5.43984300	0.80181700
H	-2.54310200	2.64606700	1.28080900
C	-6.38796700	2.38034700	0.95438200
C	-5.09908600	2.25189700	0.41581300
C	-4.69052700	3.08592400	-0.64386400
C	-5.60664400	4.01897400	-1.14699100
C	-6.89367800	4.13290400	-0.62932800
C	-7.28275700	3.30506400	0.42779100
H	-6.67927300	1.74403800	1.78132800
H	-5.29495600	4.65914000	-1.96984100
H	-7.58648000	4.86035100	-1.04302200
H	-8.28006400	3.38682200	0.85113000
C	-2.73296000	0.48789200	-1.47389700
C	-1.68985300	-0.47244100	-1.48147500
C	-3.95618000	0.22158700	-2.10379400
C	-1.92886300	-1.68286400	-2.15395900
C	-4.16616700	-0.99262900	-2.76277900
H	-4.75769000	0.95435400	-2.08442400
C	-3.14580500	-1.94368600	-2.79164700
H	-1.15822100	-2.44864600	-2.18243900
H	-5.12209200	-1.19179000	-3.24005900
H	-3.29910700	-2.89292600	-3.30151200
H	-3.36586200	2.97853300	-2.33949200

37-ts-R

B3LYP-D3 SCF energy: -3687.958691 a.u.
B3LYP-D3 enthalpy: -3687.957747 a.u.
B3LYP-D3 free energy: -3688.119336 a.u.
M06 SCF energy in solution: -3688.499680 a.u.
Imaginary frequency: -1364.04 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.78875200	-0.98151100	1.59103500
P	1.20959800	-0.00060700	-1.51509900
O	4.18814000	4.47024300	1.20793100
O	4.73042300	2.91875400	-0.42633600
O	6.19844300	0.06980200	0.23836200
O	7.04755700	-1.31163200	-1.42071000
C	2.62651900	0.66770100	1.62681300
C	2.33009300	1.60658200	2.62019100
H	1.70822300	1.31631700	3.45897100
C	2.80646900	2.93034000	2.57451500
H	2.56550000	3.64947700	3.34950200
C	3.59409900	3.26813600	1.49562600
C	4.77798300	4.30905700	-0.09000800
H	5.82038800	4.63971000	-0.05796200
H	4.19599600	4.87829300	-0.82600200
C	3.91633800	2.33568900	0.51230400
C	3.45239200	1.03293800	0.52113200
C	1.22005800	-1.25566800	3.32456600
C	0.04010200	-0.60829700	3.73365600
H	-0.50287900	0.00865000	3.02750000
C	-0.44643300	-0.77072700	5.02968700
H	-1.35785200	-0.26015400	5.32872400
C	0.21999100	-1.60567300	5.92955300
H	-0.16587600	-1.74191200	6.93640300
C	1.37632100	-2.27433400	5.52533900
H	1.89494300	-2.93439200	6.21579000
C	1.87558100	-2.10039200	4.23254200
H	2.77358000	-2.63113600	3.93660700
C	3.21077800	-2.13675200	1.38157700
C	4.41349500	-1.96984500	2.08616900
H	4.52025400	-1.14399800	2.78373700
C	5.48099600	-2.84160300	1.87267200
H	6.40514200	-2.70978700	2.42993400
C	5.36612800	-3.87413100	0.93689800
H	6.20408500	-4.54277000	0.75875400
C	4.17494100	-4.04056300	0.22704800
H	4.08621500	-4.83462600	-0.50930800
C	3.09945400	-3.18003200	0.45363100
H	2.17428400	-3.28650200	-0.10717700
C	3.02653500	-0.36949300	-1.62078400
C	3.87355700	0.12028900	-0.58083100
C	5.20029900	-0.26378400	-0.64287000
C	7.35736300	-0.65646200	-0.18270100
H	8.18766700	0.04063600	-0.33789900
H	7.60693000	-1.41140000	0.57284100
C	5.71239300	-1.09190900	-1.63779600
C	4.91714400	-1.55499500	-2.66194900
H	5.31385600	-2.18472100	-3.45044300
C	3.56302500	-1.17284400	-2.63240200
H	2.92572400	-1.51965300	-3.43543100
C	0.56768800	-0.48510100	-3.17555900
C	0.04674000	0.43047700	-4.09739500
H	0.04946400	1.49161800	-3.87484100
C	-0.50113900	-0.01488700	-5.30330800
H	-0.91348300	0.70758700	-6.00248400
C	-0.52308500	-1.37527900	-5.60906500
H	-0.94569100	-1.71738600	-6.54997100
C	-0.01297700	-2.29835700	-4.69157100
H	-0.04119300	-3.36210400	-4.91268600
C	0.51043300	-1.85719000	-3.47842100
H	0.86112000	-2.58009200	-2.74611700
C	1.25348600	1.84656600	-1.55501000
C	0.53583200	2.56959500	-0.59553500
H	-0.03840400	2.02671300	0.14514700
C	0.59483200	3.96359600	-0.56743600
H	0.04071900	4.51037700	0.19030100
C	1.36889500	4.64892800	-1.50600900
H	1.41295100	5.73482600	-1.48778500
C	2.09274100	3.93423100	-2.46636600
H	2.70158600	4.46255900	-3.19567200
C	2.04381600	2.54036500	-2.48488300
H	2.62800900	1.98779300	-3.21540500
Rh	0.03895500	-0.97059500	0.15066500
C	-2.71980000	2.70935600	0.58612000
C	-2.60034100	1.17444700	0.65969200

C	-3.63920700	0.66461900	1.67819600
N	-4.99501300	1.01897300	1.23591600
H	-2.10412500	3.14092700	1.38898500
H	-1.61560500	0.91554800	1.06500800
H	-3.55536500	-0.40980700	1.80963900
C	-5.86044500	0.09805100	0.68371900
O	-6.91752000	0.34570100	0.14123800
O	-5.37214900	-1.17381400	0.85633700
C	-6.07379300	-2.23478400	0.28967800
C	-5.38547300	-3.02493300	-0.62665000
C	-7.37806600	-2.53507400	0.67833500
C	-6.01678400	-4.15031800	-1.15905200
H	-4.38000500	-2.73883300	-0.91441900
C	-7.99970300	-3.65974200	0.13449600
H	-7.89063200	-1.88929600	1.38148000
C	-7.32284200	-4.47061600	-0.78094300
H	-5.48652100	-4.77259300	-1.87518600
H	-9.01780700	-3.90127900	0.42780800
H	-7.81301200	-5.34575600	-1.19880700
H	-3.46880500	1.14752700	2.64940500
C	-6.50860900	2.96649700	1.20075600
C	-5.22695400	2.41426000	1.04782400
C	-4.13234600	3.24506700	0.74153300
C	-4.35957000	4.61978600	0.59099400
C	-5.62978800	5.16991200	0.73093600
C	-6.70714600	4.33310400	1.03671200
H	-7.34057700	2.31437200	1.42985500
H	-3.51342500	5.26114100	0.35098500
H	-5.78037200	6.23839500	0.60296600
H	-7.70569500	4.74521900	1.15402800
C	-2.74270700	0.43487800	-0.66396700
C	-2.06102600	-0.79846800	-0.83416600
C	-3.60069100	0.90402300	-1.66645900
C	-2.30299900	-1.52842300	-2.01068100
C	-3.80012600	0.16390100	-2.83592200
H	-4.13249800	1.84301800	-1.54000000
C	-3.15643800	-1.06124800	-3.01163800
H	-1.80272000	-2.48357300	-2.14941000
H	-4.47377300	0.54248700	-3.60062300
H	-3.31405300	-1.64044300	-3.91737200
H	-2.28843000	3.07668200	-0.35212300
O	-1.45182100	-1.83433300	1.48315700
H	-1.88570900	-1.48564900	0.35945500
H	-1.31801500	-2.79685100	1.45188400

38-R

B3LYP-D3 SCF energy: -1054.657399 a.u.
B3LYP-D3 enthalpy: -1054.656455 a.u.
B3LYP-D3 free energy: -1054.726633 a.u.
M06 SCF energy in solution: -1054.494280 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.91265200	1.34047300	1.00168400
C	-1.45653700	1.47349700	1.48731800
C	-1.00261800	0.07645300	1.96476400
N	-1.00984400	-0.85527800	0.83214000
H	-3.18299900	2.19885100	0.37495800
H	-0.00530200	0.10614100	2.39439400
C	0.15169400	-1.22357600	0.18077300
O	0.22315700	-1.76053900	-0.90294700
O	1.24426200	-0.93154900	0.96363700
C	2.51301900	-1.02505700	0.39675800
C	2.83881600	-0.32469200	-0.76356100
C	3.46291300	-1.76935100	1.09003500
C	4.14978900	-0.38263200	-1.23504700
H	2.07805100	0.25141300	-1.27553200
C	4.77395400	-1.81346800	0.61081300
H	3.16701900	-2.29807700	1.99052600
C	5.11967700	-1.12323600	-0.55274100
H	4.41384500	0.15865500	-2.13953900
H	5.52179400	-2.39076400	1.14752400
H	6.13926100	-1.16085300	-0.92600400
H	-1.69863600	-0.30217700	2.72351300
C	-2.59087800	-2.18180200	-0.51227800
C	-2.26926000	-1.00119200	0.17409000
C	-3.20385400	0.04813100	0.25579400
C	-4.44992000	-0.11921000	-0.36353200
C	-4.77004200	-1.28456200	-1.05311000
C	-3.83101600	-2.31770800	-1.12648600
H	-1.85792200	-2.97562400	-0.57150300
H	-5.17303400	0.69172300	-0.30326000
H	-5.74071600	-1.38758400	-1.53001300
H	-4.06573900	-3.23538800	-1.65850000
H	-3.57174700	1.38581700	1.87953400
H	-1.44350200	2.13906900	2.35977800
C	-0.47604300	2.02864300	0.46432200
C	0.68762000	2.67080400	0.91339600
C	-0.65943600	1.87764800	-0.91681900
C	1.63652300	3.15688000	0.01527100
H	0.85125400	2.78802200	1.98290100
C	0.28713200	2.36759100	-1.82131900
H	-1.53919000	1.36825200	-1.29661500
C	1.43615900	3.01096200	-1.35994400
H	2.53059100	3.64955200	0.38760900
H	0.12367200	2.23918000	-2.88796700
H	2.17261500	3.38986500	-2.06340800

39-ts-R

B3LYP-D3 SCF energy: -3687.956862 a.u.
B3LYP-D3 enthalpy: -3687.955917 a.u.
B3LYP-D3 free energy: -3688.113865 a.u.
M06 SCF energy in solution: -3688.492946 a.u.
Imaginary frequency: -1153.43 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	2.10548600	-2.31514000	0.14913100
C	2.75432800	-2.73380700	1.51079400
C	4.30056600	-2.48556200	1.49305200
N	4.73982300	-1.66935300	0.35459400
H	1.15627600	-2.85094800	0.04874800
H	2.62974100	-3.82257500	1.60253500
H	4.81551100	-3.44874900	1.41547400
C	5.18076400	-0.39578900	0.58679000
O	5.40071400	0.09313800	1.67792500
O	5.36518800	0.26833600	-0.60664000
C	5.68180300	1.62457500	-0.57603600
C	4.86491200	2.54991700	0.07468100
C	6.79474800	2.02596900	-1.31052700
C	5.18263600	3.90490000	-0.02146600
H	4.00336400	2.20950800	0.63574500

C	7.09851500	3.38577600	-1.40085300
H	7.40035500	1.27246300	-1.80415300
C	6.29439000	4.32780700	-0.75560700
H	4.54609600	4.62892000	0.47795900
H	7.96425400	3.70533400	-1.97484700
H	6.53131900	5.38603300	-0.82629400
H	4.64152900	-1.99029900	2.40109600
C	5.23061100	-2.34873000	-1.97967300
C	4.34131200	-2.18694400	-0.91867300
C	3.00231500	-2.62345100	-0.99801100
C	2.60199600	-3.27767600	-2.17200300
C	3.47851000	-3.42633600	-3.24617200
C	4.79067600	-2.94870000	-3.16103800
H	6.25154200	-1.99597500	-1.87491500
H	1.59421100	-3.66934100	-2.23397100
H	3.13735000	-3.92651900	-4.14965900
H	5.47485500	-3.06468900	-3.99716100
C	2.07659500	-2.12320500	2.72440500
C	1.20918500	-2.89878200	3.50376200
C	2.31654800	-0.79663400	3.11861800
C	0.59090500	-2.37272000	4.64170300
H	1.01929400	-3.93179900	3.21999500
C	1.69276700	-0.26665700	4.24904000
H	3.00723400	-0.18503800	2.54681000
C	0.82306000	-1.04867100	5.01432200
H	-0.05986100	-3.00369700	5.24223700
H	1.89541500	0.76117700	4.54078900
H	0.34712600	-0.63525900	5.89974700
O	2.46651000	0.33388800	0.17733000
H	2.86279200	0.51939900	-0.69189100
H	2.37760400	-0.83183900	0.20580400
P	-0.55082100	1.64916800	0.05869300
P	-1.45356100	-1.41239300	-0.70573000
O	-5.02711100	0.28370700	3.75269000
O	-5.33960400	-0.07114300	1.48372200
O	-5.17475800	2.33188500	-0.78474300
O	-5.79534300	2.00092100	-2.99525100
C	-1.96961500	1.44234900	1.22572400
C	-1.80664400	1.67540900	2.59543300
H	-0.89421400	2.13535200	2.95456400
C	-2.78319600	1.31885000	3.54328500
H	-2.63814200	1.49691400	4.60289200
C	-3.92824700	0.72346200	3.06034500
C	-5.85526300	-0.37568600	2.78400700
H	-6.87879800	0.00160600	2.86625800
H	-5.80939400	-1.46033300	2.94436300
C	-4.11311200	0.50656500	1.69681500
C	-3.16745100	0.83352500	0.74271400
C	0.56049900	2.88807300	0.85386400
C	1.36873800	2.44532600	1.91432800
H	1.32555600	1.40788900	2.21453600
C	2.23502800	3.32200200	2.56465000
H	2.85812300	2.95739900	3.37680700
C	2.32248600	4.65378700	2.15084100
H	3.00261000	5.33750100	2.65202200
C	1.54562400	5.09633400	1.07864200
H	1.61920700	6.12658000	0.74038900
C	0.67039900	4.22089800	0.43113500
H	0.08171500	4.58438300	-0.40336500
C	-1.29187900	2.57023600	-1.35402500
C	-2.17869700	3.63959300	-1.15064200
H	-2.45353000	3.92833700	-0.14007200
C	-2.72688500	4.31463500	-2.24078900
H	-3.40560400	5.14741600	-2.07419800
C	-2.40908800	3.91724500	-3.54327200
H	-2.84760100	4.43493200	-4.39210200
C	-1.53149300	2.85117800	-3.75117000
H	-1.28846000	2.53468700	-4.76176700
C	-0.97003900	2.18434700	-2.66064000
H	-0.29556000	1.34474800	-2.80917300
C	-2.84889400	-0.46319600	-1.47313800
C	-3.47242400	0.55186700	-0.68833600
C	-4.45176100	1.29502600	-1.31908800
C	-5.96268300	2.85831100	-1.85730600
H	-7.01732900	2.87071900	-1.56308000
H	-5.60744500	3.86523800	-2.10864700
C	-4.82470400	1.09919000	-2.64614400
C	-4.25358800	0.10716000	-3.41143500
H	-4.55165900	-0.06056300	-4.44031000
C	-3.25797600	-0.67259700	-2.79423800
H	-2.80018500	-1.45865200	-3.38054800
C	-1.09051800	-2.70926100	-1.96328900
C	-1.32258700	-4.07584400	-1.75903200
H	-1.76115100	-4.42052500	-0.82823600
C	-0.99179600	-5.00271800	-2.75187300
H	-1.16814200	-6.06076500	-2.57774900
C	-0.44563800	-4.57463800	-3.96309700
H	-0.19753900	-5.29763400	-4.73526200
C	-0.20082200	-3.21412100	-4.17104400
H	0.25034500	-2.87472300	-5.09911600
C	-0.49841200	-2.29211700	-3.16957100
H	-0.26436800	-1.24086200	-3.31315000
C	-2.34742900	-2.26710100	0.66061100
C	-1.81691800	-2.21684300	1.95617400
H	-0.86785600	-1.71918000	2.13062900
C	-2.52304200	-2.77674200	3.02270000
H	-2.10901200	-2.71587400	4.02347900
C	-3.75347300	-3.39834500	2.80207100
H	-4.29902800	-3.83622200	3.63435900
C	-4.28737000	-3.45300900	1.50989600
H	-5.24790600	-3.93076200	1.33450800
C	-3.59240000	-2.88056200	0.44562400
H	-4.02243400	-2.89380200	-0.55207600
Rh	0.46146400	-0.34218500	-0.19508200

H_2O

B3LYP-D3 SCF energy: -76.383061 a.u.
B3LYP-D3 enthalpy: -76.382117 a.u.
B3LYP-D3 free energy: -76.403562 a.u.
M06 SCF energy in solution: -76.419789 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	0.00000000	0.00000000	0.11941700
H	0.00000000	0.76265600	-0.47767000
H	0.00000000	-0.76265600	-0.47767000

6b-ts-S

B3LYP-D3 SCF energy: -3631.061041 a.u.
B3LYP-D3 enthalpy: -3630.099091 a.u.
B3LYP-D3 free energy: -3630.263448 a.u.
M06 SCF energy in solution: -3630.963898 a.u.

Imaginary frequency: -1296.13 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.91595600	1.58754200	0.33192800
P	-1.82828900	-0.00395000	-0.70243500
O	-3.10204700	2.42225000	4.66658500
O	-3.73221400	2.91815800	2.49051500
O	-2.20137100	5.13971600	0.59120600
O	-3.06064100	5.81821300	-1.45295000
C	-0.23434000	1.97582000	1.72351500
C	0.13444700	1.69565500	3.04558400
H	1.14388200	1.36511900	3.25869400
C	-0.76312400	1.80932600	4.12223100
H	-0.46608100	1.57838200	5.13916500
C	-2.04219600	2.22279500	3.81988400
C	-4.21914700	2.73833500	3.82390400
H	-4.68307100	3.66767000	4.16995100
H	-4.93123200	1.90419400	3.84069400
C	-2.41784300	2.52123300	2.51293500
C	-1.56432200	2.39952500	1.43178200
C	2.54715700	1.47420500	1.22086200
C	3.31038400	2.60724100	1.55055300
H	2.96094500	3.59797300	1.27875400
C	4.53188500	2.47500600	2.21964400
H	5.10799200	3.36346400	2.46860200
C	5.00201700	1.20774000	2.58074500
H	5.94939000	1.10466900	3.10431700
C	4.24467300	0.07566300	2.26766800
H	4.60336800	-0.91608500	2.52663900
C	3.03171500	0.20975700	1.58951800
H	2.47269600	-0.67340100	1.30534200
C	1.08954300	3.19362400	-0.57304200
C	0.89715000	4.44430200	0.03159400
H	0.59743200	4.50162900	1.07383300
C	1.05385400	5.61898400	-0.70869400
H	0.90526000	6.58274600	-0.22752900
C	1.39734200	5.55603600	-2.06109000
H	1.50819900	6.47018800	-2.63876900
C	1.58096200	4.31135900	-2.67249900
H	1.82429700	4.25724000	-3.73125300
C	1.42542200	3.13520900	-1.93594800
H	1.54401900	2.15918000	-2.39948400
C	-2.34541700	1.77012200	-0.95175500
C	-2.07732100	2.72721400	0.07226600
C	-2.36635100	4.04590500	-0.22822500
C	-2.49276900	6.28066900	-0.22211800
H	-3.21536900	6.92025000	0.29452500
H	-1.56150300	6.82331400	-0.43367900
C	-2.87760600	4.45622100	-1.45512100
C	-3.15276000	3.54875100	-2.45396100
H	-3.56328400	3.86010500	-3.40822100
C	-2.87689100	2.19743600	-2.17428700
H	-3.08648200	1.46878200	-2.94752100
C	-2.76617100	-0.84353700	-2.06307900
C	-2.12765300	-0.91187300	-3.31535600
H	-1.12760300	-0.49636800	-3.42436500
C	-2.75825300	-1.50829800	-4.40674200
H	-2.24898700	-1.55159600	-5.36612800
C	-4.03532800	-2.05764900	-4.26175100
H	-4.52404600	-2.53449800	-5.10747700
C	-4.67313000	-2.00263700	-3.02266700
H	-5.65208600	-2.45344100	-2.88864300
C	-4.04581300	-1.39557600	-1.93216600
H	-4.54961600	-1.39516500	-0.97378500
C	-2.72820000	-0.43677500	0.85174600
C	-2.01182900	-1.13081400	1.83547100
H	-0.97798500	-1.39722200	1.63944800
C	-2.61366000	-1.46423500	3.04991400
H	-2.04852900	-2.01454800	3.79585400
C	-3.94271700	-1.10899100	3.28999200
H	-4.41629700	-1.37495400	4.23138200
C	-4.66382000	-0.40881200	2.31632700
H	-5.69886000	-0.13002300	2.49920900
C	-4.05582700	-0.06054400	1.11020300
H	-4.60560500	0.52285900	0.37719700
Rh	0.43333800	-0.19497200	-0.89949400
C	0.17630300	-2.76354400	-1.39035000
C	1.44334300	-2.84403100	-1.91303200
C	2.60470000	-3.36995200	-1.23394700
C	2.27095600	-4.12250400	0.07588900
C	1.08574200	-3.43310700	0.77762700
N	-0.06629800	-3.36979200	-0.11659100
H	3.23013600	-3.96292500	-1.91145300
H	-0.69349600	-2.58017700	-1.99983700
H	1.57647500	-2.43761600	-2.91322500
H	1.93420900	-5.14695600	-0.15348200
H	0.78411400	-3.96372600	1.68061400
C	-1.24866300	-3.89383500	0.29727100
O	-1.48226300	-4.36285700	1.39963900
O	-2.17952200	-3.82724200	-0.72161500
C	-3.48644000	-4.22659400	-0.49818100
C	-4.06865500	-4.99537100	-1.50444600
C	-4.23163000	-3.79464800	0.60040000
C	-5.42080000	-5.32943200	-1.41997000
H	-3.45875800	-5.29706400	-2.34967500
C	-5.58213300	-4.13682100	0.67358700
H	-3.76345900	-3.20076800	1.37189900
C	-6.18394700	-4.89971600	-0.33134000
H	-5.87651700	-5.92351600	-2.20785200
H	-6.16596000	-3.79548200	1.52446500
H	-7.23730500	-5.15843900	-0.26553800
H	1.34644000	-2.40039000	1.04073100
C	3.49370800	-4.24859200	0.97400400
C	4.57830800	-5.02525000	0.53563400
C	3.61746800	-3.59761200	2.21028200
C	5.74363500	-5.14083800	1.29091700
H	4.50367200	-5.53823800	-0.42010000
C	4.78446100	-3.71143000	2.97475600
H	2.80269600	-2.99278200	2.59506700
C	5.85523900	-4.47910700	2.51750400
H	6.56671400	-5.74871400	0.92318600
H	4.84782800	-3.20183500	3.93374600
H	6.76117300	-4.56935800	3.11122700
O	4.48732700	-1.64827000	-0.58457500
H	3.56819800	-2.42006900	-0.93784300
H	4.68684800	-1.99607200	0.29781900
Cs	5.11398700	1.05882100	-1.63594300
O	2.37866000	0.04256700	-1.49944400
H	2.88836100	-0.65942600	-1.05019000

6c-ts-S

B3LYP-D3 SCF energy: -3611.159232 a.u.
B3LYP-D3 enthalpy: -3610.201610 a.u.
B3LYP-D3 free energy: -3610.358044 a.u.
M06 SCF energy in solution: -3610.866824 a.u.
Imaginary frequency: -1122.25 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.48388000	-1.15590300	1.24126300
P	0.94300600	0.83699400	-1.39155500
O	6.18177500	0.59931100	1.76916800
O	5.46308400	-0.16213500	-0.29739000
O	4.33519900	-3.17518000	-0.70247600
O	4.17551900	-3.99658800	-2.86046700
C	2.27827600	-0.76527500	1.50397000
C	2.73748900	-0.32138400	2.75086500
H	2.06251700	-0.34193300	3.59817200
C	4.03987400	0.16718400	2.95428200
H	4.37359000	0.51402500	3.92639500
C	4.86846900	0.18958300	1.85439800
C	6.49840200	0.55585300	0.37301000
H	7.45095100	0.03350700	0.23371700
H	6.54384400	1.58058800	-0.02021700
C	4.43470400	-0.26717800	0.61513700
C	3.15579600	-0.74324000	0.37861700
C	-0.11984400	-1.48109400	2.95236800
C	-0.25118100	-2.75188100	3.52246300
H	-0.00072100	-3.63751200	2.94855800
C	-0.72333100	-2.89671900	4.83048200
H	-0.82647300	-3.89168900	5.25741900
C	-1.06509200	-1.77219500	5.58138600
H	-1.43504900	-1.88574500	6.59795500
C	-0.94648200	-0.49941000	5.01557100
H	-1.23464600	0.38114600	5.58478200
C	-0.49839400	-0.35519300	3.70396300
H	-0.44060500	0.62393700	3.24836000
C	0.60659800	-2.84441500	0.48469600
C	1.55088000	-3.79167500	0.90837500
H	2.25179100	-3.53688300	1.69813000
C	1.61115200	-5.04954600	0.30615200
H	2.34035100	-5.77913000	0.65216200
C	0.74041300	-5.36849300	-0.74003000
H	0.79374100	-6.34533400	-1.21515700
C	-0.19760300	-4.42782300	-1.17214200
H	-0.87723000	-4.66771600	-1.98587000
C	-0.26753400	-3.17440700	-0.56103300
H	-0.98411900	-2.42803400	-0.89265600
C	2.05208400	-0.54330200	-1.98109700
C	2.85166500	-1.22111300	-1.00641700
C	3.49752100	-2.36558800	-1.44048700
C	4.57176700	-4.31911900	-1.52168800
H	5.63903800	-4.56066900	-1.50843400
H	3.96508800	-5.16002200	-1.15724000
C	3.40855300	-2.85874300	-2.73813000
C	2.68447800	-2.19562000	-3.70256800
H	2.63601800	-2.55205200	-4.72595100
C	2.01013200	-1.03028300	-3.29260400
H	1.44983000	-0.48999500	-4.04329000
C	0.46079500	1.79174100	-2.91620000
C	-0.29836000	1.19566000	-3.94050800
H	-0.50919600	0.13282500	-3.91180600
C	-0.81441500	1.95004700	-4.99453700
H	-1.39270300	1.45721700	-5.77208900
C	-0.61179900	3.33008800	-5.03609700
H	-1.02430500	3.92170300	-5.84950200
C	0.10702900	3.94429700	-4.00929400
H	0.25587100	5.02148000	-4.01630100
C	0.63612200	3.18636500	-2.96365000
H	1.17826900	3.68910500	-2.17052800
C	2.23223600	1.97254400	-0.68298700
C	2.03390000	2.54402700	0.57884700
H	1.11918800	2.33040900	1.12363300
C	3.01425300	3.36653800	1.14029500
H	2.84560300	3.79276300	2.12381900
C	4.18725700	3.64273300	0.43722800
H	4.94837700	4.28425500	0.87558900
C	4.38121200	3.09438700	-0.83583900
H	5.28848100	3.31506400	-1.39454000
C	3.41338500	2.25687600	-1.38739400
H	3.57638700	1.80961000	-2.36427700
Rh	-0.76026500	0.28401900	0.01767400
C	-2.51033300	1.16747300	-1.27973800
C	-2.59663400	-0.13568100	-1.75413200
C	-3.68031300	-1.04156300	-1.43894300
C	-4.97796100	-0.23868500	-1.22051500
C	-4.72885400	0.83373000	-0.14657400
N	-3.58769900	1.70094000	-0.50622500
H	-3.79932100	-1.82729900	-2.19460600
H	-1.92421500	1.91485100	-1.79586800
H	-1.84957100	-0.43855200	-2.47860800
H	-5.22221400	0.30236700	-2.15110100
H	-5.60618300	1.47515000	-0.02582000
C	-3.40233100	2.76427000	0.31353700
O	-4.17560200	3.17864500	1.15516000
O	-2.19919000	3.42510800	0.02346400
C	-1.42454900	3.83169900	1.08395700
C	-0.65865300	4.98379700	0.90172600
C	-1.33357600	3.08323100	2.26488800
C	0.20726100	5.40301700	1.91349200
H	-0.74809400	5.52841400	-0.03334900
C	-0.46820800	3.52137500	3.26716300
H	-1.89756000	2.15758000	2.35290800
C	0.30192700	4.67904200	3.10392100
H	0.81000400	6.29612800	1.76649700
H	-0.38689500	2.94148200	4.18386400
H	0.97270200	5.00810800	3.89408200
H	-4.49856200	0.36254700	0.81278300
C	-6.20426300	-1.06178700	-0.86168800
C	-7.42406100	-0.79609500	-1.50191000
C	-6.16945100	-2.06756800	0.11946500
C	-8.58353900	-1.50607900	-1.18277500
H	-7.46327800	-0.01849300	-2.26337700
C	-7.33036300	-2.77709200	0.43671200
H	-5.22451500	-2.29976300	0.61368200
C	-8.54031600	-2.50366900	-0.20701400
H	-9.51627500	-1.28074000	-1.69660500
H	-7.28566600	-3.55381300	1.19787000
H	-9.43908300	-3.06249700	0.04711000
O	-3.22879600	-2.23410100	0.88022600
H	-3.39819500	-1.68764200	-0.29042000
H	-2.56776400	-2.92726100	0.72670700
O	-2.17020300	0.19159500	1.45686200

H	-2.55811300	-0.72038500	1.41381000