Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
This journal is © the Partner Organisations 2022

Supplementary Information

for

What is the difference between mono- and biphosphine ligand? Revealing the chemoselectivity in Pd-catalysed carbenation of bromonaphthalene

Wenting Gong,[a] Dongmin Fu,[c] Kangbao Zhong,[b] Hao Ni,[b] Xiaoqian He,[b] Chunhui Shan,*[a] Rong Li,*[a] and Yu Lan*[b,c]

[a] Chongqing Key Laboratory of Inorganic Functional Materials, College of Chemistry, Chongqing Normal University, Chongqing 401331, China.

[b] School of Chemistry and Chemical Engineering, Chongqing Key Laboratory of Theoretical and Computational Chemistry, Chongqing University, Chongqing 400030, China

[c] Green Catalysis Center, and College of Chemistry, Zhengzhou University, Zhengzhou, Henan 450001, China.

chunhui.shan@cqnu.edu (Chunhui shan); rongli258@163.com (Rong Li); lanyu@cqu.edu.cn (Yu Lan)

Table of Content

1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, 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, **2013**.

2. Mechanistic study for another possible pathway

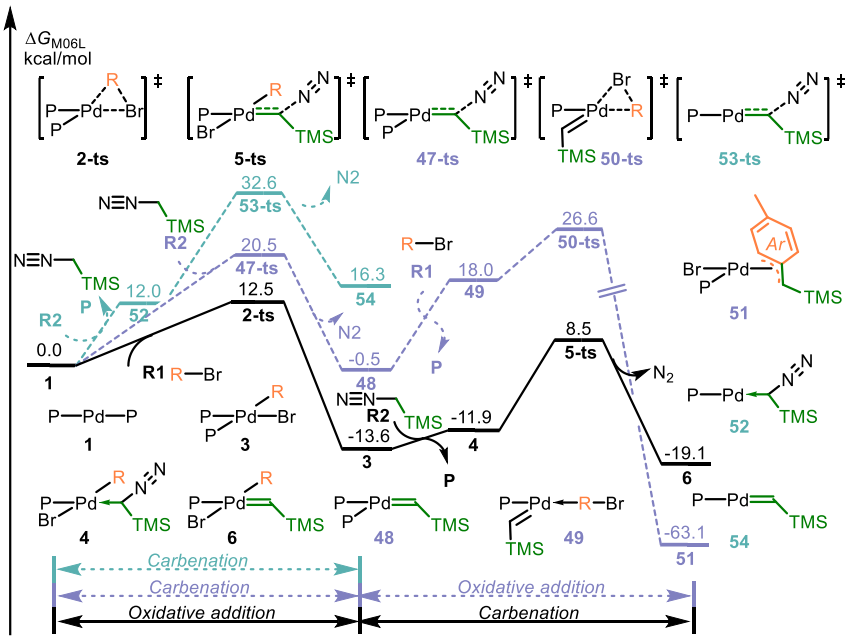

Fig S1. Free energy profiles for the carbonation and oxidative addition steps of Pd-catalysed dearomatization. Energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-L method in 1,4-dioxane.

Another possible mechanism, the order of the conversion steps is carbenation followed by oxidative addition, which is also considered in Fig. S1. The reaction starts from a phosphine-coordinated Pd(0) species **1**. The carbenation occurs via the transition state **47-ts** with an energy barrier of 20.5 kcal/mol, releasing nitrogen to give the Pd(II)-carbene complex **48**. The relative free energy of the transition state **47-ts** is 8.0 kcal/mol higher than that of transition state **2-ts**. Ligand exchange with bromonaphthalene **R1** forms intermediate **49** with an endothermic energy of 18.5 kcal/mol. Oxidative addition via a three-membered-ring transition state **50-ts** occurs with an energy barrier of 27.1 kcal/mol, giving a square-planar aryl-Pd(II) intermediate **51**, indicating that the step of carbenation is unfavorable. Similarly, carbenation occurs with assistance of one monophosphine-coordinated Pd(0) is also considered (green line). The energy barrier of this pathway is 32.6 kcal/mol, which is 20.1 kcal/mol higher than that of Path **a**. The results indicates carbenation with assistance of Pd(0) is unfavorable.

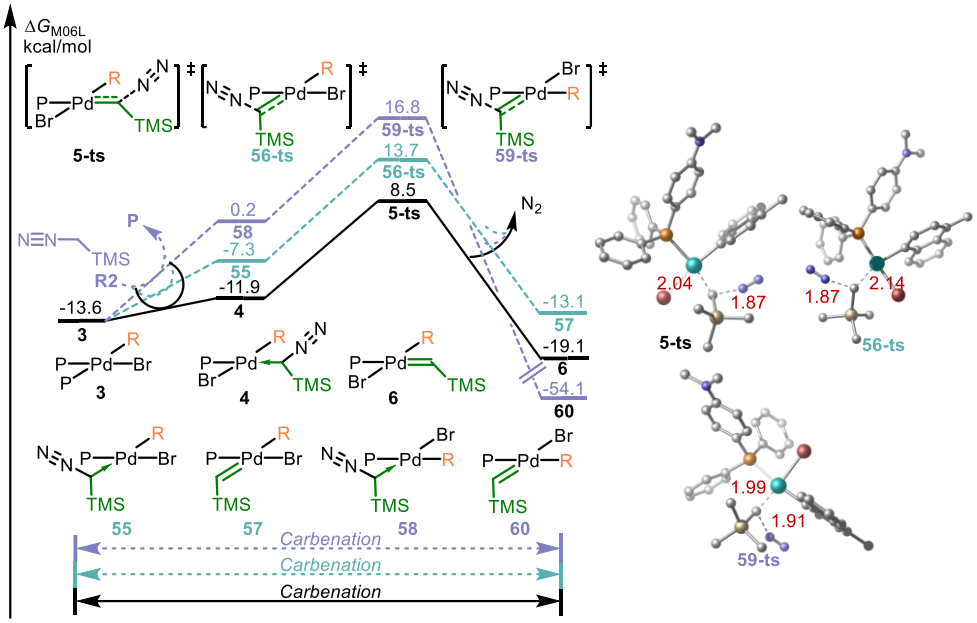

Fig S2. Free energy profiles for carbenation pathways of Pd-catalysed dearomatization. Energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-L method in 1,4-dioxane. Bond lengths are in angstroms.

When intermediate **3** is formed, the corresponding carbenation pathways (black line, green line and purple line) should be considered. The calculated free energy profiles are shown in Fig S2. Ligand exchange with TMS-diazomethane **R2** forms complex **4**, **55** and **58** with an endothermic energy of 1.7, 6.3 and 13.8 kcal/mol, respectively. Subsequent the relative activation free energies of carbonation via transition states **5-ts**, **56-ts** and **59-ts** for the generation of aryl palladium intermediate **6**, **57** and alkyl palladium **60** are 8.5, 13.7 and 16.8 kcal/mol, respectively. In **5-ts**, the smaller bromide anion is at the left side, which would engender less repulsion with the large site of the ligand. However, in **56-ts** and

59-ts, when bromide anion is at the right side, the larger TMS-diazomethane moiety would have a larger repulsion with the ligand. Therefore, the calculated relative free energy of **5-ts** is 5.2 and 8.3 kcal/mol lower than that of **56-ts** and **59-ts**. These results indicate that generation of intermediate **6** is dynamically and thermodynamically favorable.

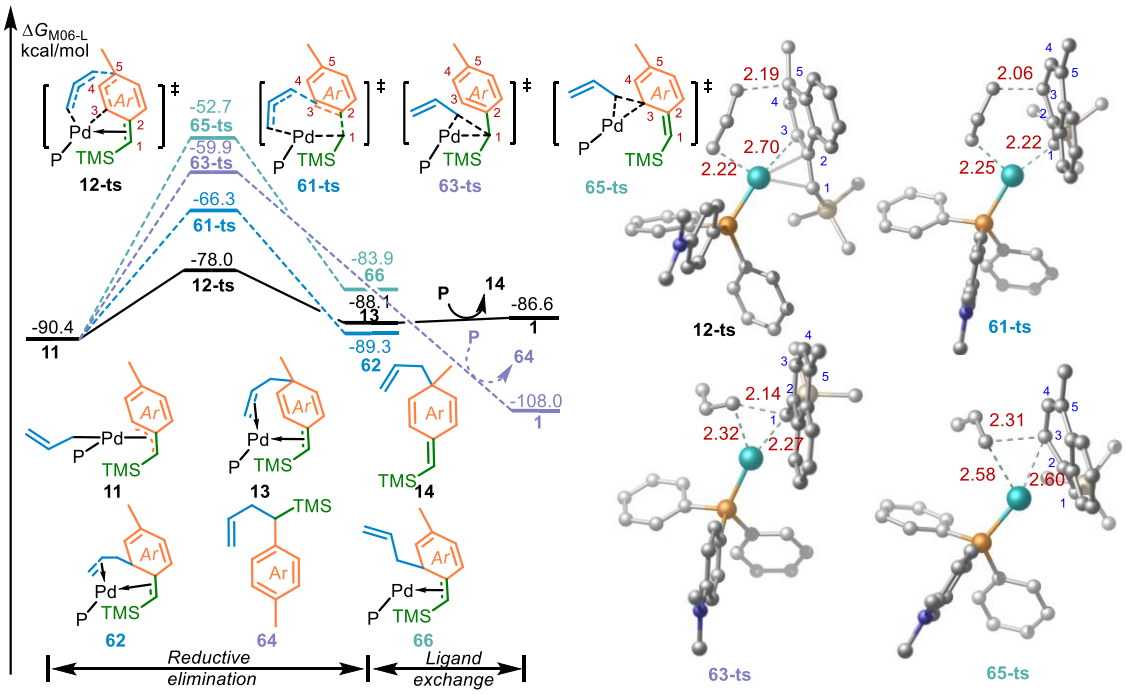

Fig S3. Free energy profiles for the dearomative product formation steps of Pd-catalysed dearomatization. Energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-L method in 1,4-dioxane. Bond lengths are in angstroms.

Having obtained key intermediate **11**, the possible pathways of reductive elimination for this intermediate was considered theoretically (Fig. S3). DFT calculations found that the free energy barrier of generate reductive elimination products via transition states **12-ts**, **61-ts**, **63-ts** and **65-ts** are 12.4, 24.1, 30.5 and 37.7 kcal/mol, respectively. As seen from all the structures, **12-ts** has four coordination sites, one more than that of **61-ts**, leading to the free energy of **12-ts** is 11.7 kcal/mol lower than **61-ts**. We also found that the three-membered-ring tension is usually stronger than the seven-membered-ring tension. Therefore, we proposed that the reductive elimination of seven-membered-ring transition states **12-ts** would be easier than that three-membered ring transition states **63-ts** and **65-ts**. The calculation supports this proposal. These pathways could also be excluded. Based on the mentioned above, these clearly showed that compound **13** was the kinetic product, which can be obtained from **11**. The final dearomative product **14** could be afford by ligand exchange and the active catalyst **1** could be regenerated.

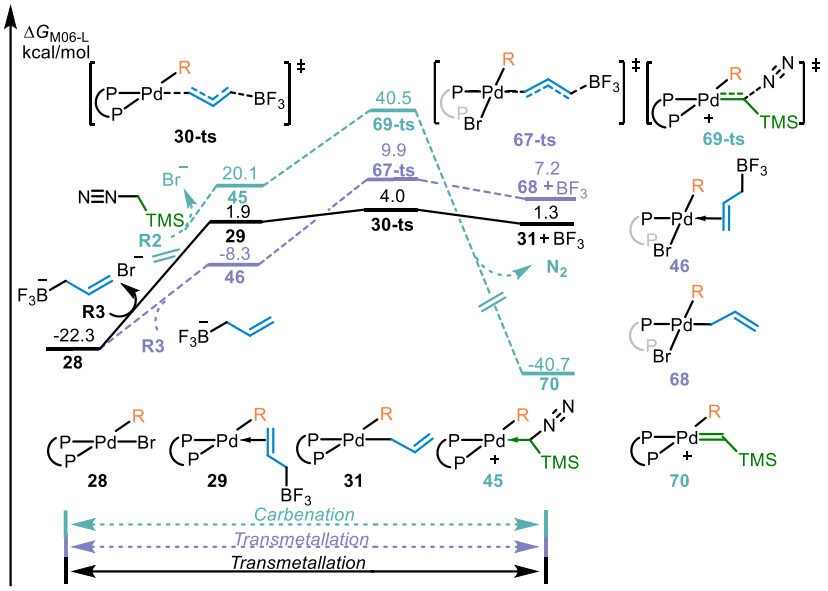

Fig S4. Free energy profiles of competitive Suzuki-Miyaura coupling with biphosphine ligand. Energies are in kcal/mol and represent the relative free energies, which were calculated using the M06-L method in 1,4-dioxane.

When arylpalladium(II) intermediate **28** is formed, the coordination of anionic allylborate **R3** gives Pd(II) intermediate **46** with an endothermic free energy of 14.0 kcal/mol owing to entropy loss. Subsequent transmetallation occurs with an endotherm of 18.2 kcal/mol to yield intermediate **68**. The relative free energy of transition state **67-ts** is 5.9 kcal/mol higher than that of path b, indicating that the transmetallation step without dissociating bromide anion is unfavorable. For the arylpalladium(II) intermediate **28**, the subsequent ligand exchange with TMS-diazomethane **R2** forms complex **45** with an endothermic energy of 42.4 kcal/mol. The calculated free energy barrier of carbenation via transition state **69-ts** is 62.8 kcal/mol, which is 36.5 kcal/mol higher than that of transmetallation via transition state **30-ts**, revealing that the carbenation step is unfavorable due to the higher ligand exchange energy.

3. Cartesian coordinates and energies of optimized structures

1

B3LYP SCF energy: -2467.17386564 a.u.
B3LYP enthalpy: -2466.433588 a.u.
B3LYP free energy: -2466.568845 a.u.
M06-L SCF energy in solution: -2468.78007925 a.u.
M06-L enthalpy in solution: -2468.039802 a.u.
M06-L free energy in solution: -2468.175059 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	2.024888	1.128519	-0.030832
C	2.280944	2.228274	-1.504498
C	1.169768	2.946495	-1.982344
C	3.507999	2.358297	-2.174047
C	1.288826	3.790532	-3.088446
H	0.202252	2.825776	-1.486119
C	3.623507	3.195738	-3.289533
H	4.379032	1.797823	-1.828037
C	2.517241	3.916383	-3.746913
H	0.415644	4.342863	-3.446000
H	4.584737	3.282434	-3.803538
H	2.608751	4.568431	-4.619696
C	3.532360	0.069420	0.006669
C	4.749452	0.443033	0.600278
C	3.469067	-1.202966	-0.588286
C	5.856793	-0.402622	0.593516
H	4.841736	1.415043	1.090902
C	4.567658	-2.056693	-0.612885
H	2.526416	-1.534875	-1.033829
C	5.800515	-1.679543	-0.020951
H	6.771924	-0.062089	1.076791
H	4.456993	-3.031491	-1.086605
C	2.297535	2.285001	1.395153
C	1.867184	1.860150	2.665189
C	2.896966	3.548970	1.273160
C	2.049222	2.670835	3.787373
H	1.374250	0.888716	2.764235
C	3.068836	4.365369	2.397095
H	3.228345	3.904741	0.295234
C	2.649667	3.928101	3.656093
H	1.710014	2.324372	4.767286
H	3.532816	5.349157	2.284845
H	2.783388	4.567736	4.532594
N	6.895339	-2.522569	-0.033898
C	8.124415	-2.125356	0.620238
H	7.985325	-1.944936	1.702980
H	8.871799	-2.921286	0.507552
H	8.550233	-1.202730	0.183992
C	6.797578	-3.829708	-0.649803
H	6.533802	-3.765237	-1.721400
H	7.766194	-4.340743	-0.576405
H	6.040142	-4.471397	-0.160977
P	-2.024501	-1.128432	0.031486
C	-2.296056	-2.287297	-1.392766
C	-2.896186	-3.550791	-1.269465
C	-1.863989	-1.864754	-2.663026
C	-3.067096	-4.368978	-2.392297
H	-3.228881	-3.904925	-0.291389
C	-2.045073	-2.677172	-3.784083
H	-1.370534	-0.893701	-2.763141
C	-2.646242	-3.933967	-3.651491
H	-3.531641	-5.352372	-2.278897
H	-1.704558	-2.332471	-4.764156
H	-2.779170	-4.574963	-4.527114
C	-3.531744	-0.069095	-0.009303
C	-4.748151	-0.443437	-0.603827
C	-3.469210	1.203810	0.584507
C	-5.855462	0.402240	-0.599385
H	-4.839922	-1.416135	-1.093131
C	-4.567809	2.057591	0.606859
H	-2.527266	1.536015	1.031265
C	-5.799604	1.680254	0.012886
H	-6.770166	0.061036	-1.083005
H	-4.457973	3.032593	1.080365
C	-2.282262	-2.225548	1.506866
C	-1.171715	-2.942723	1.987597
C	-3.510209	-2.354437	2.175009
C	-1.292216	-3.784739	3.095135
H	-0.203495	-2.822867	1.492555
C	-3.627226	-3.189836	3.291827
H	-4.380784	-1.794635	1.826825
C	-2.521511	-3.909556	3.752102
H	-0.419421	-4.336275	3.454897
H	-4.589173	-3.275694	3.804639
H	-2.614214	-4.560018	4.625959
N	-6.893751	2.524132	0.021983
C	-8.126381	2.120991	-0.621706
H	-8.552011	1.203750	-0.173579
H	-8.871949	2.919514	-0.515529
H	-7.991648	1.928378	-1.702722
C	-6.799387	3.828178	0.644878
H	-6.034389	4.468716	0.166930
H	-7.765215	4.342930	0.561378
H	-6.548089	3.759476	1.719455
Pd	0.000255	0.000096	0.000303

R1

B3LYP SCF energy: -2998.17335127 a.u.
B3LYP enthalpy: -2997.997347 a.u.
B3LYP free energy: -2998.044164 a.u.
M06-L SCF energy in solution: -2998.67215294 a.u.
M06-L enthalpy in solution: -2998.496149 a.u.
M06-L free energy in solution: -2998.542966 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.007501	2.776346	0.000002
C	-0.024126	1.861393	0.000003
C	0.231369	0.462211	0.000001
C	1.598815	0.004219	-0.000001
C	2.633291	0.983594	-0.000004
C	2.350359	2.333642	-0.000002
H	0.786056	3.846555	0.000003
H	-1.060016	2.202474	0.000005
C	-0.802063	-0.525245	0.000002
C	1.892255	-1.402125	-0.000003
H	3.673937	0.656435	-0.000007
H	3.164725	3.062618	-0.000004
C	0.839547	-2.297819	-0.000003
C	-0.508933	-1.869747	0.000000
H	1.045071	-3.371683	-0.000006
H	-1.313780	-2.606535	-0.000001
Br	-2.645651	-0.007666	0.000003
C	3.316832	-1.898179	-0.000009
H	3.872127	-1.547091	-0.885992
H	3.872127	-1.547109	0.885982
H	3.348468	-2.997102	-0.000020

2-ts

B3LYP SCF energy: -5465.31446759 a.u.
B3LYP enthalpy: -5464.398501 a.u.
B3LYP free energy: -5464.556728 a.u.
M06-L SCF energy in solution: -5467.45586166 a.u.
M06-L enthalpy in solution: -5466.539895 a.u.
M06-L free energy in solution: -5466.698122 a.u.
Imaginary frequency: -154.7186 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.276697	1.258473	0.189282
C	0.732274	2.726456	-0.820350
C	-0.563310	2.728155	-1.363298
C	1.571170	3.825359	-1.084056
C	-1.019674	3.806051	-2.128849
H	-1.214739	1.867579	-1.195537
C	1.116425	4.901398	-1.851522
H	2.592230	3.836004	-0.696600
C	-0.181415	4.896773	-2.373658
H	-2.031530	3.782732	-2.541674
H	1.782463	5.746427	-2.046570
H	-0.533448	5.737612	-2.977339
C	3.100741	1.275174	-0.118118
C	4.065734	1.465414	0.883166
C	3.569835	1.069274	-1.427558
C	5.430797	1.469245	0.596298
H	3.757608	1.621749	1.918413
C	4.925560	1.084835	-1.733710
H	2.857320	0.896874	-2.238132
C	5.902495	1.288927	-0.726195
H	6.130577	1.622043	1.417367
H	5.223913	0.918929	-2.767778
C	1.206776	1.883371	1.941654
C	1.167378	0.923409	2.968494
C	1.209390	3.242865	2.293401
C	1.145905	1.311660	4.310770
H	1.148671	-0.138103	2.707638
C	1.175492	3.631330	3.636885
H	1.233777	4.009657	1.517208
C	1.146686	2.668188	4.649293
H	1.118671	0.550515	5.095013
H	1.173253	4.694689	3.891946
H	1.119275	2.973619	5.698595
N	7.253679	1.308209	-1.023595
C	8.224556	1.482100	0.035165
H	8.184250	0.669353	0.786015
H	9.235179	1.492061	-0.393424
H	8.082152	2.435860	0.575976
C	7.701502	1.062312	-2.377944
H	7.300854	1.806975	-3.090347
H	8.796917	1.123493	-2.416843
H	7.405366	0.061291	-2.745121
P	-2.501451	-0.331967	0.788864
C	-3.146063	-1.951695	1.421934
C	-2.546568	-2.511431	2.566692
C	-4.140639	-2.686494	0.759181
C	-2.944764	-3.760468	3.044621
H	-1.762213	-1.959321	3.092363
C	-4.530140	-3.945613	1.231963
H	-4.616224	-2.275671	-0.133253
C	-3.938056	-4.485526	2.374990
H	-2.473131	-4.174321	3.940013
H	-5.303753	-4.505386	0.699371
H	-4.243803	-5.468367	2.742803

C	-3.689885	0.123478	-0.548052
C	-4.945388	0.709243	-0.308036
C	-3.338966	-0.116642	-1.888211
C	-5.812829	1.034449	-1.346931
H	-5.259781	0.924835	0.715576
C	-4.197435	0.195587	-2.939615
H	-2.368672	-0.565161	-2.116796
C	-5.466066	0.782017	-2.699637
H	-6.770560	1.490509	-1.098366
H	-3.869395	-0.017704	-3.956286
C	-2.986226	0.840859	2.145953
C	-2.419581	2.127165	2.136746
C	-3.902913	0.519744	3.162630
C	-2.766741	3.069560	3.107191
H	-1.695040	2.395838	1.366177
C	-4.243422	1.461254	4.139614
H	-4.358109	-0.471766	3.195929
C	-3.678814	2.739174	4.114191
H	-2.310592	4.062215	3.081561
H	-4.957198	1.191831	4.922950
H	-3.944585	3.473713	4.879021
N	-6.324057	1.096465	-3.734858
C	-7.607125	1.707204	-3.454956
H	-7.504280	2.681677	-2.942007
H	-8.141418	1.881778	-4.397673
H	-8.246940	1.065705	-2.820653
C	-5.940794	0.821099	-5.104397
H	-5.745714	-0.253896	-5.274490
H	-6.752874	1.123338	-5.778083
H	-5.030997	1.373619	-5.405278
Pd	-0.155419	-0.672768	-0.008495
C	3.637842	-2.208080	-3.123095
C	2.453239	-2.138737	-2.415319
C	2.403809	-2.419591	-1.026374
C	3.622346	-2.763004	-0.340966
C	4.826351	-2.796093	-1.099684
C	4.837562	-2.538365	-2.456639
H	3.644679	-2.007114	-4.197638
H	1.521714	-1.890275	-2.926032
C	1.174971	-2.407708	-0.270670
C	3.602240	-3.095957	1.059505
H	5.761363	-3.049378	-0.597413
H	5.776257	-2.594327	-3.014752
C	2.379176	-3.154014	1.702965
C	1.159990	-2.874838	1.042415
H	2.341988	-3.452316	2.755345
H	0.212487	-3.029851	1.560072
C	4.875540	-3.419974	1.798940
H	5.395215	-4.295335	1.371550
H	5.590194	-2.579323	1.770353
H	4.667102	-3.642978	2.855663
Br	-0.573115	-2.929094	-1.381199

3

B3LYP SCF energy: -5465.35747089 a.u.
B3LYP enthalpy: -5464.439103 a.u.
B3LYP free energy: -5464.594273 a.u.
M06-L SCF energy in solution: -5467.50296459 a.u.
M06-L enthalpy in solution: -5466.584597 a.u.
M06-L free energy in solution: -5466.739767 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.689021	-0.019424	1.049542
C	2.385197	1.472775	1.887790
C	1.530722	2.225668	2.713190
C	3.703142	1.914942	1.699876
C	1.993904	3.370275	3.364459
H	0.487505	1.926548	2.839233
C	4.162399	3.067778	2.344979
H	4.374671	1.370365	1.035415
C	3.314016	3.793574	3.184048
H	1.313499	3.943801	3.998512
H	5.190341	3.401747	2.181910
H	3.674884	4.695364	3.685197
C	3.065919	-0.830129	0.137861
C	4.243821	-1.246430	0.787328
C	2.938461	-1.144755	-1.225203
C	5.259088	-1.908789	0.107126
H	4.374371	-1.059925	1.856102
C	3.941441	-1.815833	-1.920293
H	2.026083	-0.864794	-1.759392
C	5.141710	-2.209186	-1.276535
H	6.148878	-2.202514	0.662552
H	3.780858	-2.031653	-2.975643
C	1.512462	-1.232226	2.456035
C	1.323812	-2.587118	2.128162
C	1.629539	-0.881568	3.810068
C	1.273911	-3.564193	3.121760
H	1.233720	-2.886442	1.081809
C	1.570136	-1.862356	4.807419
H	1.792065	0.156679	4.099606
C	1.398535	-3.204961	4.467976
H	1.131954	-4.610829	2.842943
H	1.672703	-1.568802	5.855582
H	1.361257	-3.970416	5.247339
N	6.146179	-2.861628	-1.958619
C	7.352765	-3.267790	-1.266407
H	7.146741	-3.983341	-0.448644

H	8.031891	-3.758097	-1.975399
H	7.890699	-2.407566	-0.827324
C	5.989511	-3.161073	-3.368390
H	5.841104	-2.247655	-3.972523
H	6.893415	-3.662229	-3.737260
H	5.130389	-3.830018	-3.561850
P	-1.821494	-1.267836	-0.235922
C	-1.841464	-2.474688	-1.635487
C	-0.652945	-3.167561	-1.925318
C	-2.969947	-2.703718	-2.435403
C	-0.603080	-4.090895	-2.971409
H	0.248741	-2.975504	-1.337372
C	-2.915799	-3.620978	-3.490155
H	-3.894056	-2.156061	-2.243482
C	-1.736869	-4.320688	-3.757890
H	0.328820	-4.622500	-3.181244
H	-3.801895	-3.783011	-4.109536
H	-1.696993	-5.035578	-4.583911
C	-3.502500	-0.507072	-0.174040
C	-4.625683	-1.255387	0.228918
C	-3.714427	0.846897	-0.485424
C	-5.895459	-0.693173	0.305432
H	-4.513514	-2.307781	0.498700
C	-4.977352	1.427031	-0.404163
H	-2.881342	1.462836	-0.823909
C	-6.110584	0.674216	-0.008291
H	-6.724097	-1.326157	0.620744
H	-5.073977	2.480969	-0.661598
C	-1.955525	-2.367030	1.258539
C	-2.005342	-1.740558	2.516934
C	-2.081488	-3.763064	1.197227
C	-2.199253	-2.486120	3.679423
H	-1.906366	-0.653695	2.584613
C	-2.269365	-4.512141	2.365646
H	-2.048960	-4.274273	0.233433
C	-2.335049	-3.877236	3.607285
H	-2.240487	-1.980268	4.647249
H	-2.374445	-5.598507	2.298328
H	-2.488291	-4.462318	4.517819
N	-7.364833	1.243724	0.073079
C	-8.501799	0.444578	0.480698
H	-8.376657	0.026930	1.497152
H	-9.403949	1.069739	0.486314
H	-8.685472	-0.403604	-0.205037
C	-7.548831	2.642503	-0.258420
H	-7.260185	2.865767	-1.301969
H	-8.606855	2.909182	-0.139383
H	-6.958144	3.308254	0.397697
Pd	-0.007889	0.443240	-0.534463
C	-1.134805	4.607874	0.931515
C	-0.640663	3.429204	0.411211
C	0.544383	3.387531	-0.378711
C	1.227197	4.632035	-0.637306
C	0.692918	5.828975	-0.077989
C	-0.455880	5.823823	0.687098
H	-2.051403	4.602047	1.527695
H	-1.167594	2.489991	0.596145
C	1.057648	2.160178	-0.919528
C	2.409458	4.641779	-1.450431
H	1.202434	6.776105	-0.264911
H	-0.844177	6.759923	1.097898
C	2.850121	3.440604	-1.970242
C	2.185008	2.215033	-1.712777
H	3.741670	3.427568	-2.605566
H	2.588992	1.312179	-2.171950
C	3.147419	5.925400	-1.741462
H	2.509793	6.659633	-2.263339
H	3.505562	6.414683	-0.819134
H	4.023902	5.736302	-2.378801
Br	-1.051164	0.864467	-2.789755

R2

B3LYP SCF energy: -557.15940111 a.u.
B3LYP enthalpy: -557.013600 a.u.
B3LYP free energy: -557.061434 a.u.
M06-L SCF energy in solution: -557.47275028 a.u.
M06-L enthalpy in solution: -557.326949 a.u.
M06-L free energy in solution: -557.374783 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	2.090866	-0.400558	-0.000009
N	3.095814	0.137420	0.000001
C	0.923802	-0.970952	-0.000026
H	0.964861	-2.065967	-0.000008
Si	-0.677820	0.014928	-0.000004
C	-1.681908	-0.428614	-1.539411
H	-1.900813	-1.508863	-1.573781
H	-2.646293	0.107215	-1.551244
H	-1.135175	-0.168067	-2.460070
C	-1.681754	-0.428444	1.539555
H	-1.900816	-1.508658	1.573995
H	-1.134812	-0.167963	2.460106
H	-2.646054	0.107532	1.551550
C	-0.227009	1.848691	-0.000117
H	0.361222	2.122930	-0.891203
H	-1.139530	2.467697	-0.000082
H	0.361356	2.123034	0.890846

P

B3LYP SCF energy: -1170.24765041 a.u.
B3LYP enthalpy: -1169.878489 a.u.
B3LYP free energy: -1169.951901 a.u.
M06-L SCF energy in solution: -1170.36735523 a.u.
M06-L enthalpy in solution: -1169.998194 a.u.
M06-L free energy in solution: -1170.071606 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.078593	-0.032449	-1.284923
C	1.837915	-1.448962	-0.357690
C	3.124438	-1.856149	-0.752972
C	1.195985	-2.163565	0.664619
C	3.760549	-2.928981	-0.129014
H	3.629450	-1.328401	-1.559210
C	1.827793	-3.246309	1.282097
H	0.197277	-1.874503	0.977245
C	3.111539	-3.629561	0.891014
H	4.757631	-3.224726	-0.445490
H	1.314395	-3.789788	2.071616
H	3.601119	-4.472299	1.372230
C	-0.669116	-0.019570	-0.701193
C	-1.117676	0.555237	0.498917
C	-1.640172	-0.605854	-1.529083
C	-2.459197	0.533607	0.865058
H	-0.407146	1.042413	1.161035
C	-2.984571	-0.645212	-1.175807
H	-1.339367	-1.038018	-2.481027
C	-3.431966	-0.083268	0.042687
H	-2.749080	1.004116	1.797255
H	-3.687624	-1.106740	-1.859012
C	1.796524	1.437045	-0.408053
C	1.671096	2.682883	-1.047133
C	2.473239	1.382146	0.820251
C	2.187553	3.841628	-0.467797
H	1.167120	2.742423	-2.009263
C	3.000782	2.541049	1.395950
H	2.592701	0.429988	1.328236
C	2.856992	3.773345	0.756581
H	2.077078	4.795865	-0.976774
H	3.523831	2.478768	2.347141
H	3.268813	4.673620	1.205288
N	-4.766943	-0.135748	0.417436
C	-5.216788	0.622573	1.572263
H	-5.063415	1.707636	1.457793
H	-6.282942	0.442775	1.724268
H	-4.694784	0.301914	2.482030
C	-5.759881	-0.600448	-0.535880
H	-5.550242	-1.629415	-0.852303
H	-6.742105	-0.596855	-0.059050
H	-5.813219	0.028377	-1.439094

4

B3LYP SCF energy: -4852.93493255 a.u.
B3LYP enthalpy: -4852.238407 a.u.
B3LYP free energy: -4852.371642 a.u.
M06-L SCF energy in solution: -4854.60340194 a.u.
M06-L enthalpy in solution: -4853.906876 a.u.
M06-L free energy in solution: -4854.040111 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.272250	1.491385	0.203222
C	-0.527516	2.190490	1.899580
C	0.551306	2.221558	2.800422
C	-1.767109	2.719465	2.301222
C	0.389271	2.770561	4.075344
H	1.524837	1.832105	2.492850
C	-1.923882	3.264697	3.579082
H	-2.616884	2.703933	1.616699
C	-0.847226	3.289834	4.469899
H	1.238410	2.790297	4.763334
H	-2.894247	3.669982	3.877782
H	-0.972096	3.713545	5.469943
C	-1.972339	1.121176	-0.389204
C	-2.478530	1.629483	-1.595946
C	-2.804815	0.255877	0.345123
C	-3.752372	1.297584	-2.053332
H	-1.873115	2.305116	-2.202371
C	-4.080319	-0.077160	-0.092580
H	-2.456681	-0.171948	1.286946
C	-4.595591	0.432871	-1.313161
H	-4.088317	1.724926	-2.997319
H	-4.675393	-0.750963	0.522212
C	0.223848	2.936241	-0.835885
C	0.897892	2.701059	-2.044645
C	-0.088636	4.255188	-0.473512
C	1.237964	3.763807	-2.884458
H	1.170732	1.681147	-2.321530
C	0.263032	5.318739	-1.310329
H	-0.601617	4.459539	0.468050
C	0.923264	5.075915	-2.517728
H	1.765167	3.566319	-3.821226
H	0.022025	6.342485	-1.012461
H	1.200283	5.909119	-3.168863

N	-5.860059	0.100863	-1.754981
C	-6.344860	0.616014	-3.018935
H	-5.717629	0.295439	-3.872069
H	-7.363732	0.248608	-3.196177
H	-6.380689	1.720886	-3.031261
C	-6.681475	-0.813349	-0.987654
H	-6.889787	-0.432129	0.028781
H	-7.645105	-0.950180	-1.494750
H	-6.212828	-1.809329	-0.878998
Pd	1.341629	-0.209705	0.159558
C	-0.915163	-2.590959	3.482532
C	-0.359996	-1.940390	2.399545
C	-0.658196	-2.320505	1.057345
C	-1.576611	-3.414940	0.849449
C	-2.126767	-4.065183	1.992515
C	-1.807392	-3.669094	3.275440
H	-0.667733	-2.273002	4.498627
H	0.325168	-1.103182	2.556423
C	-0.079854	-1.638258	-0.067770
C	-1.918330	-3.815218	-0.485550
H	-2.819220	-4.896877	1.850029
H	-2.245719	-4.187152	4.132653
C	-1.350687	-3.124110	-1.539456
C	-0.447170	-2.049810	-1.336815
H	-1.603978	-3.411333	-2.565046
H	-0.046499	-1.544164	-2.220193
C	-2.873131	-4.956167	-0.738649
H	-2.510916	-5.903274	-0.303187
H	-3.868586	-4.766919	-0.300852
H	-3.010880	-5.118657	-1.817758
Br	3.313362	1.457019	0.465098
C	2.977372	-1.750322	0.152687
N	2.563803	-2.929228	0.635044
N	2.166763	-3.917327	0.994478
Si	3.878619	-1.874786	-1.567198
C	5.700102	-1.552220	-1.209218
H	6.120201	-2.300861	-0.517888
H	6.292191	-1.577377	-2.139585
H	5.816773	-0.555445	-0.754031
C	3.603346	-3.633691	-2.203916
H	4.110666	-3.758060	-3.175321
H	4.009174	-4.397708	-1.520595
H	2.533382	-3.849614	-2.359142
C	3.231760	-0.629983	-2.818087
H	2.161664	-0.781408	-3.027566
H	3.376879	0.394350	-2.443830
H	3.785736	-0.743751	-3.765973
H	3.588160	-1.242832	0.916079

N_2

B3LYP SCF energy: -109.439222 a.u.
B3LYP enthalpy: -109.430243 a.u.
B3LYP free energy: -109.451988 a.u.
M06-L SCF energy in solution: -109.538382 a.u.
M06-L enthalpy in solution: -109.529403 a.u.
M06-L free energy in solution: -109.551148 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000000	0.000000	0.550198
N	0.000000	0.000000	-0.550198

5-ts

B3LYP SCF energy: -4852.90378773 a.u.
B3LYP enthalpy: -4852.209567 a.u.
B3LYP free energy: -4852.342115 a.u.
M06-L SCF energy in solution: -4854.56939371 a.u.
M06-L enthalpy in solution: -4853.875173 a.u.
M06-L free energy in solution: -4854.007721 a.u.
Imaginary frequency: -420.9980 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.328055	-1.482463	0.222989
C	0.587341	-2.184221	1.917277
C	-0.501028	-2.227941	2.806575
C	1.829491	-2.693294	2.334543
C	-0.346908	-2.773080	4.084076
H	-1.475297	-1.845794	2.491746
C	1.979274	-3.233852	3.615409
H	2.686472	-2.664920	1.659015
C	0.892500	-3.274201	4.493333
H	-1.202903	-2.802574	4.763164
H	2.951921	-3.623959	3.926823
H	1.011868	-3.694471	5.495481
C	2.027049	-1.132468	-0.385021
C	2.547613	-1.702102	-1.557875
C	2.845876	-0.220729	0.306961
C	3.822198	-1.383887	-2.023159
H	1.952944	-2.416118	-2.130267
C	4.122412	0.099365	-0.138811
H	2.486892	0.252785	1.222589
C	4.650167	-0.468977	-1.327494
H	4.170414	-1.860016	-2.938930
H	4.707944	0.808856	0.444147
C	-0.192357	-2.931354	-0.799440
C	-0.894887	-2.694511	-1.991952

C	0.117114	-4.252656	-0.441165
C	-1.265942	-3.757094	-2.819322
H	-1.164583	-1.672811	-2.266773
C	-0.264457	-5.315721	-1.265209
H	0.653069	-4.457831	0.487608
C	-0.953298	-5.070620	-2.456442
H	-1.814422	-3.557798	-3.743393
H	-0.024087	-6.340751	-0.970999
H	-1.253599	-5.903377	-3.097806
N	5.912897	-0.144796	-1.782074
C	6.432418	-0.764381	-2.983752
H	5.804586	-0.549121	-3.867950
H	7.438751	-0.376978	-3.188365
H	6.507406	-1.864338	-2.891187
C	6.739137	0.782283	-1.036041
H	6.970652	0.415543	-0.018259
H	7.690771	0.927371	-1.563277
H	6.260364	1.772808	-0.930441
Pd	-1.331930	0.254380	0.178424
C	0.987911	2.684694	3.426920
C	0.395715	2.033489	2.363919
C	0.682118	2.383125	1.011142
C	1.623212	3.451417	0.770113
C	2.213082	4.102097	1.893207
C	1.907329	3.733025	3.187579
H	0.748663	2.390406	4.452064
H	-0.313121	1.220855	2.543010
C	0.067131	1.698054	-0.092510
C	1.945514	3.827430	-0.577095
H	2.924952	4.912483	1.725404
H	2.376277	4.250489	4.028828
C	1.336894	3.138408	-1.609343
C	0.412340	2.089034	-1.374373
H	1.572827	3.408484	-2.643713
H	-0.024816	1.586700	-2.241961
C	2.922694	4.940868	-0.865227
H	2.594188	5.902524	-0.434675
H	3.922474	4.731898	-0.446609
H	3.041013	5.085932	-1.949119
Br	-3.372305	-1.332177	0.498976
C	-2.980703	1.457298	0.122284
N	-2.517826	3.239032	0.463626
N	-1.962821	4.149732	0.750865
Si	-4.079812	1.624840	-1.474678
C	-5.881796	1.304910	-1.013547
H	-6.242153	2.033868	-0.268700
H	-6.530359	1.383442	-1.902595
H	-5.995493	0.295980	-0.588359
C	-3.912789	3.383392	-2.166271
H	-4.475341	3.452757	-3.112765
H	-4.319386	4.148524	-1.485356
H	-2.863609	3.640067	-2.386282
C	-3.494957	0.426197	-2.805578
H	-2.442285	0.613798	-3.072414
H	-3.587248	-0.614278	-2.462467
H	-4.104623	0.554967	-3.716154
H	-3.555326	1.436728	1.058741

6

B3LYP SCF energy: -4743.50506858 a.u.
B3LYP enthalpy: -4742.820821 a.u.
B3LYP free energy: -4742.949762 a.u.
M06-L SCF energy in solution: -4745.05587305 a.u.
M06-L enthalpy in solution: -4744.371625 a.u.
M06-L free energy in solution: -4744.500566 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.713185	-1.446595	0.200745
C	1.000220	-2.173755	1.878216
C	-0.120498	-2.535781	2.646710
C	2.283710	-2.373666	2.411537
C	0.040479	-3.099803	3.914279
H	-1.126845	-2.371472	2.251332
C	2.442017	-2.932126	3.684387
H	3.164058	-2.087157	1.832384
C	1.322807	-3.297998	4.437035
H	-0.840187	-3.377278	4.499247
H	3.446904	-3.079646	4.088873
H	1.448618	-3.731769	5.432485
C	2.333333	-0.733830	-0.275236
C	3.201591	-1.327144	-1.205956
C	2.734792	0.486486	0.300369
C	4.418764	-0.740368	-1.545497
H	2.929723	-2.269733	-1.685463
C	3.951328	1.077361	-0.019277
H	2.082741	0.995780	1.013373
C	4.833492	0.481367	-0.958137
H	5.048934	-1.243477	-2.277791
H	4.206276	2.022740	0.457238
C	0.539996	-2.931490	-0.889965
C	-0.135480	-2.777078	-2.113606
C	1.050108	-4.195424	-0.550730
C	-0.283687	-3.858760	-2.985521
H	-0.556689	-1.803521	-2.378973
C	0.894466	-5.278458	-1.421398
H	1.568607	-4.338465	0.399672
C	0.230474	-5.112531	-2.640470
H	-0.812010	-3.722860	-3.932614

H	1.293085	-6.257633	-1.143262
H	0.107570	-5.961412	-3.318096
N	6.037715	1.069376	-1.287487
C	6.902221	0.451089	-2.271593
H	6.418569	0.367903	-3.263176
H	7.809678	1.056565	-2.391932
H	7.215697	-0.565365	-1.970057
C	6.416011	2.334166	-0.689606
H	6.489670	2.268308	0.411383
H	7.399352	2.637722	-1.071004
H	5.698300	3.141723	-0.926037
Pd	-1.310345	-0.133434	0.096192
C	-0.695911	3.148386	3.353916
C	-0.816152	2.273945	2.293287
C	-0.358771	2.606901	0.984645
C	0.249214	3.902355	0.787691
C	0.353269	4.780101	1.906343
C	-0.104430	4.418066	3.156920
H	-1.056999	2.861179	4.344938
H	-1.269694	1.290387	2.438093
C	-0.476491	1.693588	-0.118113
C	0.730827	4.275751	-0.512084
H	0.806872	5.763531	1.769890
H	-0.010050	5.112754	3.995986
C	0.599892	3.363993	-1.542537
C	0.004979	2.090794	-1.352873
H	0.966393	3.627916	-2.539745
H	-0.058117	1.419695	-2.213402
C	1.364053	5.624573	-0.752327
H	0.670498	6.452807	-0.526482
H	2.257890	5.780677	-0.123866
H	1.673719	5.729263	-1.802629
Br	-3.679271	-1.436751	0.357823
C	-3.237658	0.541623	0.080873
Si	-4.117988	1.254189	-1.442356
C	-5.990817	0.988319	-1.310879
H	-6.396798	1.453324	-0.397076
H	-6.511668	1.436545	-2.174261
H	-6.243931	-0.083819	-1.283207
C	-3.763118	3.111322	-1.466304
H	-4.290970	3.589471	-2.309032
H	-4.108569	3.595089	-0.537825
H	-2.686675	3.314654	-1.572736
C	-3.482436	0.429088	-3.019621
H	-2.400233	0.597146	-3.139241
H	-3.658840	-0.658601	-2.997012
H	-3.991690	0.835504	-3.909532
H	-3.538358	1.014027	1.028283

7-ts

B3LYP SCF energy: -4743.48472720 a.u.
B3LYP enthalpy: -4742.801606 a.u.
B3LYP free energy: -4742.930215 a.u.
M06-L SCF energy in solution: -4745.03459226 a.u.
M06-L enthalpy in solution: -4744.351471 a.u.
M06-L free energy in solution: -4744.480080 a.u.
Imaginary frequency: -387.1290 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.059394	-1.365807	0.105036
C	1.507523	-2.103734	1.744513
C	0.504546	-2.787388	2.455927
C	2.787717	-1.993360	2.310510
C	0.784259	-3.364313	3.696917
H	-0.503899	-2.861324	2.038909
C	3.062542	-2.565896	3.557288
H	3.573831	-1.452754	1.779175
C	2.064161	-3.254637	4.251162
H	-0.004844	-3.894094	4.236862
H	4.062946	-2.469831	3.987816
H	2.280444	-3.699683	5.225984
C	2.474816	-0.268328	-0.302979
C	3.608664	-0.685880	-1.019945
C	2.437716	1.069941	0.126974
C	4.663356	0.182991	-1.289381
H	3.676510	-1.712948	-1.385702
C	3.487187	1.947552	-0.124787
H	1.564513	1.439992	0.669111
C	4.636513	1.529249	-0.843985
H	5.513616	-0.194611	-1.856216
H	3.401244	2.972145	0.234504
C	1.257098	-2.782409	-1.070987
C	0.649893	-2.674604	-2.334829
C	1.969207	-3.951567	-0.759148
C	0.765392	-3.705156	-3.270263
H	0.073894	-1.778427	-2.581538
C	2.077949	-4.986294	-1.694529
H	2.437758	-4.060080	0.221237
C	1.479548	-4.864976	-2.951502
H	0.286441	-3.606622	-4.247873
H	2.631597	-5.892863	-1.436035
H	1.562499	-5.676033	-3.679685
N	5.679375	2.395726	-1.103965
C	6.834641	1.939402	-1.849082
H	6.570680	1.603011	-2.869287
H	7.554877	2.761926	-1.945063
H	7.350161	1.099711	-1.347082
C	5.613291	3.769535	-0.648982

H	5.529236	3.841924	0.451201
H	6.528163	4.296739	-0.948331
H	4.754088	4.314031	-1.083180
Pd	-1.158433	-0.466753	0.064070
C	-1.141499	2.816947	3.426153
C	-1.273115	1.985678	2.332082
C	-1.133688	2.472353	1.000800
C	-0.826629	3.868926	0.815824
C	-0.704825	4.698264	1.968439
C	-0.859319	4.190229	3.242119
H	-1.253120	2.412633	4.435404
H	-1.477706	0.921816	2.472566
C	-1.263400	1.605130	-0.144073
C	-0.634718	4.388246	-0.510060
H	-0.480110	5.758613	1.841741
H	-0.759238	4.848179	4.109309
C	-0.759770	3.522348	-1.582145
C	-1.088538	2.158705	-1.405811
H	-0.610116	3.902145	-2.597239
H	-1.193408	1.532917	-2.294125
C	-0.303806	5.841766	-0.737100
H	-1.091042	6.507436	-0.344289
H	0.635754	6.131855	-0.236666
H	-0.190900	6.055147	-1.809756
Br	-3.206141	-2.025388	0.602449
C	-2.981370	0.308335	0.026158
Si	-4.252363	0.486435	-1.398549
C	-5.920022	-0.234782	-0.870317
H	-6.256229	0.202184	0.084459
H	-6.684820	-0.004413	-1.632001
H	-5.870732	-1.325958	-0.742922
C	-4.546986	2.331811	-1.722189
H	-5.379030	2.449152	-2.437760
H	-4.831684	2.854009	-0.793673
H	-3.663499	2.840414	-2.133740
C	-3.636895	-0.379551	-2.959170
H	-2.700603	0.062548	-3.334573
H	-3.454199	-1.447030	-2.759401
H	-4.389280	-0.304904	-3.762154
H	-3.353029	0.691991	0.987372

8

B3LYP SCF energy: -4743.57306458 a.u.
B3LYP enthalpy: -4742.886474 a.u.
B3LYP free energy: -4743.011381 a.u.
M06-L SCF energy in solution: -4745.13169956 a.u.
M06-L enthalpy in solution: -4744.445109 a.u.
M06-L free energy in solution: -4744.570016 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.076058	-0.987977	0.054663
C	-1.838255	-2.289540	-1.009573
C	-0.999459	-3.134669	-1.753140
C	-3.229187	-2.465201	-1.088520
C	-1.539439	-4.154499	-2.540936
H	0.080975	-2.975936	-1.731594
C	-3.767797	-3.481250	-1.882963
H	-3.896922	-1.800502	-0.536465
C	-2.924635	-4.330029	-2.606816
H	-0.875137	-4.802204	-3.118470
H	-4.852336	-3.605046	-1.941368
H	-3.348071	-5.120633	-3.231832
C	-2.343492	0.333240	0.223568
C	-3.331052	0.300046	1.225894
C	-2.374091	1.411019	-0.680948
C	-4.303773	1.290240	1.327472
H	-3.349386	-0.512687	1.954548
C	-3.342271	2.405171	-0.590876
H	-1.632985	1.465247	-1.482427
C	-4.338753	2.378737	0.418417
H	-5.040225	1.210884	2.126252
H	-3.315866	3.214051	-1.319892
C	-1.082502	-1.745868	1.745721
C	-0.664299	-0.953724	2.831587
C	-1.472296	-3.071096	1.988882
C	-0.641629	-1.473857	4.126450
H	-0.370824	0.085560	2.661961
C	-1.443808	-3.593368	3.287722
H	-1.802767	-3.704332	1.163864
C	-1.029212	-2.799347	4.358556
H	-0.321792	-0.842164	4.959383
H	-1.750149	-4.628652	3.458728
H	-1.009544	-3.208252	5.372016
N	-5.296258	3.366707	0.514093
C	-6.293357	3.312772	1.563319
H	-5.841158	3.338210	2.572360
H	-6.962459	4.178294	1.476031
H	-6.915556	2.400619	1.502184
C	-5.300716	4.468577	-0.428024
H	-5.429693	4.124744	-1.470659
H	-6.133061	5.144423	-0.193491
H	-4.365912	5.057570	-0.386421
Pd	0.975798	-0.205261	-0.743258
C	2.510581	3.290380	2.998102
C	2.528615	2.062157	2.356692
C	2.783027	1.954022	0.969547
C	3.051182	3.146781	0.222864
C	3.021476	4.389637	0.907002

C	2.754454	4.465247	2.263765
H	2.312977	3.344232	4.071604
H	2.355889	1.155610	2.938364
C	2.815763	0.653039	0.298134
C	3.349301	3.076654	-1.195786
H	3.216220	5.308635	0.352916
H	2.739993	5.437123	2.763749
C	3.397760	1.846863	-1.799419
C	3.148010	0.638256	-1.082996
H	3.628382	1.773322	-2.864341
H	3.381880	-0.304412	-1.577426
C	3.610870	4.331507	-1.987814
H	2.742073	5.011217	-1.969907
H	4.470223	4.898123	-1.590513
H	3.822803	4.090764	-3.039001
Br	0.147041	0.305507	-3.083701
C	2.316569	-0.580872	0.869645
Si	3.219511	-2.257340	0.782024
C	2.081256	-3.626950	1.408646
H	1.241083	-3.807704	0.720464
H	2.648112	-4.568820	1.501917
H	1.656443	-3.390087	2.396794
C	3.861679	-2.753002	-0.930521
H	3.066459	-2.755438	-1.693191
H	4.673091	-2.096869	-1.283417
H	4.272714	-3.775395	-0.873164
C	4.708412	-2.127383	1.953332
H	4.394247	-1.883816	2.981843
H	5.262338	-3.081018	1.989545
H	5.408700	-1.342665	1.622672
H	1.874015	-0.469419	1.866926

R3

B3LYP SCF energy: -441.59592593 a.u.
B3LYP enthalpy: -441.506240 a.u.
B3LYP free energy: -441.547106 a.u.
M06-L SCF energy in solution: -442.04479149 a.u.
M06-L enthalpy in solution: -441.955106 a.u.
M06-L free energy in solution: -441.995972 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.701448	0.341919	-0.272528
H	1.594131	1.436765	-0.246276
C	2.843598	-0.180869	0.203842
H	3.011283	-1.264852	0.224306
H	3.639792	0.448876	0.617538
C	0.508268	-0.374092	-0.792426
H	0.683076	-1.465815	-0.820381
H	0.311818	-0.043675	-1.832562
B	-0.887891	-0.024177	0.033294
F	-1.982651	-0.637303	-0.622471
F	-0.832584	-0.489732	1.364298
F	-1.087046	1.381240	0.042348

Br^-

B3LYP SCF energy: -2573.92676920 a.u.
B3LYP enthalpy: -2573.924409 a.u.
B3LYP free energy: -2573.942945 a.u.
M06-L SCF energy in solution: -2574.14191875 a.u.
M06-L enthalpy in solution: -2574.139559 a.u.
M06-L free energy in solution: -2574.158095 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Br	0.000000	0.000000	0.000000

9

B3LYP SCF energy: -2611.17902488 a.u.
B3LYP enthalpy: -2610.402994 a.u.
B3LYP free energy: -2610.544078 a.u.
M06-L SCF energy in solution: -2613.00978316 a.u.
M06-L enthalpy in solution: -2612.233752 a.u.
M06-L free energy in solution: -2612.374836 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.087905	0.312276	0.966224
C	1.632723	2.066388	1.113998
C	0.845902	2.953751	1.873136
C	2.736230	2.572807	0.409706
C	1.172653	4.308457	1.946466
H	-0.037427	2.588119	2.402692
C	3.051317	3.934536	0.473040
H	3.347285	1.910224	-0.205114
C	2.276226	4.803379	1.243226
H	0.550921	4.984333	2.538644
H	3.902260	4.316817	-0.095560
H	2.519508	5.867719	1.282489
C	2.413066	-0.583489	0.072842
C	3.714064	-0.676820	0.604878
C	2.163756	-1.242161	-1.142306
C	4.723917	-1.366051	-0.054095

H	3.949987	-0.202188	1.560805
C	3.162420	-1.941858	-1.812644
H	1.162476	-1.212995	-1.575446
C	4.480112	-2.018506	-1.293380
H	5.711931	-1.399653	0.403165
H	2.908023	-2.431983	-2.751200
C	1.267067	-0.391406	2.673312
C	0.954647	-1.752350	2.846882
C	1.732756	0.340264	3.776133
C	1.098009	-2.363235	4.093039
H	0.610911	-2.343093	1.993682
C	1.870290	-0.273486	5.027462
H	1.997064	1.393007	3.666319
C	1.552366	-1.622716	5.190883
H	0.855905	-3.422925	4.208787
H	2.233464	0.311457	5.876406
H	1.661278	-2.099411	6.168281
N	5.477109	-2.698021	-1.955258
C	6.814348	-2.757229	-1.397544
H	6.830599	-3.245666	-0.406081
H	7.461782	-3.338617	-2.065826
H	7.264093	-1.753802	-1.283290
C	5.199308	-3.338563	-3.226624
H	4.852440	-2.616671	-3.988192
H	6.115190	-3.809645	-3.604857
H	4.428356	-4.125669	-3.136651
Pd	-0.984690	0.179939	-0.111726
C	-2.060792	-4.991509	-0.267922
C	-2.182043	-3.713664	0.255225
C	-2.582037	-2.619352	-0.545835
C	-2.889577	-2.852821	-1.925616
C	-2.751330	-4.170443	-2.433231
C	-2.343259	-5.219808	-1.626567
H	-1.752087	-5.818756	0.375885
H	-1.976595	-3.552014	1.314144
C	-2.723516	-1.271371	0.017544
C	-3.345564	-1.767249	-2.776291
H	-2.976109	-4.364288	-3.482590
H	-2.248919	-6.225056	-2.044986
C	-3.488564	-0.518640	-2.228096
C	-3.179501	-0.245890	-0.859798
H	-3.859362	0.301963	-2.847820
H	-3.503644	0.709577	-0.444470
C	-3.675750	-2.013152	-4.225778
H	-2.801565	-2.386840	-4.785321
H	-4.475494	-2.763885	-4.342872
H	-4.010734	-1.086625	-4.712749
C	-2.244729	-0.872965	1.317616
Si	-3.172846	0.277435	2.520160
C	-2.198341	0.331554	4.138291
H	-1.203826	0.787131	4.014725
H	-2.748282	0.918834	4.892694
H	-2.045938	-0.679950	4.548834
C	-3.443161	2.048330	1.900536
H	-2.517368	2.508797	1.520451
H	-4.197146	2.103613	1.098580
H	-3.814704	2.671077	2.732042
C	-4.870267	-0.497822	2.861910
H	-4.771468	-1.517805	3.268529
H	-5.436387	0.103024	3.593956
H	-5.472689	-0.561320	1.940906
H	-1.734249	-1.663665	1.878429
C	-1.070916	2.232545	-1.908605
H	-2.054481	2.043675	-2.355803
C	-0.155013	1.166114	-1.936198
H	0.897909	1.426528	-1.795427
H	-0.336945	0.377639	-2.676484
C	-0.825831	3.562727	-1.496277
H	0.058075	3.731245	-0.871079
H	-1.705035	4.141012	-1.186971
B	-0.381312	4.403119	-3.033399
F	0.777257	3.808547	-3.497129
F	-1.443191	4.258705	-3.908993
F	-0.185297	5.712981	-2.647208

10-ts

B3LYP SCF energy: -2611.17634012 a.u.
B3LYP enthalpy: -2610.401670 a.u.
B3LYP free energy: -2610.544124 a.u.
M06-L SCF energy in solution: -2612.99210217 a.u.
M06-L enthalpy in solution: -2612.217432 a.u.
M06-L free energy in solution: -2612.359886 a.u.
Imaginary frequency: -73.2361 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.983310	-0.017693	1.115816
C	1.752061	1.577168	1.641655
C	1.005884	2.440073	2.466402
C	3.007634	2.001699	1.179979
C	1.516981	3.682795	2.843749
H	0.012605	2.143002	2.812083
C	3.511524	3.254504	1.548004
H	3.595239	1.359626	0.521809
C	2.772730	4.094557	2.383799
H	0.925439	4.338793	3.487289
H	4.486875	3.574022	1.172511
H	3.167935	5.073025	2.667952
C	2.263472	-0.921286	0.161260

C	3.461878	-1.352866	0.761815
C	2.062954	-1.251070	-1.189218
C	4.424212	-2.056641	0.047963
H	3.652053	-1.142337	1.817325
C	3.014001	-1.959884	-1.917254
H	1.136178	-0.951923	-1.681833
C	4.230632	-2.379869	-1.322058
H	5.332388	-2.363753	0.564974
H	2.801006	-2.188358	-2.960478
C	0.916600	-1.027819	2.671315
C	0.361829	-2.317377	2.579690
C	1.414302	-0.593308	3.909104
C	0.305427	-3.149562	3.698021
H	-0.022051	-2.673780	1.620258
C	1.349273	-1.427141	5.032491
H	1.858869	0.398553	4.005605
C	0.795191	-2.704241	4.931772
H	-0.124467	-4.150615	3.607971
H	1.738882	-1.071886	5.990105
H	0.745561	-3.353489	5.809604
N	5.180218	-3.076885	-2.036653
C	6.407862	-3.503386	-1.394843
H	6.221003	-4.188631	-0.547338
H	7.033173	-4.035804	-2.122596
H	6.995157	-2.649768	-1.009333
C	4.948465	-3.397280	-3.431648
H	4.807826	-2.490874	-4.048233
H	5.815020	-3.940421	-3.829346
H	4.056947	-4.036274	-3.570939
Pd	-0.976159	0.327117	-0.073039
C	-2.782184	-4.492038	-1.268926
C	-2.786656	-3.318657	-0.530282
C	-2.901139	-2.051395	-1.146199
C	-3.048573	-1.992107	-2.570624
C	-3.035173	-3.209163	-3.300108
C	-2.900640	-4.434818	-2.668656
H	-2.693075	-5.456551	-0.762800
H	-2.712408	-3.375998	0.556330
C	-2.913642	-0.813969	-0.349965
C	-3.224312	-0.718160	-3.245378
H	-3.137697	-3.180975	-4.385642
H	-2.896127	-5.355231	-3.258347
C	-3.252823	0.423132	-2.487664
C	-3.084799	0.409049	-1.067703
H	-3.413990	1.387687	-2.977181
H	-3.325121	1.321802	-0.519817
C	-3.393906	-0.657315	-4.741858
H	-2.521196	-1.075998	-5.271770
H	-4.275813	-1.227920	-5.080152
H	-3.518587	0.381914	-5.078157
C	-2.570568	-0.743238	1.044202
Si	-3.420416	0.332327	2.350726
C	-2.586570	-0.007915	4.014980
H	-1.527676	0.294970	4.019722
H	-3.100279	0.542140	4.821322
H	-2.619581	-1.080127	4.268887
C	-3.380041	2.201354	2.023513
H	-2.370235	2.561508	1.769523
H	-4.055030	2.495762	1.203301
H	-3.717402	2.738925	2.926155
C	-5.241444	-0.192354	2.477566
H	-5.333473	-1.262304	2.727496
H	-5.767606	0.382716	3.258815
H	-5.769744	-0.026851	1.524017
H	-2.273139	-1.698943	1.490702
C	-0.584064	2.852173	-1.446409
H	-1.560793	2.934311	-1.941671
C	0.064239	1.552486	-1.523469
H	1.144044	1.607327	-1.338185
H	-0.143157	1.026404	-2.467721
C	-0.104579	3.983371	-0.853735
H	0.833725	3.974706	-0.291606
H	-0.732963	4.872314	-0.757210
B	0.936470	4.776716	-2.838875
F	1.864601	3.832875	-2.991599
F	-0.094371	4.801044	-3.685165
F	1.293224	5.920784	-2.250762

11

B3LYP SCF energy: -2286.85361043 a.u.
B3LYP enthalpy: -2286.096746 a.u.
B3LYP free energy: -2286.226345 a.u.
M06-L SCF energy in solution: -2288.36782399 a.u.
M06-L enthalpy in solution: -2287.610960 a.u.
M06-L free energy in solution: -2287.740559 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.037629	-1.005684	0.018353
C	-1.662512	-2.396563	-1.025436
C	-0.796578	-3.479603	-1.262920
C	-2.933046	-2.403109	-1.621682
C	-1.204809	-4.558876	-2.048662
H	0.210111	-3.473356	-0.837659
C	-3.334637	-3.478700	-2.421698
H	-3.613552	-1.563967	-1.468419
C	-2.476725	-4.561236	-2.631063
H	-0.520150	-5.393252	-2.220191
H	-4.325373	-3.466836	-2.883531

H	-2.793370	-5.400855	-3.255184
C	-2.363508	0.264795	0.037918
C	-3.603445	0.035422	0.664103
C	-2.157940	1.527595	-0.542140
C	-4.599310	1.005216	0.691230
H	-3.799526	-0.921707	1.153979
C	-3.143385	2.510471	-0.521799
H	-1.197674	1.750660	-1.010805
C	-4.400591	2.277116	0.090907
H	-5.537799	0.771114	1.192203
H	-2.923138	3.471879	-0.983607
C	-1.157984	-1.672963	1.747113
C	-0.836399	-0.799250	2.802171
C	-1.557035	-2.982505	2.053510
C	-0.915196	-1.224408	4.128468
H	-0.528521	0.225793	2.580019
C	-1.628119	-3.409844	3.385595
H	-1.818415	-3.678720	1.254923
C	-1.308609	-2.535108	4.425135
H	-0.666766	-0.530592	4.935950
H	-1.939324	-4.434280	3.606478
H	-1.365552	-2.870232	5.463930
N	-5.383875	3.243271	0.112069
C	-6.650574	2.978953	0.764267
H	-6.531562	2.770467	1.843953
H	-7.302135	3.856248	0.663731
H	-7.177907	2.117101	0.315708
C	-5.143838	4.537311	-0.495451
H	-4.922388	4.454659	-1.575253
H	-6.038729	5.162868	-0.385319
H	-4.298909	5.071717	-0.022908
Pd	0.997143	-0.181867	-0.699187
C	2.048159	3.869261	2.515822
C	2.219083	2.566453	2.072932
C	2.556978	2.272128	0.732293
C	2.755120	3.361400	-0.178824
C	2.568042	4.683671	0.302071
C	2.218086	4.937776	1.618086
H	1.787841	4.062691	3.559545
H	2.100336	1.745975	2.781417
C	2.744997	0.882906	0.279801
C	3.152315	3.115939	-1.552997
H	2.707555	5.523148	-0.380511
H	2.083726	5.968047	1.958179
C	3.336330	1.818439	-1.954920
C	3.126132	0.704600	-1.085585
H	3.659212	1.615674	-2.980073
H	3.483079	-0.271744	-1.417052
C	3.373690	4.261254	-2.508019
H	2.461812	4.868364	-2.642956
H	4.162724	4.947915	-2.155559
H	3.673601	3.889439	-3.498493
C	2.393581	-0.275715	1.052674
Si	3.365087	-1.892388	1.147994
C	2.450424	-3.058996	2.325404
H	1.464817	-3.356835	1.934631
H	3.040352	-3.976079	2.492199
H	2.283075	-2.586407	3.307320
C	3.638697	-2.794913	-0.501328
H	2.707073	-2.920855	-1.075987
H	4.359647	-2.269710	-1.149201
H	4.055213	-3.797628	-0.303687
C	5.081232	-1.538908	1.886090
H	4.999963	-1.074237	2.882783
H	5.669023	-2.466870	1.993288
H	5.654186	-0.849310	1.244107
H	1.948475	-0.056912	2.030053
C	1.042567	-0.696525	-3.592780
H	2.066983	-0.340055	-3.769501
C	0.228290	0.125236	-2.679658
H	-0.843988	-0.098252	-2.772803
H	0.394935	1.204076	-2.834405
C	0.674523	-1.835689	-4.214394
H	-0.329387	-2.255511	-4.096273
H	1.368155	-2.380155	-4.861546

BF_3

B3LYP SCF energy: -324.31363415 a.u.
B3LYP enthalpy: -324.296638 a.u.
B3LYP free energy: -324.326187 a.u.
M06-L SCF energy in solution: -324.61115257 a.u.
M06-L enthalpy in solution: -324.594156 a.u.
M06-L free energy in solution: -324.623705 a.u.

Cartesian coordinates

ATOM	X	Y	Z
F	0.000000	1.313675	-0.000016
F	-1.137676	-0.656838	-0.000016
F	1.137676	-0.656838	-0.000016
B	0.000000	0.000000	0.000085

F^-

B3LYP SCF energy: -99.68883403 a.u.
B3LYP enthalpy: -99.686474 a.u.
B3LYP free energy: -99.702993 a.u.
M06-L SCF energy in solution: -99.93940380 a.u.

M06-L enthalpy in solution: -99.937044 a.u.
M06-L free energy in solution: -99.953563 a.u.

Cartesian coordinates

ATOM	X	Y	Z
F	0.000000	0.000000	0.000000

BF_4^-

B3LYP SCF energy: -424.19568766 a.u.
B3LYP enthalpy: -424.175822 a.u.
B3LYP free energy: -424.207666 a.u.
M06-L SCF energy in solution: -424.65298671 a.u.
M06-L enthalpy in solution: -424.633121 a.u.
M06-L free energy in solution: -424.664965 a.u.

Cartesian coordinates

ATOM	X	Y	Z
B	0.000000	0.000000	0.000261
F	0.000000	1.327013	-0.469301
F	1.149227	-0.663507	-0.469301
F	-1.149227	-0.663507	-0.469301
F	0.000000	0.000000	1.407757

12-ts

B3LYP SCF energy: -2286.83565573 a.u.
B3LYP enthalpy: -2286.079694 a.u.
B3LYP free energy: -2286.207820 a.u.
M06-L SCF energy in solution: -2288.34864925 a.u.
M06-L enthalpy in solution: -2287.592688 a.u.
M06-L free energy in solution: -2287.720814 a.u.
Imaginary frequency: -367.4103 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.356375	-0.762382	0.368079
C	1.957287	-1.409613	2.001162
C	1.196953	-2.421279	2.622069
C	3.086255	-0.910101	2.673170
C	1.573683	-2.938342	3.864190
H	0.295080	-2.799917	2.128640
C	3.452916	-1.419651	3.925034
H	3.680866	-0.110400	2.224108
C	2.703518	-2.436848	4.520666
H	0.973998	-3.727495	4.326264
H	4.330460	-1.013459	4.435827
H	2.992000	-2.832835	5.497710
C	2.453683	0.663598	-0.030928
C	3.822121	0.514068	-0.345352
C	1.928162	1.970813	-0.079970
C	4.625107	1.603927	-0.661991
H	4.272689	-0.483868	-0.353358
C	2.721053	3.071103	-0.396545
H	0.861718	2.125674	0.116987
C	4.099511	2.921572	-0.688859
H	5.671939	1.422712	-0.895744
H	2.249825	4.052632	-0.428316
C	1.999037	-2.024521	-0.837656
C	1.881865	-1.733956	-2.212484
C	2.602137	-3.238498	-0.457925
C	2.365376	-2.621567	-3.173747
H	1.410529	-0.797398	-2.528802
C	3.076347	-4.131741	-1.427793
H	2.712082	-3.488867	0.601460
C	2.963241	-3.825467	-2.784722
H	2.270379	-2.374047	-4.233520
H	3.542575	-5.069222	-1.111958
H	3.338006	-4.521661	-3.538316
N	4.890013	4.004337	-0.996526
C	6.268829	3.812277	-1.388499
H	6.365716	3.160024	-2.275078
H	6.715432	4.781973	-1.639515
H	6.875744	3.364298	-0.581466
C	4.321840	5.335028	-1.015339
H	3.832757	5.585567	-0.058059
H	5.119023	6.070335	-1.179261
H	3.568966	5.467017	-1.815439
Pd	-0.911498	-0.189789	0.441429
C	-3.085151	3.230383	-2.505503
C	-2.782602	1.918560	-2.165844
C	-3.185919	1.354717	-0.934246
C	-3.936667	2.163885	-0.029249
C	-4.235255	3.495160	-0.400291
C	-3.818557	4.028314	-1.612616
H	-2.763316	3.633197	-3.470334
H	-2.232107	1.300971	-2.877318
C	-2.896952	-0.058132	-0.603076
C	-4.369725	1.622091	1.264648
H	-4.810015	4.124118	0.280356
H	-4.070360	5.060119	-1.872748
C	-4.320714	0.208695	1.397730
C	-3.580178	-0.579766	0.553582
H	-4.811338	-0.249230	2.260008
H	-3.525427	-1.651068	0.747701
C	-5.464551	2.336430	2.032754
H	-5.242613	3.394573	2.228650
H	-6.415719	2.298025	1.475368

H	-5.630592	1.851617	3.005845
C	-2.048822	-0.909747	-1.370359
Si	-2.340052	-2.761175	-1.623173
C	-1.633409	-3.874796	-0.257765
H	-2.147502	-3.723468	0.706265
H	-1.743727	-4.938429	-0.531965
H	-0.559812	-3.673740	-0.105895
C	-4.197706	-3.134286	-1.778228
H	-4.740799	-2.989946	-0.831945
H	-4.664835	-2.477318	-2.529796
H	-4.355848	-4.178337	-2.098987
C	-1.537243	-3.249384	-3.269893
H	-0.450995	-3.065435	-3.263037
H	-1.694306	-4.321681	-3.477019
H	-1.975394	-2.679627	-4.106923
H	-1.599534	-0.450944	-2.259222
C	-0.557965	0.861487	2.364601
H	-0.863624	0.149799	3.144341
H	0.517099	1.070493	2.370707
C	-1.410942	1.962662	2.107609
H	-0.995014	2.763114	1.479640
C	-2.712688	2.172187	2.584903
H	-3.068241	3.203188	2.591753
H	-3.065076	1.555503	3.416135

13

B3LYP SCF energy: -2286.86010837 a.u.
B3LYP enthalpy: -2286.101737 a.u.
B3LYP free energy: -2286.226401 a.u.
M06-L SCF energy in solution: -2288.37069266 a.u.
M06-L enthalpy in solution: -2287.612321 a.u.
M06-L free energy in solution: -2287.736985 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.388944	-0.718108	0.363857
C	1.835775	-1.310694	2.066270
C	0.993303	-2.274877	2.652981
C	2.908286	-0.811533	2.821640
C	1.237466	-2.750004	3.943402
H	0.128754	-2.647609	2.096928
C	3.143191	-1.277365	4.120695
H	3.563042	-0.045066	2.404512
C	2.315254	-2.251250	4.683107
H	0.575011	-3.503645	4.377263
H	3.980270	-0.871566	4.695140
H	2.501788	-2.614286	5.697114
C	2.537659	0.674187	-0.007011
C	3.934733	0.516012	-0.089042
C	2.023333	1.951407	-0.285690
C	4.776760	1.578479	-0.398507
H	4.383034	-0.466498	0.078700
C	2.849823	3.027016	-0.601782
H	0.941057	2.103998	-0.273883
C	4.258011	2.875204	-0.657978
H	5.849176	1.393469	-0.448127
H	2.387706	3.990034	-0.814622
C	2.119086	-2.039285	-0.727435
C	2.316777	-1.735477	-2.087573
C	2.455837	-3.325009	-0.274457
C	2.848439	-2.683510	-2.963259
H	2.060828	-0.741934	-2.464779
C	2.979277	-4.278224	-1.156289
H	2.324486	-3.590012	0.775961
C	3.181409	-3.961667	-2.500983
H	2.999856	-2.423628	-4.014260
H	3.237053	-5.272540	-0.781886
H	3.595805	-4.705069	-3.186689
N	5.087191	3.934341	-0.962313
C	6.520247	3.736513	-1.047344
H	6.799751	3.012995	-1.836153
H	7.006344	4.691894	-1.282467
H	6.946047	3.370540	-0.095301
C	4.521926	5.235364	-1.259693
H	3.928748	5.631797	-0.415723
H	5.332239	5.947640	-1.460583
H	3.862708	5.214495	-2.147757
Pd	-0.911107	-0.023985	0.351733
C	-3.547643	3.207558	-2.465342
C	-3.100847	1.919751	-2.171447
C	-3.338414	1.326291	-0.917992
C	-4.066950	2.059980	0.055872
C	-4.516104	3.350089	-0.260262
C	-4.260978	3.929280	-1.505842
H	-3.349861	3.640473	-3.449681
H	-2.569936	1.353618	-2.938669
C	-2.908056	-0.073590	-0.611456
C	-4.275783	1.446641	1.441209
H	-5.075753	3.924417	0.479657
H	-4.624813	4.936476	-1.725111
C	-4.433712	-0.048171	1.316770
C	-3.740076	-0.744992	0.402838
H	-5.039706	-0.561656	2.069885
H	-3.777598	-1.836351	0.406304
C	-5.493485	2.021349	2.185653
H	-5.391314	3.097283	2.392194
H	-6.419672	1.865827	1.610993
H	-5.608977	1.515182	3.157808
C	-2.017711	-0.823419	-1.421207

Si	-2.138324	-2.676233	-1.790957
C	-1.622151	-3.824211	-0.371934
H	-2.155595	-3.598078	0.565011
H	-1.836172	-4.874134	-0.635648
H	-0.541291	-3.743040	-0.176506
C	-3.920432	-3.114683	-2.294049
H	-4.645457	-2.973056	-1.477088
H	-4.250713	-2.487525	-3.138918
H	-3.980146	-4.168681	-2.616003
C	-1.047122	-3.037357	-3.294290
H	0.015160	-2.840923	-3.086597
H	-1.141158	-4.094388	-3.595245
H	-1.346696	-2.418036	-4.156631
H	-1.582628	-0.277054	-2.267884
C	-0.502786	1.145235	2.245381
H	-0.589114	0.480420	3.111213
H	0.487541	1.572652	2.079372
C	-1.630072	1.743208	1.710011
H	-1.481313	2.560055	0.993577
C	-2.992618	1.712056	2.342006
H	-3.138463	2.715060	2.783869
H	-3.006989	0.996459	3.180933

14

B3LYP SCF energy: -989.28419425 a.u.
B3LYP enthalpy: -988.897687 a.u.
B3LYP free energy: -988.971418 a.u.
M06-L SCF energy in solution: -989.94386482 a.u.
M06-L enthalpy in solution: -989.557358 a.u.
M06-L free energy in solution: -989.631089 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.093445	3.663291	-0.358394
C	0.081112	2.720015	-0.226060
C	0.354293	1.358381	0.021116
C	1.706056	0.956544	0.169541
C	2.716268	1.924800	0.024375
C	2.427236	3.260963	-0.239777
H	0.843474	4.710392	-0.547102
H	-0.955751	3.050150	-0.302000
C	-0.757241	0.369855	0.147050
C	2.108536	-0.496798	0.453627
H	3.762147	1.627352	0.122961
H	3.238241	3.986380	-0.342966
C	0.907096	-1.333713	0.813329
C	-0.368188	-0.942789	0.667499
H	1.114137	-2.335054	1.202825
H	-1.166553	-1.639371	0.932152
C	3.113895	-0.576999	1.627214
H	4.059539	-0.064262	1.396598
H	2.687674	-0.121067	2.533611
H	3.359948	-1.626927	1.848802
C	-2.048573	0.637012	-0.196178
Si	-3.590096	-0.448538	-0.092403
C	-3.438595	-2.000093	-1.172377
H	-2.618773	-2.659439	-0.845817
H	-4.373484	-2.585089	-1.138299
H	-3.248103	-1.729894	-2.224106
C	-3.976208	-0.959925	1.692675
H	-3.186171	-1.589130	2.132535
H	-4.092377	-0.074332	2.338829
H	-4.918779	-1.532158	1.731649
C	-5.022947	0.601906	-0.745688
H	-4.845577	0.910786	-1.789529
H	-5.971629	0.040448	-0.720588
H	-5.159667	1.516120	-0.144208
H	-2.247119	1.630312	-0.617078
C	4.455689	-2.958058	-0.869576
H	5.295537	-2.264288	-0.986930
H	4.697927	-4.023981	-0.831367
C	3.194550	-2.522025	-0.786704
H	2.391402	-3.261772	-0.680743
C	2.772389	-1.081308	-0.854463
H	2.039148	-0.955720	-1.669862
H	3.643278	-0.456262	-1.108972

15

B3LYP SCF energy: -4737.38301884 a.u.
B3LYP enthalpy: -4736.742618 a.u.
B3LYP free energy: -4736.871490 a.u.
M06-L SCF energy in solution: -4739.16851486 a.u.
M06-L enthalpy in solution: -4738.528114 a.u.
M06-L free energy in solution: -4738.656986 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.707830	-1.417142	0.178396
C	0.619841	-1.928797	1.960792
C	-0.638457	-2.160767	2.542802
C	1.774021	-2.090998	2.748828
C	-0.735176	-2.549353	3.882388
H	-1.540809	-2.055232	1.934296
C	1.671735	-2.479979	4.087766
H	2.759775	-1.902603	2.318857
C	0.416194	-2.709408	4.658445

H	-1.722102	-2.724839	4.318457
H	2.578786	-2.599740	4.687080
H	0.336226	-3.008903	5.707312
C	2.336618	-0.549702	0.084907
C	3.330350	-0.889151	-0.845404
C	2.585303	0.561784	0.910312
C	4.517989	-0.164402	-0.949254
H	3.184358	-1.737059	-1.516756
C	3.767004	1.289661	0.823886
H	1.838191	0.879656	1.639904
C	4.774309	0.945383	-0.110980
H	5.246708	-0.473913	-1.697752
H	3.890803	2.147178	1.483702
C	1.062540	-2.983305	-0.745905
C	0.708761	-3.050926	-2.103164
C	1.707868	-4.080914	-0.157342
C	1.015701	-4.183329	-2.861290
H	0.169220	-2.218559	-2.559846
C	2.002193	-5.219952	-0.913579
H	1.975623	-4.056443	0.900675
C	1.661792	-5.272219	-2.268019
H	0.728905	-4.221242	-3.915504
H	2.496255	-6.071803	-0.437945
H	1.889372	-6.164540	-2.857962
N	5.956601	1.668695	-0.199772
C	6.888341	1.386387	-1.269237
H	6.458798	1.561078	-2.276598
H	7.772500	2.029500	-1.162313
H	7.237450	0.339277	-1.238782
C	6.102496	2.897320	0.551913
H	6.001585	2.724482	1.637482
H	7.104201	3.313386	0.378103
H	5.357464	3.668082	0.270215
Pd	-1.228330	-0.304695	-0.645956
C	-0.584521	3.073990	2.563788
C	-0.696572	2.171458	1.525570
C	-0.131140	2.422659	0.241036
C	0.568170	3.669859	0.041551
C	0.660572	4.580277	1.134894
C	0.103293	4.294134	2.365081
H	-1.035705	2.850613	3.534094
H	-1.235200	1.232274	1.671488
C	-0.241628	1.466178	-0.827567
C	1.153474	3.960643	-1.235247
H	1.183089	5.528940	0.994550
H	0.186511	5.013974	3.184555
C	1.026753	3.018394	-2.238268
C	0.342430	1.792627	-2.040544
H	1.466333	3.223165	-3.220632
H	0.281900	1.097266	-2.883242
C	1.886062	5.257144	-1.482108
H	1.238605	6.136871	-1.321361
H	2.755380	5.378235	-0.811121
H	2.257359	5.304248	-2.517070
Br	-2.495820	-2.556981	-0.540398
C	-3.366858	1.200837	-0.554658
H	-2.921900	2.180075	-0.342727
C	-2.963118	0.574721	-1.733147
H	-2.458318	1.174306	-2.496144
H	-3.518304	-0.299803	-2.080259
C	-4.430960	0.798857	0.328199
H	-4.240223	1.061255	1.380233
H	-4.729660	-0.252645	0.220414
B	-5.793573	1.781054	-0.060156
F	-6.813316	1.425966	0.826361
F	-5.436884	3.126114	0.113317
F	-6.178062	1.540151	-1.381115

16-ts

B3LYP SCF energy: -4737.36817291 a.u.
B3LYP enthalpy: -4736.729369 a.u.
B3LYP free energy: -4736.859684 a.u.
M06-L SCF energy in solution: -4739.13390000 a.u.
M06-L enthalpy in solution: -4738.495096 a.u.
M06-L free energy in solution: -4738.625411 a.u.
Imaginary frequency: -24.7730 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.012779	-1.394852	0.132525
C	1.280173	-2.112796	1.831513
C	0.209071	-2.784085	2.449928
C	2.499415	-2.003295	2.523144
C	0.363285	-3.334941	3.725286
H	-0.742616	-2.881658	1.916874
C	2.646776	-2.552207	3.801620
H	3.341098	-1.481514	2.063910
C	1.578876	-3.219833	4.407234
H	-0.480005	-3.854156	4.189367
H	3.602477	-2.454332	4.325090
H	1.692975	-3.646221	5.408277
C	2.496611	-0.307811	-0.063458
C	3.522466	-0.530121	-0.992789
C	2.577092	0.865114	0.708844
C	4.583504	0.365568	-1.145652
H	3.500671	-1.418751	-1.626558
C	3.632347	1.761031	0.577166
H	1.789809	1.097994	1.428346
C	4.673055	1.534865	-0.356588

H	5.343432	0.141642	-1.894188
H	3.624164	2.656608	1.196981
C	1.430392	-2.813641	-0.988732
C	0.872053	-2.820434	-2.277423
C	2.289249	-3.860091	-0.617550
C	1.184319	-3.838901	-3.181736
H	0.171839	-2.030756	-2.559344
C	2.592789	-4.885304	-1.519167
H	2.721766	-3.880472	0.385216
C	2.044116	-4.875183	-2.804985
H	0.737019	-3.831283	-4.179421
H	3.258379	-5.697339	-1.212251
H	2.278097	-5.679115	-3.508917
N	5.731491	2.428676	-0.490649
C	6.676323	2.256298	-1.570460
H	6.210822	2.332517	-2.574869
H	7.456174	3.027167	-1.499659
H	7.178669	1.274378	-1.517472
C	5.679008	3.703226	0.192916
H	5.609709	3.574688	1.287024
H	6.600813	4.264588	-0.013207
H	4.818602	4.328848	-0.119188
Pd	-1.166169	-0.423874	-0.356597
C	-0.979939	3.033033	2.812758
C	-0.987819	2.125135	1.772008
C	-0.482355	2.450317	0.479445
C	0.033889	3.784093	0.271626
C	0.020956	4.697913	1.366945
C	-0.467704	4.335415	2.606752
H	-1.377686	2.748817	3.791005
H	-1.394172	1.120962	1.913205
C	-0.472062	1.472348	-0.579351
C	0.548336	4.152490	-1.014822
H	0.409077	5.708988	1.222901
H	-0.463114	5.058077	3.428739
C	0.532659	3.196923	-2.014979
C	0.034927	1.887812	-1.804397
H	0.919646	3.459846	-3.006442
H	0.058284	1.191342	-2.648200
C	1.091369	5.536883	-1.276124
H	0.335561	6.323583	-1.101715
H	1.951155	5.779716	-0.625273
H	1.430972	5.631046	-2.319182
Br	-2.242605	-2.814977	-0.237366
C	-3.949913	0.321206	0.244528
H	-4.221578	-0.689748	0.574370
C	-3.051851	0.377154	-0.910149
H	-2.966388	1.385955	-1.335973
H	-3.326046	-0.357080	-1.681758
C	-4.453009	1.375181	0.938312
H	-4.181483	2.404883	0.682947
H	-5.042265	1.227852	1.848246
B	-6.638096	1.222352	-0.622128
F	-7.419488	1.030328	0.433904
F	-6.448285	2.457827	-1.062826
F	-6.390334	0.204673	-1.428887

17

B3LYP SCF energy: -4413.04149677 a.u.
B3LYP enthalpy: -4412.420448 a.u.
B3LYP free energy: -4412.536992 a.u.
M06-L SCF energy in solution: -4414.51077740 a.u.
M06-L enthalpy in solution: -4413.889729 a.u.
M06-L free energy in solution: -4414.006273 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.909315	0.971471	0.159239
C	1.453657	1.335011	1.905754
C	2.618614	0.704255	2.381674
C	0.750834	2.194249	2.768651
C	3.066251	0.937803	3.684961
H	3.176715	0.035262	1.717503
C	1.200529	2.420316	4.074380
H	-0.159037	2.688974	2.423834
C	2.360168	1.792982	4.537232
H	3.973978	0.438785	4.036039
H	0.637830	3.090473	4.731215
H	2.710146	1.967394	5.559064
C	-0.787342	1.708836	0.123062
C	-1.153614	2.813734	-0.658281
C	-1.809624	1.078354	0.855481
C	-2.469890	3.278950	-0.704720
H	-0.402134	3.330298	-1.258247
C	-3.122688	1.535870	0.829287
H	-1.581978	0.196486	1.457610
C	-3.492236	2.657353	0.047383
H	-2.691317	4.135295	-1.341567
H	-3.866813	0.991430	1.409119
C	1.877937	2.209787	-0.828454
C	2.186896	1.894576	-2.161481
C	2.292425	3.447853	-0.311889
C	2.872914	2.808125	-2.966848
H	1.905281	0.915511	-2.555483
C	2.987977	4.357410	-1.114645
H	2.075134	3.704032	0.727614
C	3.276229	4.041255	-2.445983
H	3.109748	2.544593	-4.001310
H	3.308955	5.315659	-0.695627

H	3.823696	4.751047	-3.073107
N	-4.805736	3.120530	0.019885
C	-5.176941	4.146802	-0.927212
H	-5.045887	3.836312	-1.984756
H	-6.233008	4.413560	-0.781303
H	-4.583165	5.065996	-0.781264
C	-5.852079	2.326370	0.627627
H	-5.672797	2.176493	1.706262
H	-6.812331	2.850904	0.525431
H	-5.957972	1.322117	0.169685
Pd	1.163752	-1.327629	-0.626816
C	-1.845750	-3.369398	2.359317
C	-1.081164	-2.773894	1.374833
C	-1.647065	-2.319660	0.148190
C	-3.064211	-2.517131	-0.056686
C	-3.822430	-3.139431	0.979059
C	-3.234082	-3.552323	2.158569
H	-1.376335	-3.708357	3.287170
H	-0.004873	-2.643640	1.507542
C	-0.828787	-1.672585	-0.847230
C	-3.670245	-2.081126	-1.280443
H	-4.895135	-3.291676	0.837337
H	-3.841965	-4.026036	2.935999
C	-2.858313	-1.477319	-2.224006
C	-1.471878	-1.277874	-2.014949
H	-3.303160	-1.138697	-3.167276
H	-0.901221	-0.790873	-2.811705
C	-5.146108	-2.270207	-1.537223
H	-5.446237	-3.333044	-1.501800
H	-5.772069	-1.744504	-0.792920
H	-5.420621	-1.882732	-2.530652
Br	3.781783	-1.030206	-0.597403
C	2.000356	-4.158885	-0.320603
H	3.021685	-3.891906	-0.019774
C	1.414754	-3.296004	-1.362468
H	0.484163	-3.710242	-1.774988
H	2.133704	-3.086175	-2.169890
C	1.408950	-5.204991	0.291694
H	0.386747	-5.513110	0.044487
H	1.921432	-5.771623	1.076450

18-ts

B3LYP SCF energy: -4413.00548153 a.u.
B3LYP enthalpy: -4412.385800 a.u.
B3LYP free energy: -4412.501298 a.u.
M06-L SCF energy in solution: -4414.47905878 a.u.
M06-L enthalpy in solution: -4413.859377 a.u.
M06-L free energy in solution: -4413.974875 a.u.

Imaginary frequency: -334.3387 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.837112	1.016343	0.123059
C	1.403970	1.470852	1.838596
C	2.645625	0.963738	2.269023
C	0.657270	2.270910	2.720232
C	3.125354	1.264999	3.546225
H	3.232209	0.327663	1.595560
C	1.138853	2.561719	4.001895
H	-0.310674	2.667873	2.407652
C	2.375283	2.061826	4.418712
H	4.092464	0.863921	3.862859
H	0.541414	3.183263	4.675835
H	2.751184	2.288102	5.421018
C	-0.895161	1.662953	0.085145
C	-1.326578	2.747821	-0.693054
C	-1.880572	0.965714	0.808520
C	-2.667518	3.134387	-0.738076
H	-0.606550	3.310552	-1.290240
C	-3.218734	1.346706	0.784381
H	-1.601791	0.091494	1.400543
C	-3.651917	2.451712	0.012522
H	-2.938809	3.978865	-1.371621
H	-3.929335	0.752617	1.357426
C	1.740706	2.270751	-0.911666
C	2.131303	1.901918	-2.208500
C	2.047449	3.563859	-0.455902
C	2.790285	2.812701	-3.039890
H	1.934447	0.883330	-2.550630
C	2.714062	4.472172	-1.283705
H	1.768032	3.863745	0.556916
C	3.083569	4.099711	-2.580498
H	3.092167	2.505895	-4.045107
H	2.949985	5.473636	-0.911625
H	3.609608	4.808535	-3.226843
N	-4.990039	2.842798	-0.008800
C	-5.420932	3.845712	-0.955371
H	-5.279726	3.541413	-2.013651
H	-6.488940	4.056065	-0.803474
H	-4.876504	4.795538	-0.813926
C	-5.989325	1.985205	0.591271
H	-5.794205	1.826836	1.665699
H	-6.976311	2.460898	0.504531
H	-6.046924	0.984102	0.117431
Pd	1.266044	-1.197007	-0.503262
C	-1.889926	-2.966197	2.535642
C	-1.010704	-2.706118	1.496825
C	-1.456755	-2.473818	0.169188
C	-2.878048	-2.511373	-0.091511

C	-3.753290	-2.794324	0.999755
C	-3.277447	-3.015204	2.278978
H	-1.509478	-3.133823	3.547053
H	0.061402	-2.660993	1.690818
C	-0.507835	-2.171971	-0.894178
C	-3.377211	-2.239354	-1.405369
H	-4.830314	-2.827295	0.819755
H	-3.978587	-3.224099	3.093475
C	-2.450702	-1.922481	-2.393039
C	-1.067564	-1.898278	-2.161416
H	-2.814702	-1.690916	-3.401174
H	-0.398490	-1.692512	-3.002128
C	-4.854061	-2.271491	-1.709454
H	-5.310130	-3.257553	-1.501536
H	-5.426557	-1.534552	-1.114445
H	-5.036522	-2.043536	-2.771422
Br	3.944126	-1.099368	-0.600642
C	1.723159	-4.054630	-0.038270
H	2.708933	-3.601739	0.120911
C	0.901926	-3.445292	-1.115879
H	0.140707	-4.155975	-1.456296
H	1.511222	-3.157572	-1.987400
C	1.343788	-5.090946	0.731889
H	0.362702	-5.565851	0.619719
H	1.999324	-5.485761	1.514409

19

B3LYP SCF energy: -541.52880157 a.u.
B3LYP enthalpy: -541.279464 a.u.
B3LYP free energy: -541.330843 a.u.
M06-L SCF energy in solution: -541.97587257 a.u.
M06-L enthalpy in solution: -541.726535 a.u.
M06-L free energy in solution: -541.777914 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.659495	-2.608913	-0.013879
C	0.411615	-2.019222	0.015063
C	0.253142	-0.603469	0.023961
C	1.438497	0.213774	-0.006424
C	2.708276	-0.430534	-0.031849
C	2.821708	-1.805962	-0.035158
H	1.748398	-3.698327	-0.020549
H	-0.472276	-2.658213	0.027565
C	-1.043785	0.019464	0.052598
C	1.323019	1.646283	-0.014774
H	3.613895	0.177749	-0.051160
H	3.809144	-2.274183	-0.055927
C	0.058325	2.199220	0.001087
C	-1.108633	1.398357	0.032357
H	-0.051148	3.287467	-0.011104
H	-2.083089	1.891527	0.034167
C	2.546770	2.527592	-0.044896
H	3.196639	2.357739	0.830163
H	3.163421	2.343858	-0.940966
H	2.263131	3.589934	-0.047995
C	-2.305515	-0.831948	0.076024
H	-2.418748	-1.350857	-0.893252
H	-2.174326	-1.631860	0.827389
C	-3.578067	-0.100339	0.403243
C	-4.646735	-0.013651	-0.393746
H	-3.612848	0.377940	1.390704
H	-5.552741	0.513136	-0.081047
H	-4.658124	-0.469826	-1.389631

20

B3LYP SCF energy: -3332.96251586 a.u.
B3LYP enthalpy: -3331.954291 a.u.
B3LYP free energy: -3332.127078 a.u.
M06-L SCF energy in solution: -3335.37388241 a.u.
M06-L enthalpy in solution: -3334.365658 a.u.
M06-L free energy in solution: -3334.538445 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.978452	-0.352692	-1.056813
C	-2.598472	0.893900	-2.274913
C	-1.769159	1.227559	-3.360860
C	-3.826010	1.559826	-2.137729
C	-2.175347	2.168856	-4.308790
H	-0.786445	0.761357	-3.462266
C	-4.226169	2.511280	-3.081251
H	-4.470953	1.351688	-1.283808
C	-3.408906	2.812015	-4.173188
H	-1.514358	2.415027	-5.143257
H	-5.182840	3.024553	-2.954230
H	-3.723854	3.557046	-4.908185
C	-3.320340	-0.603748	0.177199
C	-4.614525	-1.009379	-0.203350
C	-3.068866	-0.479003	1.552915
C	-5.614789	-1.241207	0.733271
H	-4.851616	-1.157701	-1.259688
C	-4.055818	-0.714299	2.507060
H	-2.067837	-0.196635	1.890276
C	-5.368012	-1.091567	2.124743
H	-6.597178	-1.548481	0.376942

H	-3.795883	-0.599787	3.558469
C	-2.137917	-1.957662	-1.999774
C	-2.204319	-3.152533	-1.259089
C	-2.238906	-2.034579	-3.398159
C	-2.387965	-4.380791	-1.893810
H	-2.137432	-3.123315	-0.169551
C	-2.415870	-3.268742	-4.034499
H	-2.209376	-1.129665	-4.005209
C	-2.497510	-4.444235	-3.286612
H	-2.444086	-5.293361	-1.295771
H	-2.504761	-3.302496	-5.123685
H	-2.646488	-5.405861	-3.784347
N	-6.356439	-1.310851	3.058787
C	-7.684316	-1.709391	2.635577
H	-7.679071	-2.672152	2.091800
H	-8.326862	-1.828374	3.517090
H	-8.154992	-0.957038	1.976355
C	-6.070118	-1.145409	4.470538
H	-5.730498	-0.120765	4.707324
H	-6.980226	-1.338669	5.052221
H	-5.289555	-1.844372	4.824030
P	1.467698	-1.633421	0.373164
C	1.632878	-2.141345	2.143806
C	0.465449	-2.537161	2.825266
C	2.835621	-2.057176	2.861278
C	0.508832	-2.870939	4.179979
H	-0.490417	-2.573512	2.295064
C	2.873673	-2.377129	4.223412
H	3.748794	-1.726874	2.363930
C	1.715538	-2.790568	4.884076
H	-0.406153	-3.180931	4.691366
H	3.816481	-2.292423	4.769243
H	1.748103	-3.037171	5.948200
C	3.172951	-1.275646	-0.219594
C	4.177502	-2.263938	-0.220352
C	3.511992	-0.020311	-0.749577
C	5.458737	-2.005594	-0.690746
H	3.957265	-3.267230	0.152652
C	4.788059	0.255019	-1.233079
H	2.765014	0.773434	-0.782479
C	5.807848	-0.729409	-1.210245
H	6.195014	-2.807618	-0.656540
H	4.987362	1.251621	-1.623763
C	1.195905	-3.246890	-0.511692
C	1.202695	-3.215065	-1.918077
C	1.076341	-4.486854	0.133351
C	1.114331	-4.393159	-2.658627
H	1.299862	-2.259596	-2.440333
C	0.980458	-5.668616	-0.612063
H	1.078422	-4.543127	1.222918
C	1.005621	-5.626775	-2.006937
H	1.126838	-4.347978	-3.750244
H	0.898374	-6.627180	-0.092537
H	0.939589	-6.550885	-2.586896
N	7.076677	-0.464407	-1.674056
C	8.105471	-1.483536	-1.605279
H	7.837668	-2.383330	-2.188507
H	9.040191	-1.085291	-2.019627
H	8.307706	-1.806632	-0.567051
C	7.410517	0.862409	-2.156417
H	7.278401	1.636105	-1.377883
H	8.460878	0.880716	-2.473273
H	6.793144	1.154603	-3.025171
Pd	-0.033406	0.382394	0.229643
C	1.280705	3.655391	-2.698801
C	0.742468	2.788095	-1.770770
C	-0.314219	3.170494	-0.894942
C	-0.826593	4.515000	-1.007475
C	-0.249291	5.384145	-1.978316
C	0.778095	4.972972	-2.802792
H	2.094230	3.326711	-3.351288
H	1.121962	1.766613	-1.694300
C	-0.862940	2.264282	0.075870
C	-1.890610	4.948662	-0.148145
H	-0.626578	6.404226	-2.068817
H	1.204477	5.665543	-3.533467
C	-2.385623	4.048702	0.774843
C	-1.877958	2.729870	0.890646
H	-3.190805	4.360133	1.447800
H	-2.313949	2.090589	1.660920
C	-2.447736	6.347820	-0.237223
H	-1.676588	7.111321	-0.037431
H	-2.860134	6.565244	-1.237550
H	-3.255500	6.493680	0.494906
C	2.157765	1.766676	1.737206
H	2.995927	1.063419	1.667218
C	0.883241	1.213965	2.052269
H	0.155871	1.940483	2.423246
H	0.920226	0.296748	2.650345
C	2.485191	3.116147	1.637201
H	1.670787	3.844049	1.558488
H	3.403703	3.381376	1.103884
B	3.121517	3.428017	3.394915
F	3.475609	4.748871	3.321520
F	2.072226	3.184692	4.241051
F	4.189877	2.581757	3.572085

21-ts

B3LYP SCF energy: -3332.96399138 a.u.

B3LYP enthalpy: -3331.957036 a.u.

B3LYP free energy: -3332.127063 a.u.
M06-L SCF energy in solution: -3335.36917250 a.u.
M06-L enthalpy in solution: -3334.362217 a.u.
M06-L free energy in solution: -3334.532244 a.u.
Imaginary frequency: -26.0356 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.997356	-0.399605	-1.022591
C	-2.744015	0.839781	-2.176601
C	-2.015181	1.198160	-3.325112
C	-3.971806	1.475196	-1.936727
C	-2.519275	2.133939	-4.230397
H	-1.032975	0.757080	-3.509476
C	-4.470287	2.421373	-2.837923
H	-4.541751	1.246490	-1.035892
C	-3.752161	2.747251	-3.990548
H	-1.934501	2.400178	-5.114167
H	-5.425511	2.910401	-2.629826
H	-4.143243	3.488290	-4.692349
C	-3.229945	-0.672703	0.316860
C	-4.538681	-1.119814	0.050929
C	-2.873338	-0.504448	1.664366
C	-5.454024	-1.354414	1.070216
H	-4.855238	-1.298403	-0.979545
C	-3.773690	-0.742492	2.700293
H	-1.857293	-0.186441	1.912132
C	-5.100359	-1.164780	2.433371
H	-6.453240	-1.694908	0.801432
H	-3.433656	-0.595240	3.724466
C	-2.209981	-2.001051	-1.963592
C	-2.183586	-3.203834	-1.233699
C	-2.416119	-2.071271	-3.350729
C	-2.372296	-4.433212	-1.865057
H	-2.037624	-3.180627	-0.151972
C	-2.599162	-3.305550	-3.985125
H	-2.460876	-1.161145	-3.948945
C	-2.582538	-4.489641	-3.246562
H	-2.354127	-5.351855	-1.273734
H	-2.769178	-3.333469	-5.064828
H	-2.733879	-5.451989	-3.742193
N	-6.005079	-1.389032	3.448658
C	-7.350380	-1.831533	3.140887
H	-7.360833	-2.804896	2.616333
H	-7.917378	-1.949493	4.073003
H	-7.893563	-1.106468	2.507166
C	-5.613599	-1.181370	4.828924
H	-5.289086	-0.141693	5.016903
H	-6.468292	-1.388314	5.485361
H	-4.785651	-1.847812	5.134309
P	1.483377	-1.644948	0.247984
C	1.458933	-2.256680	1.994946
C	0.247325	-2.761906	2.504226
C	2.555119	-2.140969	2.864214
C	0.145290	-3.168366	3.835643
H	-0.630391	-2.834495	1.857454
C	2.447261	-2.536341	4.202512
H	3.500139	-1.731998	2.503709
C	1.247232	-3.056086	4.690768
H	-0.803057	-3.563740	4.208723
H	3.309681	-2.429789	4.865247
H	1.165923	-3.364446	5.736159
C	3.247688	-1.291833	-0.139817
C	4.251673	-2.270686	-0.009456
C	3.632063	-0.047043	-0.662227
C	5.574782	-2.011563	-0.345472
H	3.999066	-3.267374	0.360830
C	4.950988	0.229158	-1.011854
H	2.880052	0.730901	-0.802027
C	5.969376	-0.743793	-0.852203
H	6.307783	-2.806922	-0.216276
H	5.184823	1.216507	-1.407355
C	1.269533	-3.186500	-0.764894
C	1.184826	-3.027649	-2.159307
C	1.292751	-4.484689	-0.232742
C	1.144507	-4.138509	-3.001775
H	1.162637	-2.023140	-2.590532
C	1.244552	-5.598791	-1.079105
H	1.360796	-4.634621	0.846322
C	1.176362	-5.429667	-2.463428
H	1.081755	-3.996236	-4.083318
H	1.269527	-6.603942	-0.649459
H	1.144387	-6.300574	-3.123190
N	7.280501	-0.475660	-1.178071
C	8.297451	-1.493660	-1.005964
H	8.098011	-2.391641	-1.619559
H	9.271156	-1.090874	-1.312242
H	8.386178	-1.822197	0.046122
C	7.651130	0.835352	-1.675393
H	7.403726	1.637059	-0.956224
H	8.733897	0.865275	-1.850859
H	7.148615	1.077032	-2.630228
Pd	0.059008	0.375600	0.075306
C	1.078107	3.632917	-3.015597
C	0.649012	2.778770	-2.019871
C	-0.343235	3.156144	-1.069581
C	-0.899961	4.482897	-1.170023
C	-0.441004	5.336666	-2.214704
C	0.522453	4.929304	-3.115659
H	1.845830	3.310394	-3.724412
H	1.072047	1.773577	-1.940259

C	-0.773003	2.260547	-0.029953
C	-1.883093	4.917317	-0.218829
H	-0.855769	6.342770	-2.300305
H	0.859203	5.610184	-3.902219
C	-2.254042	4.035937	0.777534
C	-1.706450	2.730588	0.874626
H	-2.994846	4.350042	1.520094
H	-2.051043	2.102118	1.698774
C	-2.488071	6.297472	-0.293745
H	-1.723943	7.089055	-0.208024
H	-3.014923	6.465593	-1.248989
H	-3.214843	6.450079	0.517705
C	1.974402	2.504017	1.306104
H	2.860863	2.435748	0.663337
C	1.313741	1.251456	1.620152
H	0.594324	1.349008	2.445787
H	2.055701	0.477555	1.852288
C	1.682909	3.744588	1.804826
H	0.764993	3.905762	2.377485
H	2.145934	4.630675	1.363107
B	3.032775	3.640711	3.409185
F	2.772442	4.872453	3.901446
F	2.590987	2.604391	4.153990
F	4.240133	3.485938	2.818206

22

B3LYP SCF energy: -3008.63969006 a.u.
B3LYP enthalpy: -3007.650164 a.u.
B3LYP free energy: -3007.808263 a.u.
M06-L SCF energy in solution: -3010.74105796 a.u.
M06-L enthalpy in solution: -3009.751532 a.u.
M06-L free energy in solution: -3009.909631 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.717267	0.003177	0.958085
C	2.419661	1.555913	1.680319
C	1.583185	2.330937	2.503941
C	3.716964	2.019421	1.416392
C	2.043434	3.517025	3.078656
H	0.554916	2.012449	2.691913
C	4.173734	3.214130	1.982791
H	4.375537	1.455217	0.755155
C	3.343581	3.961967	2.820707
H	1.376208	4.104681	3.713990
H	5.185717	3.562582	1.760205
H	3.702253	4.895882	3.261088
C	3.086468	-0.796022	0.015605
C	4.293678	-1.187082	0.625289
C	2.927254	-1.108559	-1.344096
C	5.301589	-1.827086	-0.087432
H	4.453760	-0.995876	1.689189
C	3.921994	-1.756862	-2.073125
H	1.991625	-0.841392	-1.844053
C	5.148397	-2.127437	-1.467044
H	6.214498	-2.102399	0.439333
H	3.736000	-1.972881	-3.124409
C	1.701071	-1.132465	2.443880
C	1.444800	-2.497161	2.218312
C	1.965185	-0.714302	3.757663
C	1.463477	-3.415503	3.267686
H	1.238850	-2.852033	1.206175
C	1.978724	-1.635476	4.812200
H	2.179755	0.333634	3.969100
C	1.731674	-2.987785	4.572601
H	1.263467	-4.470593	3.065264
H	2.194994	-1.287620	5.826080
H	1.747471	-3.706711	5.395885
N	6.146144	-2.757937	-2.181710
C	7.384925	-3.130918	-1.529609
H	7.225315	-3.849849	-0.704345
H	8.052799	-3.604949	-2.260187
H	7.914784	-2.256265	-1.109167
C	5.953634	-3.055870	-3.586553
H	5.772165	-2.143853	-4.184493
H	6.854362	-3.541353	-3.983358
H	5.100334	-3.738576	-3.757181
P	-1.825098	-1.250466	-0.224661
C	-1.855338	-2.747147	-1.315052
C	-0.631551	-3.404618	-1.534174
C	-3.006719	-3.240059	-1.946804
C	-0.564570	-4.542472	-2.341634
H	0.283159	-3.013114	-1.080712
C	-2.938058	-4.374799	-2.762559
H	-3.961404	-2.729050	-1.815063
C	-1.720560	-5.032062	-2.958568
H	0.395930	-5.040590	-2.497537
H	-3.843931	-4.742960	-3.251536
H	-1.670081	-5.917585	-3.597517
C	-3.524897	-0.531595	-0.248849
C	-4.641896	-1.221828	0.258378
C	-3.737484	0.778312	-0.706577
C	-5.909720	-0.649789	0.283878
H	-4.526525	-2.230893	0.660683
C	-4.996413	1.371701	-0.678075
H	-2.894636	1.352228	-1.091555
C	-6.126791	0.671110	-0.188310
H	-6.734395	-1.234861	0.689299
H	-5.092821	2.393491	-1.042819

C	-1.877128	-2.012909	1.471767
C	-1.766374	-1.149947	2.575695
C	-2.106529	-3.377735	1.704620
C	-1.897704	-1.634654	3.877303
H	-1.579778	-0.085015	2.411982
C	-2.235789	-3.864072	3.010842
H	-2.194630	-4.070016	0.865213
C	-2.136312	-2.995217	4.099203
H	-1.806847	-0.948756	4.723157
H	-2.419011	-4.929653	3.174251
H	-2.237811	-3.375767	5.118801
N	-7.379608	1.249215	-0.162087
C	-8.508467	0.514848	0.370756
H	-8.372630	0.247294	1.435723
H	-9.413410	1.131142	0.294310
H	-8.694705	-0.422604	-0.184877
C	-7.559223	2.612009	-0.620887
H	-7.268091	2.735493	-1.679970
H	-8.617080	2.890352	-0.531134
H	-6.968643	3.335882	-0.028711
Pd	-0.088141	0.431045	-0.749742
C	-1.281983	4.602167	0.739489
C	-0.771344	3.437388	0.203005
C	0.414715	3.418821	-0.587688
C	1.083080	4.676604	-0.823323
C	0.531550	5.859816	-0.251039
C	-0.619202	5.830262	0.510904
H	-2.196844	4.575975	1.338024
H	-1.278119	2.484755	0.377155
C	0.935148	2.194045	-1.137390
C	2.273299	4.711686	-1.623811
H	1.030588	6.815659	-0.421920
H	-1.019626	6.755923	0.933860
C	2.733067	3.520804	-2.151257
C	2.074575	2.286827	-1.917376
H	3.635928	3.525000	-2.771184
H	2.504344	1.394274	-2.379148
C	3.001943	6.006527	-1.887956
H	2.363167	6.745230	-2.402392
H	3.349086	6.483090	-0.954718
H	3.885258	5.835325	-2.521113
C	-1.589042	-0.193393	-3.426023
H	-1.032278	-1.119072	-3.623850
C	-2.851997	-0.126668	-3.883193
H	-3.470120	0.765224	-3.738802
H	-3.309192	-0.964658	-4.417297
C	-0.841173	0.867935	-2.719246
H	-1.392603	1.819989	-2.692617
H	0.111879	1.047867	-3.236219

23

B3LYP SCF energy: -3448.43218690 a.u.
B3LYP enthalpy: -3447.367476 a.u.
B3LYP free energy: -3447.540238 a.u.
M06-L SCF energy in solution: -3450.78388257 a.u.
M06-L enthalpy in solution: -3449.719172 a.u.
M06-L free energy in solution: -3449.891934 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.784588	-0.332314	-1.162860
C	-2.463874	0.970363	-2.279064
C	-1.658773	1.458313	-3.324395
C	-3.742446	1.520756	-2.097622
C	-2.137430	2.440942	-4.193101
H	-0.643526	1.080037	-3.461807
C	-4.215202	2.511652	-2.963389
H	-4.373112	1.188005	-1.273047
C	-3.420141	2.967743	-4.017321
H	-1.499322	2.805397	-5.001487
H	-5.212994	2.929156	-2.807979
H	-3.793994	3.739383	-4.694582
C	-3.137748	-0.869693	-0.052708
C	-4.361351	-1.331423	-0.581058
C	-2.977245	-0.938663	1.340072
C	-5.380985	-1.796182	0.237124
H	-4.524384	-1.336814	-1.661320
C	-3.984157	-1.409770	2.177343
H	-2.032917	-0.624667	1.789746
C	-5.229971	-1.844257	1.651636
H	-6.304884	-2.134083	-0.229893
H	-3.795948	-1.435195	3.249552
C	-1.659621	-1.831476	-2.261372
C	-1.641802	-3.095036	-1.641801
C	-1.681019	-1.774656	-3.664323
C	-1.661845	-4.264776	-2.400529
H	-1.646368	-3.171583	-0.552810
C	-1.694974	-2.949827	-4.423904
H	-1.722941	-0.817636	-4.182305
C	-1.690301	-4.196581	-3.796831
H	-1.658185	-5.234342	-1.897632
H	-1.726876	-2.882554	-5.514256
H	-1.713978	-5.112668	-4.391952
N	-6.237627	-2.296817	2.464412
C	-7.495713	-2.743614	1.890646
H	-7.360220	-3.604957	1.212257
H	-8.171650	-3.055802	2.695890
H	-7.998395	-1.941333	1.321777
C	-6.050353	-2.339492	3.903576

H	-5.835247	-1.340047	4.322109
H	-6.966375	-2.710450	4.379059
H	-5.223594	-3.012277	4.195792
P	1.654265	-1.546360	0.224739
C	1.571835	-2.283458	1.921391
C	0.343675	-2.830679	2.341563
C	2.645486	-2.267444	2.827507
C	0.202040	-3.370447	3.621489
H	-0.513750	-2.835361	1.664049
C	2.497252	-2.797663	4.114886
H	3.606760	-1.843801	2.531655
C	1.280004	-3.354481	4.513510
H	-0.756432	-3.798607	3.924789
H	3.343357	-2.778268	4.806307
H	1.168955	-3.771991	5.517094
C	3.379250	-0.970451	-0.016941
C	4.472660	-1.861439	0.035716
C	3.653864	0.355154	-0.392664
C	5.768390	-1.446514	-0.233905
H	4.309569	-2.913949	0.280036
C	4.945925	0.787936	-0.678492
H	2.835790	1.073950	-0.476257
C	6.051607	-0.099758	-0.599152
H	6.570354	-2.180833	-0.175688
H	5.091927	1.825242	-0.975697
C	1.651808	-3.011823	-0.904295
C	1.747239	-2.757852	-2.283976
C	1.676986	-4.339475	-0.451602
C	1.883299	-3.809169	-3.189766
H	1.729826	-1.728995	-2.653400
C	1.808775	-5.392798	-1.364236
H	1.609824	-4.561891	0.614597
C	1.917827	-5.131057	-2.731355
H	1.962416	-3.596842	-4.258454
H	1.836445	-6.422431	-0.998563
H	2.029504	-5.954687	-3.440768
N	7.330045	0.314894	-0.870235
C	8.435499	-0.626236	-0.802129
H	8.318967	-1.457254	-1.520726
H	9.370563	-0.105608	-1.041442
H	8.543664	-1.063541	0.206212
C	7.583207	1.690556	-1.260805
H	7.260527	2.405772	-0.483251
H	8.659312	1.832255	-1.417666
H	7.067171	1.958285	-2.200662
Pd	0.040630	0.404472	0.206045
C	0.915110	4.134138	-2.305526
C	0.499184	3.097210	-1.495453
C	-0.583787	3.239384	-0.580331
C	-1.257389	4.514092	-0.523662
C	-0.800581	5.562449	-1.374069
C	0.257649	5.384268	-2.241654
H	1.748771	3.990334	-2.997699
H	1.001424	2.127679	-1.554206
C	-1.016113	2.164475	0.268806
C	-2.361108	4.701575	0.377292
H	-1.300403	6.531542	-1.338188
H	0.585955	6.207652	-2.880736
C	-2.737778	3.639626	1.176285
C	-2.075697	2.385109	1.125399
H	-3.574168	3.761511	1.870813
H	-2.443040	1.595943	1.783509
C	-3.093731	6.017842	0.451594
H	-2.423054	6.847097	0.732443
H	-3.547593	6.288330	-0.516530
H	-3.900042	5.975509	1.197468
N	0.336023	0.777733	3.012862
N	-0.454638	0.531237	3.773988
C	1.219462	1.167060	2.077317
Si	1.922406	2.947746	2.554428
C	0.519990	4.095399	3.037695
H	-0.107806	3.672644	3.838455
H	0.954299	5.032573	3.425251
H	-0.130559	4.345473	2.188200
C	3.011858	2.601424	4.059412
H	2.441898	2.162055	4.894629
H	3.841871	1.918361	3.815435
H	3.454585	3.543167	4.426040
C	2.977394	3.627355	1.161569
H	2.410672	3.776618	0.231779
H	3.368603	4.608358	1.480922
H	3.839459	2.974944	0.957451
H	2.058020	0.456009	2.103896

24-ts

B3LYP SCF energy: -3448.39705991 a.u.
B3LYP enthalpy: -3447.334972 a.u.
B3LYP free energy: -3447.508503 a.u.
M06-L SCF energy in solution: -3450.74812603 a.u.
M06-L enthalpy in solution: -3449.686038 a.u.
M06-L free energy in solution: -3449.859569 a.u.
Imaginary frequency: -285.1519 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.788337	-0.375578	-1.175871
C	-2.473963	0.948487	-2.263299
C	-1.663537	1.458467	-3.294067
C	-3.755537	1.490855	-2.081323

C	-2.139672	2.454283	-4.149011
H	-0.646350	1.084252	-3.432221
C	-4.226138	2.495538	-2.932688
H	-4.391169	1.140308	-1.267908
C	-3.425881	2.972839	-3.973099
H	-1.497559	2.835382	-4.946484
H	-5.226800	2.906264	-2.777303
H	-3.798175	3.754631	-4.639504
C	-3.135479	-0.923575	-0.061133
C	-4.368284	-1.379160	-0.572018
C	-2.952104	-1.004273	1.327837
C	-5.374614	-1.849400	0.259844
H	-4.548582	-1.376356	-1.649574
C	-3.944780	-1.481165	2.179297
H	-1.997113	-0.696076	1.758199
C	-5.199911	-1.909059	1.671064
H	-6.306613	-2.183280	-0.193821
H	-3.739377	-1.518063	3.248142
C	-1.691592	-1.856478	-2.304721
C	-1.628420	-3.129779	-1.709101
C	-1.761334	-1.776199	-3.704559
C	-1.646227	-4.286687	-2.487501
H	-1.597632	-3.225257	-0.621802
C	-1.774033	-2.938304	-4.484674
H	-1.839451	-0.810480	-4.202606
C	-1.720546	-4.195288	-3.881054
H	-1.605760	-5.264526	-2.002347
H	-1.842901	-2.852931	-5.572099
H	-1.742632	-5.101271	-4.491564
N	-6.194909	-2.367124	2.497293
C	-7.462514	-2.808641	1.940885
H	-7.339714	-3.666887	1.256038
H	-8.126762	-3.123080	2.754988
H	-7.972036	-2.002414	1.383900
C	-5.981491	-2.427615	3.931742
H	-5.756495	-1.433748	4.358617
H	-6.889561	-2.802049	4.419652
H	-5.151190	-3.105798	4.201235
P	1.711564	-1.508071	0.203246
C	1.602539	-2.274317	1.883201
C	0.384885	-2.876411	2.256363
C	2.640274	-2.213736	2.828043
C	0.219657	-3.423912	3.529936
H	-0.444964	-2.919148	1.546642
C	2.468099	-2.753132	4.108991
H	3.592892	-1.749395	2.567094
C	1.262329	-3.362638	4.461982
H	-0.728905	-3.896633	3.796298
H	3.287183	-2.699949	4.830516
H	1.132970	-3.788556	5.459868
C	3.441265	-0.936587	-0.005146
C	4.530676	-1.829563	0.079125
C	3.727426	0.385013	-0.386235
C	5.832998	-1.419949	-0.166007
H	4.360069	-2.879187	0.330821
C	5.026578	0.813031	-0.646203
H	2.911798	1.102958	-0.501853
C	6.127720	-0.077116	-0.536882
H	6.631665	-2.155493	-0.083395
H	5.181570	1.846986	-0.950336
C	1.700598	-2.941095	-0.963639
C	1.759089	-2.647201	-2.337470
C	1.757484	-4.280585	-0.549622
C	1.889799	-3.670314	-3.275877
H	1.716222	-1.608970	-2.677849
C	1.882727	-5.305380	-1.494712
H	1.719588	-4.534361	0.511092
C	1.954565	-5.003644	-2.856133
H	1.938714	-3.426833	-4.339665
H	1.934084	-6.344378	-1.159341
H	2.059879	-5.805289	-3.591185
N	7.412395	0.331234	-0.786569
C	8.512546	-0.614367	-0.696504
H	8.401720	-1.450076	-1.410518
H	9.453045	-0.099720	-0.927275
H	8.605378	-1.044631	0.316401
C	7.677466	1.703295	-1.182264
H	7.339326	2.424971	-0.417481
H	8.757127	1.841390	-1.316120
H	7.182935	1.964887	-2.135385
Pd	0.092066	0.437462	0.246977
C	0.856571	4.206218	-2.261367
C	0.483522	3.164297	-1.436996
C	-0.616577	3.265893	-0.536452
C	-1.357267	4.504592	-0.515894
C	-0.945303	5.558591	-1.382141
C	0.133282	5.420810	-2.231627
H	1.706250	4.093122	-2.939687
H	1.036266	2.221700	-1.471473
C	-1.003092	2.184820	0.326947
C	-2.481017	4.652576	0.366890
H	-1.497013	6.499711	-1.373127
H	0.426500	6.247776	-2.883029
C	-2.811767	3.588246	1.182635
C	-2.080419	2.372299	1.169530
H	-3.663450	3.679537	1.863305
H	-2.412938	1.580895	1.843591
C	-3.282288	5.929887	0.405726
H	-2.660336	6.798710	0.679056
H	-3.736283	6.157945	-0.573267
H	-4.095744	5.859146	1.141718
N	0.116249	0.715842	3.314089

N	-0.665691	0.443084	4.041970
C	1.266443	1.199578	1.753695
Si	1.883125	2.916469	2.469355
C	0.502314	4.101421	2.932584
H	-0.183563	3.673632	3.680084
H	0.960653	4.998521	3.382845
H	-0.092767	4.419801	2.065849
C	2.899787	2.503764	4.010308
H	2.288490	2.063292	4.814904
H	3.720554	1.803473	3.784069
H	3.353176	3.424351	4.415275
C	3.020668	3.659260	1.163004
H	2.492950	3.867672	0.221376
H	3.397807	4.616732	1.561446
H	3.889429	3.016666	0.957615
H	1.984952	0.448867	2.126290

25

B3LYP SCF energy: -3339.07327977 a.u.
B3LYP enthalpy: -3338.018473 a.u.
B3LYP free energy: -3338.183649 a.u.
M06-L SCF energy in solution: -3341.31686382 a.u.
M06-L enthalpy in solution: -3340.262057 a.u.
M06-L free energy in solution: -3340.427233 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.877774	-0.279590	-0.936228
C	-1.892577	1.105059	-2.163128
C	-0.665225	1.462222	-2.752804
C	-3.053091	1.791941	-2.552292
C	-0.605971	2.457289	-3.731228
H	0.254135	0.954386	-2.449233
C	-2.990695	2.792214	-3.528603
H	-4.013786	1.552363	-2.095431
C	-1.771089	3.122969	-4.125271
H	0.354354	2.716453	-4.183293
H	-3.905180	3.311917	-3.825855
H	-1.727290	3.899482	-4.892944
C	-3.533949	-0.374138	-0.158585
C	-4.698488	-0.624464	-0.915344
C	-3.688599	-0.290426	1.235252
C	-5.948770	-0.730514	-0.322169
H	-4.629799	-0.756317	-1.997721
C	-4.931681	-0.402675	1.850596
H	-2.808119	-0.154739	1.865882
C	-6.110846	-0.611424	1.086790
H	-6.809905	-0.921605	-0.960844
H	-4.981661	-0.338631	2.936536
C	-1.934640	-1.782192	-2.024754
C	-2.347272	-2.998016	-1.449673
C	-1.663253	-1.741728	-3.401500
C	-2.509780	-4.136842	-2.238237
H	-2.568802	-3.051732	-0.381301
C	-1.823074	-2.887794	-4.188763
H	-1.351542	-0.811281	-3.877595
C	-2.254413	-4.084111	-3.612756
H	-2.841595	-5.069838	-1.776925
H	-1.623338	-2.835207	-5.262045
H	-2.392947	-4.973917	-4.231846
N	-7.344847	-0.708686	1.677252
C	-8.526482	-0.954259	0.868024
H	-8.468612	-1.916443	0.327868
H	-9.410323	-0.987121	1.516529
H	-8.687623	-0.156886	0.121051
C	-7.473239	-0.605409	3.120038
H	-7.093107	0.359990	3.498947
H	-8.531811	-0.678102	3.397424
H	-6.930544	-1.411652	3.646605
P	1.466710	-1.507172	0.595096
C	1.894478	-2.009027	2.323565
C	0.841623	-2.130945	3.248813
C	3.195951	-2.338749	2.733068
C	1.079606	-2.601191	4.542819
H	-0.176362	-1.861382	2.953351
C	3.434293	-2.795640	4.033805
H	4.034013	-2.238225	2.042429
C	2.378269	-2.937754	4.937765
H	0.249408	-2.697978	5.246745
H	4.453748	-3.043728	4.339102
H	2.567469	-3.300416	5.950859
C	2.992811	-1.081271	-0.314204
C	4.020054	-2.021854	-0.541381
C	3.144973	0.186525	-0.900241
C	5.154375	-1.701021	-1.273433
H	3.928495	-3.039100	-0.154252
C	4.267095	0.521113	-1.651074
H	2.359340	0.934485	-0.771665
C	5.320506	-0.410691	-1.851078
H	5.915204	-2.467906	-1.410517
H	4.321454	1.518159	-2.085622
C	1.033365	-3.143692	-0.168211
C	1.174580	-3.302116	-1.559213
C	0.633656	-4.249834	0.600019
C	0.958986	-4.543770	-2.157695
H	1.481721	-2.458205	-2.179969
C	0.410344	-5.491026	-0.004996
H	0.521389	-4.162641	1.681189
C	0.583186	-5.644759	-1.381875

H	1.086712	-4.650818	-3.237139
H	0.116425	-6.344394	0.611304
H	0.424837	-6.619112	-1.850581
N	6.439865	-0.089775	-2.575105
C	7.493682	-1.071545	-2.769048
H	7.136034	-1.962878	-3.315072
H	8.304302	-0.623152	-3.356041
H	7.922328	-1.411919	-1.809806
C	6.574715	1.231208	-3.162310
H	6.550716	2.027277	-2.396601
H	7.535980	1.300748	-3.685605
H	5.776094	1.444042	-3.895998
Pd	-0.086365	0.287625	0.627724
C	2.280819	4.623283	-0.770172
C	1.861555	3.630311	0.101224
C	0.500309	3.468688	0.443437
C	-0.463456	4.338175	-0.164476
C	-0.003661	5.353892	-1.042065
C	1.340109	5.501131	-1.338592
H	3.341935	4.725688	-1.010096
H	2.599705	2.952977	0.523565
C	0.056248	2.450198	1.401706
C	-1.879643	4.172623	0.099598
H	-0.724959	6.029660	-1.501930
H	1.666981	6.292263	-2.017526
C	-2.284044	3.135225	0.906099
C	-1.344927	2.284394	1.545257
H	-3.346837	2.982128	1.105667
H	-1.706505	1.637627	2.346287
C	-2.888760	5.116700	-0.494473
H	-2.696838	6.157479	-0.185593
H	-2.860448	5.094657	-1.596039
H	-3.907336	4.853007	-0.178034
C	0.902742	1.551196	2.157706
Si	2.563076	1.955896	3.051301
C	2.560829	3.803566	3.474276
H	1.638859	4.084566	4.009204
H	3.410114	4.015123	4.146144
H	2.655800	4.461328	2.598413
C	2.483358	1.026184	4.693237
H	1.588942	1.315052	5.269878
H	2.466167	-0.065068	4.562729
H	3.364703	1.276737	5.306984
C	4.185420	1.505230	2.193152
H	4.369597	2.046591	1.253615
H	5.009001	1.757272	2.882767
H	4.250071	0.429497	1.974406
H	0.307886	1.062060	2.946455

26

B3LYP SCF energy: -2273.36752179 a.u.
B3LYP enthalpy: -2272.798773 a.u.
B3LYP free energy: -2272.906356 a.u.
M06-L SCF energy in solution: -2274.81988069 a.u.
M06-L enthalpy in solution: -2274.251132 a.u.
M06-L free energy in solution: -2274.358715 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-2.078862	0.043015	-0.450965
P	2.188093	0.004423	-0.428223
O	0.173105	-1.020362	1.435829
C	-2.208907	-1.111838	1.018539
C	-3.436699	-1.702540	1.373575
C	-3.549233	-2.588312	2.447183
C	-2.416636	-2.922829	3.193495
C	-1.182744	-2.365723	2.858916
C	-1.078692	-1.462633	1.793424
C	0.524598	0.461378	3.334125
C	0.858090	-0.014756	2.063263
C	1.955206	0.520499	1.344518
C	2.719737	1.517759	1.966961
C	2.405032	1.987473	3.246997
C	1.302111	1.464246	3.922207
C	-3.570409	-0.462793	-1.438635
C	-3.431355	-1.582921	-2.278977
C	-4.492167	-2.010976	-3.078710
C	-5.705253	-1.312665	-3.069479
C	-5.848627	-0.189024	-2.252084
C	-4.790343	0.232871	-1.438658
C	-2.599960	1.675313	0.262806
C	-3.256578	1.825927	1.495140
C	-3.616202	3.096252	1.958847
C	-3.331297	4.231614	1.196162
C	-2.675369	4.093283	-0.031824
C	-2.304031	2.827113	-0.489022
C	3.591264	1.086278	-0.980011
C	3.259871	2.292349	-1.622081
C	4.258822	3.159626	-2.071478
C	5.606016	2.824227	-1.902059
C	5.947047	1.620495	-1.277939
C	4.947532	0.757547	-0.817146
C	2.983239	-1.663680	-0.298603
C	2.994578	-2.473455	-1.447583
C	3.584029	-3.739443	-1.421215
C	4.155426	-4.222987	-0.239330
C	4.137614	-3.431175	0.912197
C	3.557664	-2.158337	0.883172
H	-4.326728	-1.467448	0.786957

H	-4.520988	-3.024145	2.691470
H	-2.487973	-3.627315	4.025942
H	3.569629	1.947392	1.433791
H	3.016592	2.767518	3.706299
H	1.037616	1.833003	4.916625
H	-2.476916	-2.116996	-2.309094
H	-4.368046	-2.886377	-3.721687
H	-6.532876	-1.640350	-3.703969
H	-6.790517	0.366265	-2.243961
H	-4.919342	1.111866	-0.803751
H	-3.489614	0.949684	2.102910
H	-4.122118	3.196404	2.922928
H	-3.612450	5.223166	1.560571
H	-2.440211	4.976884	-0.630992
H	-1.765122	2.722727	-1.434894
H	2.205808	2.542689	-1.774795
H	3.984052	4.094971	-2.566195
H	6.389025	3.496415	-2.262860
H	6.998273	1.348977	-1.148905
H	5.228364	-0.179775	-0.332041
H	2.527615	-2.108342	-2.366786
H	3.586947	-4.355761	-2.324167
H	4.608131	-5.217746	-0.215082
H	4.577991	-3.804577	1.840764
H	3.551633	-1.547380	1.788876
H	-0.338476	0.051181	3.859854
H	-0.275864	-2.634475	3.404367
Pd	0.052218	0.084433	-1.308721

27-ts

B3LYP SCF energy: -5271.52565880 a.u.
B3LYP enthalpy: -5270.780942 a.u.
B3LYP free energy: -5270.912853 a.u.
M06-L SCF energy in solution: -5273.50622082 a.u.
M06-L enthalpy in solution: -5272.761504 a.u.
M06-L free energy in solution: -5272.893415 a.u.
Imaginary frequency: -144.8710 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.052718	1.518118	-0.107046
P	2.363474	-0.541236	0.091991
O	1.326227	1.518555	1.823850
C	-0.882036	2.434796	1.518593
C	-1.915628	3.217609	2.066180
C	-1.799884	3.813939	3.324881
C	-0.641481	3.630829	4.082853
C	0.404943	2.867670	3.562897
C	0.290085	2.296942	2.291961
C	2.802313	3.380249	1.274042
C	2.395506	2.048940	1.144867
C	3.092956	1.144454	0.317332
C	4.223147	1.617417	-0.366680
C	4.644434	2.944455	-0.239576
C	3.929779	3.822903	0.577059
C	-2.843141	1.830750	-0.484924
C	-3.808457	1.174473	0.301410
C	-5.170356	1.361639	0.062083
C	-5.595024	2.183904	-0.987147
C	-4.645800	2.819100	-1.790714
C	-3.279743	2.649328	-1.539779
C	-0.213182	2.667794	-1.299381
C	-0.053548	4.044059	-1.068023
C	0.554315	4.859856	-2.027013
C	1.002577	4.314489	-3.233861
C	0.844046	2.946942	-3.476551
C	0.247261	2.129554	-2.512699
C	3.418365	-1.248931	-1.255927
C	2.922669	-1.209122	-2.570126
C	3.675928	-1.716698	-3.632945
C	4.931034	-2.283527	-3.394861
C	5.430249	-2.338499	-2.089331
C	4.680518	-1.825309	-1.027295
C	2.957684	-1.476416	1.578334
C	2.678848	-2.855655	1.635984
C	3.062457	-3.615001	2.742583
C	3.716852	-3.007204	3.820525
C	3.991396	-1.638706	3.775788
C	3.618832	-0.877929	2.661377
H	-2.836805	3.357430	1.499866
H	-2.624838	4.415117	3.714846
H	-0.550537	4.077147	5.076197
H	4.777075	0.940259	-1.018951
H	5.526490	3.289691	-0.783827
H	4.247726	4.863764	0.678148
H	-3.492932	0.515667	1.114086
H	-5.903057	0.848065	0.688456
H	-6.661968	2.322691	-1.180163
H	-4.965948	3.459543	-2.617074
H	-2.554270	3.165244	-2.170404
H	-0.407205	4.485998	-0.134046
H	0.676462	5.928236	-1.829745
H	1.478003	4.953875	-3.982285
H	1.194129	2.511433	-4.416027
H	0.134969	1.057070	-2.694472
H	1.932354	-0.788028	-2.756273
H	3.274217	-1.679274	-4.648882
H	5.517421	-2.688153	-4.223999
H	6.409549	-2.784250	-1.895356

H	5.081224	-1.875722	-0.012400
H	2.162769	-3.340387	0.802353
H	2.844718	-4.686083	2.765468
H	4.011238	-3.599869	4.690503
H	4.504784	-1.155168	4.611350
H	3.853199	0.187889	2.637906
H	2.241908	4.063246	1.913180
H	1.321008	2.697318	4.132167
Pd	-0.093780	-0.689246	-0.229786
C	-4.764053	-1.758707	-2.109467
C	-3.428126	-1.823633	-1.763955
C	-3.020556	-2.149211	-0.446080
C	-4.026071	-2.392253	0.555726
C	-5.391770	-2.312490	0.160731
C	-5.755761	-2.011764	-1.137555
H	-5.051766	-1.511249	-3.134160
H	-2.657142	-1.637286	-2.512946
C	-1.634005	-2.265428	-0.065288
C	-3.645794	-2.717623	1.906099
H	-6.170237	-2.502870	0.901592
H	-6.813163	-1.967283	-1.411474
C	-2.300368	-2.849891	2.197531
C	-1.293706	-2.693439	1.215990
H	-1.994375	-3.122518	3.211877
H	-0.257565	-2.920366	1.469134
Br	-0.332036	-2.972312	-1.583307
C	-4.687684	-2.951562	2.971125
H	-5.339412	-2.072279	3.114148
H	-5.350088	-3.799124	2.723058
H	-4.214071	-3.173772	3.938456

28

B3LYP SCF energy: -5271.57140590 a.u.
B3LYP enthalpy: -5270.824366 a.u.
B3LYP free energy: -5270.955267 a.u.
M06-L SCF energy in solution: -5273.55340523 a.u.
M06-L enthalpy in solution: -5272.806365 a.u.
M06-L free energy in solution: -5272.937266 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.891711	1.496378	0.032526
P	-2.277084	-0.675276	-0.033721
O	-1.789186	1.784918	-1.364589
C	0.410268	2.741318	-1.274693
C	1.298699	3.709956	-1.776414
C	0.922038	4.585832	-2.798323
C	-0.356389	4.506710	-3.354815
C	-1.264597	3.567649	-2.863835
C	-0.887984	2.715195	-1.822754
C	-3.136047	3.341986	-0.047877
C	-2.659000	2.061485	-0.333627
C	-3.070563	0.937007	0.404008
C	-3.987859	1.130837	1.446011
C	-4.475504	2.407567	1.745234
C	-4.047836	3.507847	0.999466
C	2.709353	1.808107	0.212859
C	3.559369	1.639603	-0.895944
C	4.937013	1.819831	-0.769669
C	5.493021	2.156443	0.468814
C	4.660111	2.314531	1.577176
C	3.277258	2.143806	1.451830
C	0.220585	2.244993	1.587926
C	0.122569	3.635962	1.762398
C	-0.307651	4.167538	2.980204
C	-0.642192	3.318395	4.040241
C	-0.548025	1.934331	3.875877
C	-0.122027	1.401414	2.655465
C	-3.069451	-1.824793	1.176885
C	-2.391918	-2.108375	2.373773
C	-2.971327	-2.931578	3.341684
C	-4.230096	-3.497663	3.118090
C	-4.904807	-3.235657	1.922523
C	-4.329393	-2.403543	0.957061
C	-3.093472	-1.079055	-1.652777
C	-2.531190	-2.067994	-2.478537
C	-3.127607	-2.390758	-3.700997
C	-4.286867	-1.732306	-4.119887
C	-4.852367	-0.747550	-3.305236
C	-4.260899	-0.422365	-2.080972
H	2.306012	3.780148	-1.366908
H	1.637989	5.325346	-3.164504
H	-0.649195	5.174745	-4.168445
H	-4.322077	0.273715	2.032938
H	-5.188657	2.539128	2.562183
H	-4.424287	4.507960	1.228738
H	3.148864	1.356186	-1.865325
H	5.578926	1.682162	-1.642996
H	6.573392	2.287739	0.569125
H	5.083727	2.569700	2.551734
H	2.646697	2.269687	2.332425
H	0.387081	4.311224	0.945894
H	-0.380655	5.251348	3.101814
H	-0.978543	3.736410	4.992508
H	-0.810990	1.263170	4.697164
H	-0.052521	0.318910	2.528326
H	-1.391194	-1.704376	2.537062
H	-2.428162	-3.147232	4.265229
H	-4.679389	-4.151556	3.870081

H	-5.883767	-3.684490	1.734911
H	-4.865243	-2.212360	0.025154
H	-1.632080	-2.597107	-2.154950
H	-2.677198	-3.163909	-4.328840
H	-4.748849	-1.985176	-5.077938
H	-5.760134	-0.226617	-3.621554
H	-4.717523	0.350980	-1.460261
H	-2.799043	4.198240	-0.633424
H	-2.271056	3.476133	-3.276760
Pd	0.244837	-0.799265	-0.204246
C	3.875253	-1.963495	2.615565
C	2.908762	-1.624343	1.692105
C	3.174432	-1.616290	0.293667
C	4.495171	-1.989853	-0.151543
C	5.469117	-2.331476	0.831241
C	5.172864	-2.318718	2.178881
H	3.638202	-1.967298	3.682826
H	1.899119	-1.370781	2.020467
C	2.174578	-1.268489	-0.669266
C	4.793295	-2.024322	-1.555554
H	6.472582	-2.616677	0.510046
H	5.939424	-2.590898	2.909617
C	3.787148	-1.700920	-2.446546
C	2.489497	-1.327438	-2.012515
H	3.991275	-1.738318	-3.521548
H	1.735357	-1.096731	-2.770694
Br	-0.042127	-3.293452	-0.126225
C	6.161512	-2.422479	-2.052956
H	6.952729	-1.755534	-1.669063
H	6.431245	-3.446067	-1.740967
H	6.202905	-2.389944	-3.151726

29

B3LYP SCF energy: -3139.17961758 a.u.
B3LYP enthalpy: -3138.342773 a.u.
B3LYP free energy: -3138.490232 a.u.
M06-L SCF energy in solution: -3141.42599057 a.u.
M06-L enthalpy in solution: -3140.589146 a.u.
M06-L free energy in solution: -3140.736605 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.204313	-1.711178	-0.172062
P	2.284271	-0.105482	0.179764
O	1.493129	-2.327517	-1.319506
C	-0.813311	-2.890227	-1.567077
C	-1.791059	-3.614598	-2.271797
C	-1.446691	-4.455201	-3.334391
C	-0.111897	-4.583277	-3.725523
C	0.880205	-3.880162	-3.039547
C	0.526706	-3.060711	-1.964927
C	2.563173	-4.182087	-0.133981
C	2.282672	-2.826792	-0.313291
C	2.831157	-1.840542	0.528310
C	3.701708	-2.248020	1.547264
C	4.000097	-3.602526	1.733627
C	3.424883	-4.563179	0.899537
C	-3.054736	-1.715292	-0.193751
C	-3.722422	-1.193333	-1.316798
C	-5.116249	-1.143188	-1.355023
C	-5.866723	-1.598655	-0.266003
C	-5.213218	-2.107077	0.857601
C	-3.816030	-2.167540	0.895129
C	-0.818592	-2.727886	1.328872
C	-0.932266	-4.128381	1.337658
C	-0.689352	-4.852054	2.507828
C	-0.336188	-4.186996	3.686242
C	-0.222665	-2.794294	3.688420
C	-0.457484	-2.069871	2.515775
C	3.197940	0.878609	1.448832
C	2.832159	0.713894	2.799401
C	3.421212	1.490034	3.798610
C	4.369311	2.463303	3.463768
C	4.724122	2.649620	2.126976
C	4.146796	1.861026	1.125166
C	3.175624	0.216301	-1.412599
C	2.481009	0.765792	-2.500753
C	3.131982	0.990083	-3.718174
C	4.482632	0.663681	-3.861647
C	5.180855	0.104810	-2.785596
C	4.531045	-0.122031	-1.570256
H	-2.839551	-3.519982	-1.988970
H	-2.229667	-5.005534	-3.861263
H	0.159305	-5.225819	-4.566641
H	4.149109	-1.502450	2.206494
H	4.680502	-3.903490	2.533336
H	3.649582	-5.622682	1.045397
H	-3.153412	-0.814451	-2.167005
H	-5.616015	-0.732316	-2.235364
H	-6.958224	-1.549991	-0.291944
H	-5.789952	-2.458314	1.716877
H	-3.325433	-2.565435	1.784006
H	-1.215172	-4.659800	0.426604
H	-0.778933	-5.941366	2.498947
H	-0.148383	-4.754490	4.601241
H	0.052066	-2.267209	4.605562
H	-0.361499	-0.981183	2.519102
H	2.074995	-0.025824	3.072460
H	3.128257	1.345029	4.841525

H	4.819204	3.082762	4.243382
H	5.448117	3.420286	1.852435
H	4.436360	2.027909	0.086647
H	1.422676	1.015426	-2.395960
H	2.578638	1.421626	-4.555835
H	4.992035	0.841427	-4.812227
H	6.236352	-0.158033	-2.893363
H	5.083676	-0.568470	-0.740279
H	2.116583	-4.929441	-0.790664
H	1.930436	-3.947245	-3.329991
Pd	-0.149165	0.537282	0.031073
C	-3.729632	1.579401	2.979704
C	-2.767820	1.334168	2.021604
C	-2.966439	1.661544	0.650071
C	-4.213132	2.285171	0.275727
C	-5.186294	2.517899	1.290116
C	-4.956941	2.174813	2.607154
H	-3.542791	1.320637	4.025271
H	-1.812378	0.887262	2.304601
C	-1.963874	1.406343	-0.342745
C	-4.438915	2.666463	-1.090071
H	-6.134611	2.986322	1.021010
H	-5.720637	2.371397	3.364382
C	-3.434395	2.427625	-2.008723
C	-2.211070	1.809742	-1.641363
H	-3.579863	2.728247	-3.051237
H	-1.455866	1.665316	-2.420331
C	-5.726416	3.330277	-1.512923
H	-6.606178	2.696902	-1.305896
H	-5.890505	4.284485	-0.983744
H	-5.718794	3.547550	-2.591129
C	1.003401	3.155728	-0.485599
H	2.056628	2.891817	-0.638859
C	0.346306	2.563665	0.643071
H	-0.573079	3.073781	0.942092
H	1.006431	2.363190	1.495246
C	0.488530	4.112041	-1.342675
H	-0.582933	4.332359	-1.315736
H	0.993911	4.290808	-2.296496
B	1.203064	5.710903	-0.447383
F	0.726758	6.668596	-1.290678
F	0.646351	5.718373	0.794161
F	2.560515	5.560903	-0.471595

30-ts

B3LYP SCF energy: -3139.17957259 a.u.
B3LYP enthalpy: -3138.343760 a.u.
B3LYP free energy: -3138.489983 a.u.
M06-L SCF energy in solution: -3141.42278104 a.u.
M06-L enthalpy in solution: -3140.586968 a.u.
M06-L free energy in solution: -3140.733191 a.u.
Imaginary frequency: -48.5112 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.227467	-1.703831	-0.148530
P	2.268570	-0.148934	0.168047
O	1.440976	-2.337720	-1.387072
C	-0.882601	-2.885670	-1.553409
C	-1.886350	-3.604609	-2.227250
C	-1.584308	-4.432468	-3.312244
C	-0.266504	-4.552235	-3.759567
C	0.751067	-3.856831	-3.103992
C	0.441038	-3.052438	-2.004615
C	2.494965	-4.223448	-0.241586
C	2.226264	-2.861465	-0.388133
C	2.788147	-1.900852	0.473498
C	3.661356	-2.341987	1.476782
C	3.946614	-3.703010	1.630668
C	3.357189	-4.638363	0.777847
C	-3.078708	-1.687839	-0.130281
C	-3.763676	-1.151831	-1.236358
C	-5.157342	-1.089515	-1.247377
C	-5.891029	-1.546119	-0.147340
C	-5.220463	-2.068279	0.959679
C	-3.823234	-2.141331	0.969532
C	-0.824998	-2.720286	1.347718
C	-0.916632	-4.122105	1.356226
C	-0.659688	-4.842241	2.525772
C	-0.314494	-4.172352	3.703707
C	-0.223697	-2.777805	3.706490
C	-0.472333	-2.057028	2.534580
C	3.182761	0.788586	1.471866
C	2.813822	0.578320	2.815269
C	3.395417	1.324773	3.841170
C	4.339795	2.313139	3.542169
C	4.697123	2.545135	2.213223
C	4.126176	1.787542	1.184124
C	3.178679	0.195019	-1.408862
C	2.483098	0.711903	-2.512225
C	3.143116	0.940252	-3.723912
C	4.504482	0.651870	-3.845986
C	5.204482	0.126226	-2.754398
C	4.545268	-0.106283	-1.545327
H	-2.923193	-3.513418	-1.903284
H	-2.387373	-4.978091	-3.813258
H	-0.028523	-5.183369	-4.619226
H	4.121084	-1.617152	2.150433

H	4.628374	-4.028915	2.419449
H	3.571528	-5.703294	0.897653
H	-3.207924	-0.771340	-2.094564
H	-5.670196	-0.668269	-2.115246
H	-6.982374	-1.487443	-0.151949
H	-5.783469	-2.420881	1.827530
H	-3.319645	-2.551397	1.845671
H	-1.193132	-4.657566	0.445570
H	-0.731939	-5.932862	2.516615
H	-0.115502	-4.737238	4.618006
H	0.043907	-2.246689	4.623510
H	-0.394828	-0.966712	2.537874
H	2.060274	-0.174030	3.062577
H	3.099932	1.143614	4.877744
H	4.784869	2.908119	4.343381
H	5.418950	3.327211	1.966173
H	4.417581	1.992321	0.152924
H	1.417568	0.935123	-2.421244
H	2.588739	1.345958	-4.573777
H	5.021090	0.833405	-4.791991
H	6.268439	-0.107207	-2.845556
H	5.099335	-0.530332	-0.704484
H	2.038762	-4.949906	-0.914961
H	1.789577	-3.919482	-3.434896
Pd	-0.149106	0.535350	0.020562
C	-3.708522	1.702385	2.947775
C	-2.753347	1.418015	1.993903
C	-2.943544	1.729576	0.617326
C	-4.175667	2.375109	0.232414
C	-5.142407	2.648782	1.242889
C	-4.920533	2.322732	2.565505
H	-3.528433	1.455330	3.997408
H	-1.809121	0.951128	2.282885
C	-1.944366	1.436867	-0.368996
C	-4.393217	2.736662	-1.140012
H	-6.079461	3.135131	0.966071
H	-5.678714	2.550963	3.319476
C	-3.393401	2.460512	-2.053593
C	-2.182758	1.824980	-1.674486
H	-3.532870	2.745329	-3.101494
H	-1.429503	1.653536	-2.449936
C	-5.666263	3.420230	-1.575364
H	-6.560288	2.813782	-1.349705
H	-5.805644	4.391267	-1.069987
H	-5.657522	3.610029	-2.658792
C	1.048931	3.160046	-0.529370
H	2.093653	2.876405	-0.703285
C	0.390843	2.549970	0.599474
H	-0.513473	3.078370	0.914180
H	1.059650	2.353902	1.446639
C	0.538002	4.125139	-1.364345
H	-0.520578	4.394357	-1.305816
H	1.051174	4.353309	-2.302452
B	1.366055	5.743133	-0.385372
F	0.811246	6.708571	-1.154881
F	0.905443	5.667352	0.882700
F	2.700214	5.560099	-0.548326

31

B3LYP SCF energy: -2814.85932810 a.u.
B3LYP enthalpy: -2814.041301 a.u.
B3LYP free energy: -2814.177257 a.u.
M06-L SCF energy in solution: -2816.79580684 a.u.
M06-L enthalpy in solution: -2815.977780 a.u.
M06-L free energy in solution: -2816.113736 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.876695	1.461650	-0.083618
P	-2.281056	-0.750514	0.072857
O	-1.883613	1.735163	-1.195169
C	0.292001	2.706059	-1.351003
C	1.129373	3.650203	-1.971269
C	0.642240	4.522437	-2.949319
C	-0.697580	4.462679	-3.340767
C	-1.552137	3.536655	-2.739631
C	-1.058342	2.685748	-1.747661
C	-3.209524	3.249767	0.190127
C	-2.723338	1.983143	-0.138789
C	-3.095019	0.835793	0.588021
C	-3.997940	0.991777	1.648240
C	-4.499605	2.253838	1.985626
C	-4.099613	3.377938	1.260796
C	2.704784	1.751631	-0.128364
C	3.407908	1.403540	-1.296191
C	4.791721	1.566162	-1.369017
C	5.500033	2.062903	-0.269684
C	4.813678	2.396997	0.898798
C	3.424526	2.244624	0.970604
C	0.382695	2.279296	1.507055
C	0.290313	3.674426	1.649350
C	-0.041142	4.242307	2.882129
C	-0.282809	3.425504	3.991461
C	-0.192897	2.037264	3.861406
C	0.133251	1.468668	2.626329
C	-3.083951	-1.971872	1.210630
C	-2.685593	-1.965306	2.561253
C	-3.213809	-2.885355	3.468374
C	-4.135798	-3.845317	3.036794

C	-4.522856	-3.874547	1.695774
C	-4.002973	-2.944351	0.788068
C	-3.090848	-1.036370	-1.570278
C	-2.316466	-1.493711	-2.647394
C	-2.898471	-1.693805	-3.903592
C	-4.257750	-1.436273	-4.097835
C	-5.036051	-0.972708	-3.031387
C	-4.455869	-0.770087	-1.776906
H	2.181458	3.702350	-1.689528
H	1.318203	5.246023	-3.411236
H	-1.078302	5.131038	-4.116950
H	-4.312185	0.119305	2.223038
H	-5.201073	2.354525	2.816976
H	-4.483023	4.367145	1.523370
H	2.873499	0.993749	-2.154858
H	5.319300	1.288252	-2.284579
H	6.585380	2.180794	-0.322806
H	5.358760	2.777050	1.766604
H	2.907673	2.508835	1.894034
H	0.480923	4.325100	0.793251
H	-0.109893	5.329256	2.976419
H	-0.541957	3.871433	4.955227
H	-0.380142	1.391685	4.723296
H	0.198137	0.382404	2.523844
H	-1.950033	-1.233799	2.906398
H	-2.894675	-2.860955	4.513491
H	-4.542420	-4.573371	3.743264
H	-5.233489	-4.628038	1.346464
H	-4.315761	-2.985932	-0.256318
H	-1.253022	-1.694085	-2.500450
H	-2.282554	-2.051604	-4.732506
H	-4.711478	-1.592395	-5.080131
H	-6.099145	-0.763735	-3.177547
H	-5.070397	-0.396545	-0.954334
H	-2.896689	4.123713	-0.382336
H	-2.600061	3.452195	-3.034215
Pd	0.202326	-0.984642	-0.059068
C	3.915513	-1.573883	2.862411
C	2.926424	-1.453685	1.907707
C	3.178915	-1.667737	0.522353
C	4.517669	-2.039924	0.130589
C	5.516840	-2.148247	1.141087
C	5.229843	-1.920716	2.471999
H	3.685124	-1.405936	3.918040
H	1.905332	-1.198436	2.199662
C	2.139392	-1.540451	-0.460177
C	4.808043	-2.302857	-1.250165
H	6.534302	-2.423339	0.856555
H	6.016946	-2.015523	3.225235
C	3.774145	-2.202235	-2.162290
C	2.460514	-1.833462	-1.774456
H	3.970988	-2.418129	-3.217904
H	1.690165	-1.797807	-2.551456
C	6.195257	-2.696916	-1.695906
H	6.943081	-1.921133	-1.456035
H	6.537727	-3.626835	-1.209907
H	6.224405	-2.861812	-2.783254
C	-0.513752	-3.847273	-0.819320
H	-1.596997	-3.767331	-0.982016
C	0.032603	-3.083912	0.320490
H	1.015033	-3.461551	0.624308
H	-0.643789	-3.103830	1.187012
C	0.178907	-4.626045	-1.671417
H	1.261092	-4.757729	-1.575026
H	-0.317838	-5.153697	-2.491128

32-ts

B3LYP SCF energy: -2814.82838448 a.u.
B3LYP enthalpy: -2814.012190 a.u.
B3LYP free energy: -2814.149887 a.u.
M06-L SCF energy in solution: -2816.76163608 a.u.
M06-L enthalpy in solution: -2815.945442 a.u.
M06-L free energy in solution: -2816.083139 a.u.
Imaginary frequency: -370.2384 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.792884	1.545349	0.060704
P	-2.323374	-0.785711	-0.115935
O	-2.032576	1.856882	-1.041165
C	0.122028	2.917792	-1.023313
C	0.923441	3.968110	-1.507850
C	0.411254	4.944885	-2.366410
C	-0.923415	4.889751	-2.774591
C	-1.743290	3.860240	-2.309581
C	-1.225802	2.900079	-1.435451
C	-3.401581	3.112705	0.547607
C	-2.879771	1.922766	0.036284
C	-3.220960	0.671261	0.587754
C	-4.125214	0.643771	1.658003
C	-4.663723	1.827956	2.173740
C	-4.295465	3.056656	1.621887
C	2.605736	1.911527	-0.029320
C	3.273880	1.578686	-1.221384
C	4.640140	1.825888	-1.363475
C	5.366627	2.387879	-0.308486
C	4.716295	2.702073	0.887039
C	3.343693	2.469475	1.026555
C	0.347615	2.144293	1.760318

C	0.039581	3.482393	2.057826
C	-0.265023	3.868723	3.366584
C	-0.259303	2.926464	4.399021
C	0.050241	1.592958	4.115700
C	0.344046	1.204328	2.805860
C	-2.954791	-2.181066	0.926390
C	-2.407013	-2.314917	2.217460
C	-2.785230	-3.369437	3.050763
C	-3.701166	-4.326225	2.599205
C	-4.234947	-4.216256	1.313379
C	-3.867226	-3.151547	0.482494
C	-3.187422	-1.013741	-1.740085
C	-2.434000	-1.431250	-2.848183
C	-3.041130	-1.618340	-4.094095
C	-4.409547	-1.381449	-4.248776
C	-5.167993	-0.953607	-3.153703
C	-4.561353	-0.768826	-1.908495
H	1.971993	4.019190	-1.212568
H	1.063387	5.746267	-2.722110
H	-1.326217	5.640985	-3.458429
H	-4.404692	-0.313973	2.101070
H	-5.366135	1.787464	3.009487
H	-4.706695	3.985589	2.025127
H	2.723175	1.115360	-2.042997
H	5.141517	1.562549	-2.297984
H	6.438662	2.572683	-0.415992
H	5.277366	3.133579	1.720190
H	2.851220	2.726422	1.965686
H	0.037027	4.232595	1.264533
H	-0.506074	4.913588	3.579749
H	-0.497484	3.230434	5.421652
H	0.058042	0.849206	4.916748
H	0.579915	0.160297	2.586191
H	-1.673199	-1.584773	2.570327
H	-2.354889	-3.450860	4.052340
H	-3.990055	-5.158649	3.245913
H	-4.943895	-4.964277	0.948782
H	-4.295124	-3.082785	-0.519004
H	-1.359232	-1.593034	-2.731817
H	-2.439831	-1.942688	-4.947328
H	-4.884794	-1.523337	-5.222978
H	-6.237573	-0.759238	-3.270179
H	-5.162002	-0.426811	-1.062268
H	-3.112715	4.070539	0.113194
H	-2.785779	3.776709	-2.623344
Pd	0.177293	-0.809645	-0.298923
C	3.800185	-1.854072	2.523453
C	2.785676	-1.819705	1.587256
C	3.047947	-1.805424	0.191411
C	4.418998	-1.852740	-0.245209
C	5.442296	-1.883448	0.746440
C	5.146415	-1.881031	2.095010
H	3.564565	-1.866775	3.590889
H	1.741633	-1.818431	1.908867
C	1.969740	-1.759729	-0.772160
C	4.726524	-1.869543	-1.648308
H	6.487001	-1.908240	0.431354
H	5.954163	-1.905793	2.831672
C	3.671089	-1.839852	-2.543219
C	2.321798	-1.802837	-2.122611
H	3.882871	-1.860524	-3.617493
H	1.540499	-1.825276	-2.887858
C	6.152608	-1.929621	-2.135810
H	6.744742	-1.063110	-1.792579
H	6.677574	-2.831857	-1.776247
H	6.190045	-1.941940	-3.235430
C	1.354647	-4.242871	-0.151851
H	2.133454	-4.481393	-0.885970
C	0.469623	-3.091586	-0.480893
H	-0.354615	-3.087399	0.249091
H	0.065075	-3.198790	-1.497520
C	1.250294	-5.000825	0.948622
H	0.492342	-4.800542	1.713645
H	1.924888	-5.843187	1.125007

33

B3LYP SCF energy: -2814.86544890 a.u.
B3LYP enthalpy: -2814.047436 a.u.
B3LYP free energy: -2814.186503 a.u.
M06-L SCF energy in solution: -2816.79091892 a.u.
M06-L enthalpy in solution: -2815.972906 a.u.
M06-L free energy in solution: -2816.111973 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-3.126992	0.613178	-0.498746
P	1.573273	-1.560512	-0.005303
O	-1.104279	-0.884926	1.038606
C	-3.424800	-0.925836	0.501346
C	-4.660540	-1.589534	0.577598
C	-4.811576	-2.770681	1.309574
C	-3.713464	-3.315527	1.978879
C	-2.469955	-2.684382	1.913290
C	-2.329935	-1.501280	1.180047
C	-0.569836	-0.487895	3.360212
C	-0.186145	-0.849580	2.064618
C	1.160826	-1.121524	1.750680
C	2.106094	-1.031484	2.784060
C	1.729491	-0.682194	4.083539

C	0.390354	-0.406370	4.369257
C	-4.771321	0.843911	-1.331439
C	-4.945393	0.200796	-2.571540
C	-6.133725	0.339573	-3.292205
C	-7.163754	1.145109	-2.795259
C	-6.997133	1.803471	-1.573850
C	-5.811996	1.653101	-0.845622
C	-3.153563	1.922430	0.816645
C	-3.764288	1.769284	2.074021
C	-3.739306	2.808524	3.009481
C	-3.105928	4.017029	2.702150
C	-2.492871	4.180150	1.456413
C	-2.510567	3.137886	0.524756
C	3.381384	-1.965450	0.019654
C	4.308725	-0.943109	0.298985
C	5.681537	-1.193454	0.245417
C	6.154738	-2.460925	-0.108467
C	5.243872	-3.476118	-0.408413
C	3.867789	-3.233200	-0.343547
C	0.778699	-3.236947	-0.107216
C	0.035289	-3.605403	-1.235175
C	-0.553266	-4.872597	-1.319103
C	-0.403274	-5.786626	-0.274536
C	0.335239	-5.427904	0.859111
C	0.918001	-4.161831	0.944770
H	-5.522498	-1.167406	0.057687
H	-5.786566	-3.261715	1.355612
H	-3.816645	-4.242447	2.548643
H	3.155087	-1.242718	2.573735
H	2.486046	-0.621685	4.869196
H	0.088547	-0.118278	5.379322
H	-4.136321	-0.412760	-2.979183
H	-6.250712	-0.172318	-4.251083
H	-8.090410	1.264768	-3.362604
H	-7.794851	2.440266	-1.181893
H	-5.698739	2.173930	0.107259
H	-4.267640	0.832334	2.324204
H	-4.219570	2.673849	3.982608
H	-3.086233	4.828230	3.434643
H	-1.986148	5.116854	1.210944
H	-2.008847	3.266940	-0.437895
H	3.959722	0.060494	0.545651
H	6.382254	-0.384858	0.467335
H	7.229634	-2.653294	-0.157784
H	5.601648	-4.468261	-0.696137
H	3.175062	-4.040369	-0.584298
H	-0.085405	-2.889145	-2.047117
H	-1.133960	-5.141758	-2.205098
H	-0.862538	-6.776473	-0.339421
H	0.457276	-6.137587	1.681743
H	1.490357	-3.893787	1.835919
H	-1.617848	-0.261985	3.563982
H	-1.602147	-3.111780	2.417002
Pd	1.140714	0.140490	-1.599239
C	5.178309	2.525998	-2.082062
C	3.980802	1.905294	-1.789584
C	3.146249	2.331029	-0.714387
C	3.594494	3.450480	0.081347
C	4.838498	4.065580	-0.246135
C	5.613063	3.620613	-1.298340
H	5.791140	2.172491	-2.915742
H	3.643787	1.052983	-2.384755
C	1.899280	1.671540	-0.423174
C	2.784765	3.919593	1.169291
H	5.186432	4.912806	0.347989
H	6.561604	4.114479	-1.526901
C	1.588442	3.272471	1.412794
C	1.153444	2.170620	0.632384
H	0.951525	3.616194	2.234463
H	0.191947	1.719542	0.888176
C	3.219481	5.085964	2.023040
H	4.181612	4.894159	2.529186
H	3.353219	6.007414	1.430068
H	2.472333	5.298273	2.802135
C	0.712009	0.333943	-3.766282
H	1.590283	0.195796	-4.409272
C	0.553256	1.579852	-3.105752
H	-0.433226	1.870681	-2.729917
H	1.230798	2.402153	-3.344383
C	-0.025304	-0.797316	-3.408257
H	-1.016688	-0.696237	-2.955902
H	0.206701	-1.755345	-3.879291

34-ts

B3LYP SCF energy: -2814.83412986 a.u.
B3LYP enthalpy: -2814.017447 a.u.
B3LYP free energy: -2814.157154 a.u.
M06-L SCF energy in solution: -2816.75665842 a.u.
M06-L enthalpy in solution: -2815.939976 a.u.
M06-L free energy in solution: -2816.079683 a.u.
Imaginary frequency: -326.9015 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	3.166351	-0.580674	-0.350269
P	-1.792069	1.510879	-0.032256
O	1.045139	1.121555	0.856701
C	3.369094	1.149670	0.300725
C	4.568837	1.878255	0.224706

C	4.662331	3.185094	0.709974
C	3.541574	3.793697	1.281044
C	2.332875	3.101090	1.356818
C	2.247747	1.792531	0.866788
C	0.698908	0.921537	3.235398
C	0.200144	1.124838	1.943810
C	-1.183898	1.268571	1.709298
C	-2.044080	1.188700	2.816928
C	-1.553733	0.988572	4.110240
C	-0.178937	0.857223	4.318253
C	4.749515	-0.818368	-1.292534
C	4.729252	-0.476097	-2.657512
C	5.863520	-0.642993	-3.455634
C	7.034177	-1.176039	-2.906441
C	7.062449	-1.535797	-1.556083
C	5.930431	-1.356916	-0.753835
C	3.465183	-1.600413	1.173490
C	4.041748	-1.112506	2.358662
C	4.219711	-1.951781	3.463904
C	3.829292	-3.292440	3.400795
C	3.255844	-3.790741	2.226626
C	3.068459	-2.949450	1.126637
C	-3.628016	1.670002	0.188571
C	-4.370805	0.481901	0.325686
C	-5.759602	0.521187	0.465447
C	-6.433847	1.746882	0.450952
C	-5.708262	2.930650	0.298586
C	-4.315137	2.894831	0.170688
C	-1.249494	3.257658	-0.359720
C	-0.865240	3.608003	-1.662462
C	-0.472932	4.916593	-1.962629
C	-0.454552	5.891093	-0.961503
C	-0.830788	5.552078	0.342717
C	-1.224124	4.244592	0.642296
H	5.448695	1.408036	-0.218357
H	5.609615	3.725202	0.640713
H	3.600052	4.818071	1.657593
H	-3.119525	1.291485	2.664528
H	-2.248186	0.935326	4.951995
H	0.215892	0.692797	5.324015
H	3.810846	-0.081251	-3.101761
H	5.828577	-0.367544	-4.512977
H	7.919739	-1.317280	-3.531545
H	7.972003	-1.958951	-1.121118
H	5.969160	-1.641707	0.299801
H	4.360465	-0.069409	2.418560
H	4.669981	-1.555086	4.377998
H	3.968533	-3.946805	4.265225
H	2.943801	-4.836789	2.168488
H	2.604152	-3.345788	0.219225
H	-3.859425	-0.482529	0.312197
H	-6.315284	-0.413885	0.571334
H	-7.522109	1.777731	0.550222
H	-6.226467	3.893128	0.276722
H	-3.767802	3.830574	0.049927
H	-0.863774	2.838009	-2.438728
H	-0.173868	5.172584	-2.982473
H	-0.143739	6.912967	-1.194538
H	-0.817739	6.309312	1.131411
H	-1.514727	3.992252	1.665156
H	1.773751	0.800355	3.379862
H	1.443558	3.574215	1.775197
Pd	-1.198051	-0.124890	-1.547886
C	-4.878811	-3.028606	-2.224953
C	-3.637623	-2.448305	-2.055705
C	-2.823003	-2.731258	-0.922467
C	-3.326147	-3.654042	0.065550
C	-4.615102	-4.228009	-0.138775
C	-5.374041	-3.927771	-1.252283
H	-5.479796	-2.790914	-3.106500
H	-3.264389	-1.738495	-2.797035
C	-1.529895	-2.121817	-0.751501
C	-2.531626	-3.969821	1.218983
H	-5.010760	-4.924944	0.602346
H	-6.357822	-4.386565	-1.383238
C	-1.288226	-3.373912	1.336167
C	-0.787299	-2.476069	0.364916
H	-0.665911	-3.599735	2.207718
H	0.208855	-2.051959	0.512316
C	-3.030968	-4.926637	2.272764
H	-3.970290	-4.577960	2.735958
H	-3.235555	-5.929043	1.858429
H	-2.289419	-5.044846	3.076494
C	-0.488600	-1.000935	-3.457379
H	-1.282862	-1.122760	-4.204562
C	-0.381703	-2.045791	-2.433573
H	0.601519	-2.145322	-1.962947
C	0.245391	0.169593	-3.488149
H	1.143418	0.296057	-2.876891
H	0.076607	0.898099	-4.284875
H	-0.804723	-3.007176	-2.734558

35

B3LYP SCF energy: -5828.72907373 a.u.
B3LYP enthalpy: -5827.834438 a.u.
B3LYP free energy: -5827.997154 a.u.
M06-L SCF energy in solution: -5831.03284123 a.u.
M06-L enthalpy in solution: -5830.138205 a.u.
M06-L free energy in solution: -5830.300921 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.875890	1.577205	-0.050004
P	3.201007	-0.297609	0.448007
O	1.035781	1.721272	0.756214
C	-1.160407	2.289098	1.507861
C	-1.964950	2.868466	2.506019
C	-1.410482	3.440276	3.652180
C	-0.023638	3.437550	3.826123
C	0.799124	2.875503	2.852202
C	0.238130	2.313778	1.696553
C	2.204095	3.696576	0.007776
C	2.189844	2.329214	0.304701
C	3.320780	1.519961	0.087392
C	4.470319	2.136097	-0.437008
C	4.500710	3.502155	-0.725044
C	3.362553	4.281902	-0.502293
C	-3.690045	1.435404	0.325497
C	-4.132257	0.719049	1.454146
C	-5.495992	0.570980	1.713474
C	-6.444647	1.119891	0.845500
C	-6.017725	1.826344	-0.280312
C	-4.652370	1.987843	-0.537107
C	-1.834324	3.014401	-1.216098
C	-1.711111	4.335908	-0.755196
C	-1.751639	5.406804	-1.653272
C	-1.923547	5.171415	-3.020054
C	-2.051281	3.859986	-3.485594
C	-1.999420	2.786679	-2.592274
C	4.631595	-0.955818	-0.532744
C	4.478409	-0.991560	-1.933940
C	5.473821	-1.541637	-2.743736
C	6.630539	-2.083097	-2.170368
C	6.786054	-2.062720	-0.782538
C	5.795834	-1.500274	0.032090
C	3.814379	-0.391617	2.198845
C	3.456655	-1.533946	2.938231
C	3.866205	-1.687245	4.265929
C	4.626057	-0.689462	4.883817
C	4.977163	0.457370	4.164871
C	4.577035	0.604935	2.832852
H	-3.047709	2.881292	2.379841
H	-2.062950	3.884762	4.407100
H	0.421854	3.869886	4.725621
H	5.357757	1.528956	-0.626069
H	5.409248	3.953816	-1.130413
H	3.367460	5.348396	-0.741078
H	-3.410482	0.275229	2.139935
H	-5.816067	0.011861	2.596025
H	-7.511822	0.996514	1.047105
H	-6.748330	2.263289	-0.965960
H	-4.343256	2.553925	-1.416185
H	-1.588987	4.538588	0.310061
H	-1.651269	6.429168	-1.279501
H	-1.953685	6.008970	-3.721880
H	-2.174428	3.664667	-4.553642
H	-2.067313	1.766587	-2.970613
H	3.575566	-0.574867	-2.393229
H	5.342410	-1.552118	-3.829048
H	7.406245	-2.520180	-2.804607
H	7.686246	-2.482899	-0.325545
H	5.936093	-1.486850	1.114978
H	2.845301	-2.310454	2.469662
H	3.581487	-2.584621	4.821615
H	4.939935	-0.802893	5.924801
H	5.569747	1.242575	4.642385
H	4.863297	1.503564	2.281824
H	1.300127	4.289056	0.156976
H	1.883199	2.857986	2.976466
Pd	-0.817709	-0.405792	-0.748074
C	-4.695712	-3.066493	-0.480573
C	-3.573657	-2.267130	-0.402220
C	-2.800815	-2.166284	0.789576
C	-3.232429	-2.916933	1.944371
C	-4.389661	-3.740815	1.824303
C	-5.104088	-3.818427	0.645874
H	-5.270685	-3.116413	-1.408914
H	-3.257699	-1.673135	-1.261866
C	-1.632086	-1.333799	0.864229
C	-2.503059	-2.813333	3.177062
H	-4.721109	-4.322702	2.686235
H	-5.989252	-4.457209	0.584238
C	-1.396843	-1.985905	3.212277
C	-0.963389	-1.257106	2.074176
H	-0.829399	-1.888862	4.143226
H	-0.073914	-0.629544	2.174606
Br	0.525730	0.585977	-2.759464
C	-2.925407	-3.587270	4.401713
H	-3.951336	-3.333988	4.719657
H	-2.908251	-4.676571	4.225513
H	-2.254167	-3.377435	5.247297
N	0.516757	-3.052021	-0.270662
N	0.677654	-3.683285	0.644973
C	0.265374	-2.285844	-1.338580
Si	-0.422720	-3.277197	-2.865246
C	-1.206387	-4.859687	-2.196762
H	-2.055909	-4.637439	-1.531127
H	-1.588872	-5.465222	-3.035601
H	-0.486957	-5.484239	-1.642064
C	-1.657966	-2.285072	-3.872972
H	-2.586416	-2.090749	-3.316578

H	-1.217890	-1.319997	-4.165142
H	-1.916994	-2.853110	-4.783147
C	1.085679	-3.671605	-3.930243
H	1.844242	-4.246333	-3.374314
H	0.794399	-4.261186	-4.816031
H	1.552987	-2.737478	-4.281860
H	1.185713	-1.728622	-1.578851

36-ts

B3LYP SCF energy: -5828.69933304 a.u.
B3LYP enthalpy: -5827.806848 a.u.
B3LYP free energy: -5827.969889 a.u.
M06-L SCF energy in solution: -5830.99949280 a.u.
M06-L enthalpy in solution: -5830.107008 a.u.
M06-L free energy in solution: -5830.270049 a.u.
Imaginary frequency: -444.1186 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.848329	1.608566	-0.176195
P	3.177289	-0.264822	0.527554
O	1.048917	1.816681	0.551946
C	-1.120458	2.448490	1.310927
C	-1.903734	3.098912	2.280127
C	-1.323285	3.759589	3.364933
C	0.067293	3.777319	3.501997
C	0.870154	3.142891	2.555313
C	0.281789	2.488587	1.464639
C	2.273302	3.673203	-0.380240
C	2.225586	2.346444	0.061951
C	3.340948	1.494560	-0.049004
C	4.506908	2.023216	-0.630073
C	4.569447	3.348428	-1.066475
C	3.449107	4.174227	-0.938404
C	-3.666242	1.553346	0.196253
C	-4.132390	0.913034	1.360516
C	-5.501161	0.811220	1.616544
C	-6.430470	1.333293	0.711857
C	-5.979506	1.965198	-0.448618
C	-4.609052	2.078391	-0.704126
C	-1.757282	2.936308	-1.465378
C	-1.677007	4.297505	-1.123101
C	-1.670631	5.279782	-2.117484
C	-1.749963	4.916284	-3.465327
C	-1.835148	3.565992	-3.813447
C	-1.834168	2.580692	-2.821434
C	4.605240	-1.066418	-0.343669
C	4.446383	-1.309776	-1.723392
C	5.437389	-1.975437	-2.447266
C	6.595792	-2.428202	-1.804704
C	6.756696	-2.203859	-0.435540
C	5.770676	-1.525299	0.290998
C	3.771718	-0.149117	2.284502
C	3.331082	-1.149141	3.170109
C	3.721600	-1.143152	4.512442
C	4.547407	-0.124117	4.996040
C	4.982887	0.883713	4.129509
C	4.600075	0.871053	2.784471
H	-2.989554	3.096870	2.180299
H	-1.958791	4.258228	4.100272
H	0.532442	4.281520	4.352849
H	5.381668	1.379915	-0.744209
H	5.490323	3.732422	-1.511894
H	3.481578	5.208629	-1.289682
H	-3.426159	0.492489	2.076806
H	-5.840255	0.308858	2.525724
H	-7.501631	1.246482	0.911462
H	-6.695344	2.379437	-1.163386
H	-4.279573	2.583088	-1.613026
H	-1.624853	4.598256	-0.075151
H	-1.605795	6.334000	-1.835434
H	-1.742452	5.684995	-4.242514
H	-1.888963	3.270679	-4.864199
H	-1.873090	1.529002	-3.106770
H	3.539983	-0.968456	-2.234523
H	5.300133	-2.147964	-3.518081
H	7.367885	-2.956449	-2.370263
H	7.657568	-2.555015	0.075202
H	5.915211	-1.354069	1.359837
H	2.668122	-1.938005	2.803277
H	3.371410	-1.931635	5.183865
H	4.847718	-0.112322	6.047098
H	5.627511	1.684675	4.501837
H	4.951159	1.661617	2.117290
H	1.381154	4.296864	-0.303522
H	1.956861	3.138419	2.654909
Pd	-0.834466	-0.520661	-0.709073
C	-4.699771	-3.140763	-0.123047
C	-3.566380	-2.353962	-0.145247
C	-2.810270	-2.087058	1.031754
C	-3.267965	-2.656236	2.276980
C	-4.440591	-3.467213	2.261948
C	-5.139832	-3.707077	1.096373
H	-5.260166	-3.322249	-1.043888
H	-3.224456	-1.901253	-1.077991
C	-1.628793	-1.269792	1.001148
C	-2.545345	-2.393799	3.489815
H	-4.794784	-3.909480	3.194919
H	-6.036087	-4.332997	1.115728

C	-1.418001	-1.596478	3.417980
C	-0.961254	-1.043796	2.193529
H	-0.854459	-1.382818	4.331862
H	-0.058263	-0.428252	2.208652
Br	0.538919	0.081930	-2.859814
C	-2.996282	-2.973055	4.808365
H	-4.018249	-2.652481	5.074202
H	-3.004959	-4.076523	4.792325
H	-2.327395	-2.658464	5.622789
N	0.218938	-3.437501	0.076295
N	0.256111	-3.891932	1.082308
C	0.124109	-2.225507	-1.320456
Si	-0.405198	-3.361269	-2.809490
C	-1.043487	-5.013605	-2.130080
H	-1.882088	-4.870468	-1.429058
H	-1.414662	-5.626909	-2.968717
H	-0.260126	-5.596611	-1.619320
C	-1.787251	-2.588610	-3.831016
H	-2.687492	-2.403887	-3.224841
H	-1.465742	-1.634931	-4.272675
H	-2.064399	-3.281498	-4.643939
C	1.113827	-3.678712	-3.886821
H	1.930160	-4.142143	-3.308265
H	0.863613	-4.356054	-4.720983
H	1.487448	-2.732530	-4.307696
H	1.210604	-2.084911	-1.233667

37

B3LYP SCF energy: -5719.29678501 a.u.
B3LYP enthalpy: -5718.414236 a.u.
B3LYP free energy: -5718.571190 a.u.
M06-L SCF energy in solution: -5721.48389234 a.u.
M06-L enthalpy in solution: -5720.601343 a.u.
M06-L free energy in solution: -5720.758297 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.267045	-1.604539	0.079969
P	3.892870	0.609569	-0.119897
O	1.800770	-1.538601	0.102250
C	-0.077727	-2.683512	-0.873021
C	-0.525762	-3.673608	-1.766980
C	0.361580	-4.461418	-2.502292
C	1.737143	-4.270413	-2.360025
C	2.212794	-3.301080	-1.479337
C	1.319049	-2.515654	-0.739882
C	2.877141	-2.955864	1.728886
C	2.882512	-1.811253	0.923931
C	3.953268	-0.894445	0.969778
C	4.995008	-1.154566	1.878296
C	4.991286	-2.289757	2.691894
C	3.931300	-3.196009	2.610283
C	-2.901490	-2.423787	-0.213580
C	-3.479810	-2.290960	-1.490393
C	-4.731560	-2.842203	-1.768401
C	-5.441601	-3.513389	-0.767898
C	-4.891426	-3.624564	0.510094
C	-3.630767	-3.084480	0.787138
C	-0.846492	-2.022256	1.831441
C	-0.706073	-3.351763	2.268807
C	-0.410269	-3.630729	3.605321
C	-0.235440	-2.585230	4.518965
C	-0.355244	-1.261450	4.089936
C	-0.660901	-0.981581	2.753772
C	5.358228	1.578457	0.476352
C	5.143488	2.417149	1.587230
C	6.168498	3.223416	2.085998
C	7.423132	3.225367	1.466580
C	7.642985	2.413641	0.350903
C	6.620304	1.594165	-0.140097
C	4.471814	-0.082049	-1.740969
C	3.968633	0.519167	-2.907368
C	4.359104	0.064443	-4.170929
C	5.251493	-1.004852	-4.286017
C	5.752908	-1.617665	-3.132464
C	5.365212	-1.160851	-1.869270
H	-1.595670	-3.843136	-1.882937
H	-0.026697	-5.223040	-3.182440
H	2.445151	-4.870735	-2.936700
H	5.829980	-0.454355	1.941538
H	5.818590	-2.466399	3.383544
H	3.914987	-4.088504	3.240864
H	-2.954639	-1.739417	-2.272325
H	-5.160740	-2.729032	-2.766872
H	-6.426699	-3.935813	-0.981921
H	-5.445635	-4.130533	1.304778
H	-3.227968	-3.174007	1.796068
H	-0.830309	-4.175035	1.560682
H	-0.312117	-4.668627	3.934582
H	0.000007	-2.804420	5.563624
H	-0.208593	-0.439560	4.795068
H	-0.745480	0.055607	2.418930
H	4.158026	2.441966	2.062057
H	5.983209	3.862938	2.953083
H	8.223640	3.864353	1.848349
H	8.617923	2.415465	-0.144054
H	6.809802	0.965871	-1.012508
H	3.256330	1.344398	-2.821905
H	3.957131	0.542874	-5.067827

H	5.553438	-1.364310	-5.273269
H	6.450452	-2.455570	-3.216662
H	5.762599	-1.647076	-0.974704
H	2.035149	-3.645810	1.669067
H	3.284096	-3.131780	-1.365106
Pd	-1.359159	0.791191	-0.393536
C	-5.079006	0.645433	2.508410
C	-4.084010	0.724715	1.555549
C	-4.373032	0.866255	0.168005
C	-5.759794	0.930660	-0.229904
C	-6.761125	0.840966	0.780497
C	-6.435861	0.702647	2.114542
H	-4.819591	0.539017	3.565048
H	-3.034845	0.683474	1.853220
C	-3.333827	0.948285	-0.820032
C	-6.100036	1.089511	-1.615235
H	-7.812833	0.886291	0.492017
H	-7.226842	0.639893	2.866831
C	-5.069692	1.186253	-2.531002
C	-3.707216	1.125685	-2.142585
H	-5.307878	1.319823	-3.591353
H	-2.946877	1.218042	-2.923045
Br	0.865881	2.322587	-0.506073
C	-7.539224	1.162787	-2.063397
H	-8.102817	0.252243	-1.796274
H	-8.073011	2.011993	-1.602988
H	-7.603118	1.284293	-3.154835
C	-1.084123	2.783626	-0.748089
Si	-1.628589	4.213657	0.376345
C	-3.437131	4.611321	-0.001570
H	-4.095607	3.764864	0.244687
H	-3.765439	5.485977	0.585423
H	-3.579348	4.849858	-1.068311
C	-1.415438	3.763453	2.200272
H	-2.083678	2.935582	2.484783
H	-0.377950	3.461515	2.417228
H	-1.656650	4.627469	2.842133
C	-0.576427	5.746693	-0.001914
H	-0.673089	6.046501	-1.058790
H	-0.893536	6.602168	0.618753
H	0.491193	5.560870	0.198308
H	-1.200102	3.008401	-1.819958

38-ts

B3LYP SCF energy: -5719.28388502 a.u.
B3LYP enthalpy: -5718.402418 a.u.
B3LYP free energy: -5718.559811 a.u.
M06-L SCF energy in solution: -5721.46852207 a.u.
M06-L enthalpy in solution: -5720.587055 a.u.
M06-L free energy in solution: -5720.744448 a.u.
Imaginary frequency: -367.3331 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.864457	1.823360	-0.100258
P	3.166950	-0.314705	0.389743
O	1.037531	1.790283	0.577880
C	-1.083556	2.394206	1.486185
C	-1.820534	2.886275	2.575851
C	-1.190349	3.319892	3.745436
C	0.201888	3.263623	3.844291
C	0.958993	2.771513	2.780555
C	0.321019	2.339331	1.611941
C	2.299184	3.703617	-0.159962
C	2.228069	2.339651	0.148650
C	3.331625	1.485726	-0.045915
C	4.502200	2.048408	-0.585497
C	4.583996	3.407338	-0.896042
C	3.479762	4.236394	-0.676867
C	-3.676717	1.977454	0.249479
C	-4.265089	1.020983	1.098259
C	-5.633892	1.056032	1.370347
C	-6.442933	2.034747	0.783041
C	-5.872153	2.977709	-0.074618
C	-4.498064	2.952829	-0.338929
C	-1.517762	3.253342	-1.226562
C	-1.494295	4.583321	-0.768798
C	-1.247212	5.633998	-1.656131
C	-1.018406	5.369399	-3.011355
C	-1.035750	4.051245	-3.473370
C	-1.280890	2.997629	-2.585987
C	4.555758	-1.058308	-0.591110
C	4.278811	-1.365611	-1.937605
C	5.250309	-1.961684	-2.744897
C	6.506377	-2.279743	-2.216795
C	6.786070	-1.992361	-0.878248
C	5.819338	-1.382959	-0.070322
C	3.835974	-0.353890	2.122975
C	3.615959	-1.534063	2.858223
C	4.065331	-1.654868	4.175291
C	4.726695	-0.587059	4.791077
C	4.941199	0.595088	4.077302
C	4.503105	0.710346	2.753061
H	-2.908231	2.936841	2.506261
H	-1.789086	3.701044	4.575923
H	0.705142	3.593716	4.756562
H	5.366426	1.404887	-0.761833
H	5.507874	3.816568	-1.311839
H	3.528682	5.299703	-0.924902

H	-3.649214	0.237226	1.544193
H	-6.070451	0.304556	2.032888
H	-7.516264	2.057087	0.988862
H	-6.497069	3.741731	-0.544588
H	-4.070544	3.698210	-1.011254
H	-1.671133	4.800484	0.287344
H	-1.233137	6.663451	-1.288153
H	-0.822144	6.191757	-3.704390
H	-0.848460	3.835680	-4.528303
H	-1.270639	1.967419	-2.950582
H	3.293420	-1.137259	-2.355842
H	5.019861	-2.188919	-3.789092
H	7.262954	-2.755530	-2.846339
H	7.764072	-2.240838	-0.456984
H	6.053961	-1.161035	0.972942
H	3.085807	-2.369172	2.390502
H	3.890745	-2.583037	4.726030
H	5.070620	-0.675822	5.824848
H	5.458325	1.434217	4.550770
H	4.689495	1.636421	2.204754
H	1.418558	4.331287	-0.013422
H	2.045705	2.703444	2.852493
Pd	-1.113325	-0.323702	-0.824823
C	-5.026087	-2.799671	-0.051461
C	-3.776592	-2.232802	-0.207062
C	-2.753550	-2.395386	0.766979
C	-3.055944	-3.156925	1.952295
C	-4.355417	-3.726942	2.081125
C	-5.317334	-3.559121	1.104572
H	-5.790797	-2.657007	-0.819145
H	-3.547397	-1.629054	-1.087807
C	-1.449367	-1.802520	0.604408
C	-2.054907	-3.320884	2.971690
H	-4.597217	-4.309618	2.971549
H	-6.305577	-4.010050	1.227665
C	-0.816621	-2.736493	2.778628
C	-0.510243	-1.999481	1.609845
H	-0.045719	-2.846859	3.547141
H	0.488387	-1.568004	1.508503
Br	0.296809	-0.643096	-3.051682
C	-2.342965	-4.111553	4.222721
H	-3.187832	-3.686424	4.790817
H	-2.608523	-5.157696	3.993795
H	-1.467487	-4.127059	4.887747
C	-0.326991	-2.099365	-1.212348
Si	-0.761188	-3.709400	-2.160345
C	-1.151050	-5.066902	-0.896400
H	-2.094729	-4.883422	-0.362711
H	-1.235445	-6.035433	-1.418757
H	-0.348773	-5.159160	-0.146473
C	-2.204947	-3.489993	-3.353847
H	-2.007457	-2.665801	-4.056385
H	-2.345871	-4.414483	-3.939102
H	-3.147090	-3.280409	-2.825845
C	0.777773	-4.264427	-3.114048
H	1.656304	-4.337110	-2.451740
H	0.607873	-5.261103	-3.556552
H	1.023230	-3.562269	-3.924777
H	0.683581	-2.137513	-0.774845

39

B3LYP SCF energy: -5719.36365844 a.u.
B3LYP enthalpy: -5718.478914 a.u.
B3LYP free energy: -5718.633405 a.u.
M06-L SCF energy in solution: -5721.55546019 a.u.
M06-L enthalpy in solution: -5720.670716 a.u.
M06-L free energy in solution: -5720.825207 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.492003	1.815690	-0.171844
P	3.277438	-0.694025	0.138898
O	1.436067	1.718528	-0.302322
C	-0.315604	2.596678	1.021343
C	-0.718968	3.260258	2.190501
C	0.213130	3.814864	3.072859
C	1.576876	3.706417	2.793522
C	2.010481	3.030277	1.651510
C	1.073302	2.464385	0.778359
C	2.887175	3.024352	-1.685677
C	2.659887	1.865436	-0.932828
C	3.604929	0.824301	-0.888042
C	4.775749	0.979554	-1.654593
C	5.013483	2.130581	-2.405978
C	4.066469	3.159881	-2.415663
C	-3.176497	2.464617	0.269642
C	-4.263442	1.577443	0.274415
C	-5.564677	2.040492	0.499770
C	-5.796564	3.398363	0.725235
C	-4.723010	4.295861	0.704266
C	-3.426503	3.835753	0.467046
C	-1.224902	2.774429	-1.736080
C	-0.679083	4.068868	-1.726079
C	-0.598349	4.813119	-2.907021
C	-1.063423	4.273251	-4.109757
C	-1.609610	2.987334	-4.124635
C	-1.689823	2.238996	-2.946710
C	4.103230	-1.996765	-0.896075
C	3.350931	-2.506014	-1.972647

C	3.876978	-3.507852	-2.791687
C	5.149764	-4.031635	-2.539147
C	5.896744	-3.542247	-1.464539
C	5.379599	-2.529186	-0.648861
C	4.480838	-0.478365	1.540066
C	4.425599	-1.442484	2.566150
C	5.252647	-1.351432	3.687076
C	6.139450	-0.277148	3.819685
C	6.193474	0.696110	2.819497
C	5.375002	0.595444	1.687983
H	-1.781973	3.352400	2.416353
H	-0.129647	4.329254	3.973244
H	2.315543	4.136461	3.474545
H	5.513643	0.174346	-1.659211
H	5.932736	2.220535	-2.989901
H	4.234879	4.061537	-3.009912
H	-4.092993	0.517530	0.078227
H	-6.397122	1.332341	0.492162
H	-6.811778	3.761542	0.904661
H	-4.897414	5.363365	0.861943
H	-2.608383	4.557035	0.422749
H	-0.313882	4.505943	-0.793854
H	-0.171369	5.819469	-2.884667
H	-0.998376	4.854053	-5.033562
H	-1.967974	2.553322	-5.061406
H	-2.092611	1.225930	-2.974884
H	2.347796	-2.113182	-2.170404
H	3.282775	-3.886325	-3.627802
H	5.556280	-4.821827	-3.176099
H	6.891506	-3.947031	-1.258308
H	5.977253	-2.155151	0.185287
H	3.723627	-2.277628	2.484399
H	5.197715	-2.117098	4.465593
H	6.781552	-0.198514	4.700801
H	6.881812	1.540573	2.913794
H	5.443410	1.360343	0.912037
H	2.116765	3.795637	-1.713544
H	3.075184	2.916350	1.444197
Pd	-1.339562	-0.519777	-0.155009
C	-6.118616	-2.755287	0.466330
C	-4.914451	-2.247126	0.927383
C	-3.674542	-2.723611	0.439937
C	-3.674008	-3.780438	-0.527475
C	-4.923177	-4.274082	-0.984903
C	-6.121640	-3.773067	-0.505006
H	-7.061969	-2.371196	0.862633
H	-4.922555	-1.471782	1.694848
C	-2.403798	-2.193943	0.936611
C	-2.423820	-4.333470	-1.013734
H	-4.941836	-5.070653	-1.729500
H	-7.068278	-4.175364	-0.874623
C	-1.245393	-3.841977	-0.515097
C	-1.212214	-2.788813	0.445961
H	-0.294840	-4.249675	-0.864649
H	-0.254613	-2.555947	0.918333
Br	-0.287156	-0.893409	-2.432122
C	-2.420633	-5.431958	-2.044512
H	-2.959794	-6.328473	-1.694100
H	-2.906637	-5.108097	-2.980227
H	-1.392298	-5.731143	-2.290719
C	-2.255686	-0.993430	1.736575
Si	-1.230509	-0.960674	3.350360
C	-1.411449	-2.658115	4.179073
H	-0.958977	-3.455859	3.567946
H	-0.915773	-2.667227	5.164742
H	-2.471882	-2.918259	4.331920
C	0.603822	-0.571611	3.160001
H	1.109810	-1.236540	2.443636
H	0.764890	0.458983	2.810838
H	1.108894	-0.678020	4.135109
C	-2.031652	0.341117	4.468986
H	-3.094704	0.114313	4.654905
H	-1.521685	0.379760	5.446166
H	-1.971600	1.346383	4.023086
H	-3.195874	-0.455889	1.907391

40

B3LYP SCF energy: -3586.97697124 a.u.
B3LYP enthalpy: -3586.002332 a.u.
B3LYP free energy: -3586.170001 a.u.
M06-L SCF energy in solution: -3589.43564170 a.u.
M06-L enthalpy in solution: -3588.461002 a.u.
M06-L free energy in solution: -3588.628671 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.839739	-1.662572	0.764350
P	3.253928	-0.075838	-0.479011
O	1.150272	-1.986306	0.708112
C	-0.867779	-3.061296	0.035826
C	-1.482259	-4.112414	-0.666740
C	-0.737230	-5.136159	-1.256266
C	0.655449	-5.119597	-1.157559
C	1.297309	-4.081373	-0.482526
C	0.547293	-3.054385	0.105536
C	2.521958	-3.001783	2.398606
C	2.385346	-2.103067	1.332347
C	3.445055	-1.259556	0.948134
C	4.634030	-1.332027	1.699762

C	4.780268	-2.224278	2.761656
C	3.719909	-3.067691	3.107253
C	-3.613316	-2.208063	0.721719
C	-4.593607	-1.322469	0.251744
C	-5.949483	-1.665795	0.299572
C	-6.341701	-2.900900	0.817724
C	-5.373582	-3.786808	1.304482
C	-4.022350	-3.440022	1.267354
C	-1.544353	-1.790046	2.586073
C	-1.077289	-2.964359	3.196973
C	-0.970326	-3.041961	4.589085
C	-1.330122	-1.950164	5.384029
C	-1.801453	-0.779798	4.782029
C	-1.908395	-0.699574	3.391364
C	4.347445	1.320271	0.066322
C	3.802144	2.219720	1.003418
C	4.534309	3.325493	1.441242
C	5.818982	3.557698	0.938511
C	6.366674	2.676452	0.001334
C	5.638565	1.562571	-0.432593
C	4.241403	-0.897954	-1.817257
C	4.172090	-0.311559	-3.096271
C	4.843557	-0.873745	-4.183524
C	5.581949	-2.050852	-4.019334
C	5.647663	-2.651737	-2.760127
C	4.986862	-2.079104	-1.666961
H	-2.568666	-4.135080	-0.753167
H	-1.246935	-5.940008	-1.791649
H	1.252052	-5.910434	-1.618857
H	5.460602	-0.666897	1.441281
H	5.717062	-2.255588	3.322940
H	3.816347	-3.764710	3.943402
H	-4.292065	-0.348605	-0.135513
H	-6.699461	-0.959845	-0.065814
H	-7.400054	-3.171177	0.854255
H	-5.673490	-4.749364	1.726494
H	-3.285285	-4.132931	1.677951
H	-0.800825	-3.827516	2.587135
H	-0.603632	-3.961192	5.053478
H	-1.241541	-2.010045	6.471590
H	-2.079562	0.081105	5.394724
H	-2.268683	0.223212	2.932064
H	2.798624	2.079391	1.411013
H	4.073784	3.998410	2.168150
H	6.391256	4.427047	1.273279
H	7.369885	2.853095	-0.396617
H	6.081260	0.883337	-1.164507
H	3.585002	0.600433	-3.240540
H	4.782634	-0.396336	-5.165104
H	6.101027	-2.498029	-4.870978
H	6.222417	-3.571606	-2.621893
H	5.060931	-2.557574	-0.688579
H	1.675512	-3.629682	2.677442
H	2.385892	-4.047666	-0.422563
Pd	-1.345108	0.359272	-0.302372
C	-5.055366	3.779141	-1.407695
C	-4.249021	2.696092	-1.715580
C	-2.838252	2.805069	-1.732005
C	-2.245228	4.082675	-1.459078
C	-3.098775	5.169391	-1.133818
C	-4.474272	5.024806	-1.104291
H	-6.142250	3.665308	-1.400387
H	-4.714071	1.739764	-1.958147
C	-1.981458	1.656374	-2.041749
C	-0.806504	4.259475	-1.513545
H	-2.658715	6.138043	-0.896749
H	-5.107691	5.877809	-0.849190
C	-0.022410	3.169192	-1.819140
C	-0.580524	1.886604	-2.056843
H	1.063522	3.280926	-1.858031
H	0.088597	1.090819	-2.389456
C	-0.175373	5.587911	-1.199171
H	-0.620718	6.408388	-1.784082
H	-0.291461	5.820803	-0.127160
H	0.902707	5.563277	-1.410265
C	-2.439197	0.287984	-2.184027
Si	-1.894258	-0.850450	-3.611697
C	-2.067780	0.134909	-5.223794
H	-1.373251	0.990618	-5.245404
H	-1.845785	-0.500236	-6.098260
H	-3.089227	0.531367	-5.346294
C	-0.127808	-1.514629	-3.507730
H	0.631534	-0.717859	-3.553941
H	0.044903	-2.088383	-2.585245
H	0.057445	-2.188649	-4.361351
C	-3.112526	-2.297652	-3.659424
H	-4.148080	-1.942613	-3.791531
H	-2.881143	-2.971547	-4.501104
H	-3.076459	-2.893397	-2.734893
H	-3.517964	0.164445	-2.034430
C	-0.478394	2.274443	1.467907
H	-0.530168	2.975593	0.629892
C	0.157657	1.060899	1.234207
H	0.325727	0.383555	2.075178
H	0.898206	0.995043	0.429281
C	-0.920603	2.820726	2.716523
H	-0.916308	2.128889	3.569210
H	-1.843930	3.414934	2.657853
B	0.237495	4.088743	3.031708
F	-0.051462	4.592565	4.284826
F	1.536681	3.565716	2.975097
F	0.057837	5.059672	2.030335

41-ts

B3LYP SCF energy: -3586.96929659 a.u.
B3LYP enthalpy: -3585.996140 a.u.
B3LYP free energy: -3586.166345 a.u.
M06-L SCF energy in solution: -3589.41500822 a.u.
M06-L enthalpy in solution: -3588.441852 a.u.
M06-L free energy in solution: -3588.612057 a.u.
Imaginary frequency: -11.3557 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-2.029879	-1.499055	0.765383
P	3.173138	-0.308784	-0.477636
O	0.953560	-1.929534	0.875229
C	-1.068522	-2.964684	0.155337
C	-1.689247	-4.033076	-0.513535
C	-0.958348	-5.118305	-1.003531
C	0.426281	-5.149797	-0.831424
C	1.075362	-4.098100	-0.183652
C	0.339286	-3.008835	0.299738
C	2.227339	-2.820979	2.702142
C	2.164643	-2.047015	1.536035
C	3.284402	-1.324843	1.079602
C	4.458183	-1.389988	1.855132
C	4.529414	-2.158859	3.016898
C	3.409110	-2.881785	3.438208
C	-3.810251	-1.998136	0.553989
C	-4.657363	-1.223252	-0.249777
C	-6.013183	-1.546259	-0.378703
C	-6.538346	-2.649799	0.295510
C	-5.704076	-3.425701	1.108660
C	-4.353974	-3.098826	1.243717
C	-1.923034	-1.635565	2.610115
C	-1.459974	-2.781483	3.274479
C	-1.494329	-2.854559	4.671404
C	-1.996126	-1.786198	5.418975
C	-2.463788	-0.642807	4.763362
C	-2.424807	-0.565843	3.369252
C	4.452055	0.995367	-0.135383
C	4.061591	2.056133	0.704822
C	4.940157	3.103734	0.988019
C	6.218655	3.121633	0.419663
C	6.612172	2.081125	-0.425845
C	5.737950	1.022685	-0.699931
C	4.032504	-1.392259	-1.716872
C	3.972635	-0.979328	-3.061660
C	4.567799	-1.735215	-4.073677
C	5.216155	-2.935451	-3.763327
C	5.270162	-3.365470	-2.435243
C	4.687493	-2.599024	-1.419307
H	-2.770552	-4.019094	-0.651807
H	-1.473404	-5.932351	-1.518142
H	1.012747	-5.989384	-1.212766
H	5.334074	-0.822075	1.534962
H	5.456185	-2.189162	3.594850
H	3.447854	-3.480768	4.351514
H	-4.246048	-0.358004	-0.769877
H	-6.659168	-0.927553	-1.006785
H	-7.597103	-2.902863	0.196362
H	-6.109253	-4.285412	1.648665
H	-3.723353	-3.703027	1.899080
H	-1.082041	-3.630794	2.701119
H	-1.130996	-3.754033	5.175679
H	-2.022912	-1.843684	6.510089
H	-2.856373	0.198828	5.339582
H	-2.780414	0.337270	2.868092
H	3.064239	2.067637	1.150984
H	4.614249	3.908970	1.650972
H	6.904519	3.945621	0.633308
H	7.609119	2.087400	-0.875019
H	6.063835	0.214984	-1.358525
H	3.453694	-0.051329	-3.318905
H	4.514853	-1.391589	-5.110059
H	5.673711	-3.534207	-4.555074
H	5.774714	-4.302207	-2.183058
H	4.752633	-2.944807	-0.385715
H	1.335525	-3.352956	3.034030
H	2.159536	-4.106090	-0.066327
Pd	-1.345096	0.451591	-0.282824
C	-4.566791	4.247127	-1.984564
C	-3.840107	3.076770	-2.133561
C	-2.441579	3.035559	-1.924762
C	-1.767392	4.253818	-1.578115
C	-2.539540	5.435456	-1.428284
C	-3.910076	5.437336	-1.622546
H	-5.647013	4.244071	-2.150874
H	-4.360950	2.164476	-2.425718
C	-1.674983	1.791265	-2.096249
C	-0.328553	4.277687	-1.392284
H	-2.040558	6.364991	-1.151667
H	-4.478444	6.362838	-1.499406
C	0.367265	3.103423	-1.537779
C	-0.274950	1.873210	-1.857117
H	1.451970	3.097915	-1.402872
H	0.362931	1.021521	-2.101449
C	0.387731	5.557648	-1.045795
H	0.195410	6.350944	-1.787582
H	0.076844	5.946348	-0.061790

H	1.473828	5.392896	-1.004024
C	-2.255101	0.492955	-2.344820
Si	-1.664857	-0.721863	-3.666291
C	-1.639077	0.167593	-5.346464
H	-0.917747	1.001740	-5.342314
H	-1.352767	-0.520880	-6.160157
H	-2.628605	0.587247	-5.592801
C	0.045323	-1.481085	-3.392103
H	0.846471	-0.725893	-3.409299
H	0.109728	-2.013945	-2.431672
H	0.263448	-2.205143	-4.195462
C	-2.945383	-2.116140	-3.764666
H	-3.957320	-1.718861	-3.950476
H	-2.702861	-2.806692	-4.589838
H	-2.982121	-2.705274	-2.835331
H	-3.351679	0.503949	-2.366727
C	-0.742299	2.432137	1.761470
H	-0.783023	3.192512	0.971634
C	-0.162984	1.148449	1.377009
H	-0.073481	0.436360	2.206074
H	0.797819	1.244475	0.851345
C	-1.229039	2.798056	2.977161
H	-1.200272	2.119240	3.834578
H	-1.750217	3.749178	3.112946
B	0.877953	4.285780	3.278361
F	0.673391	4.303819	4.586134
F	1.856424	3.531073	2.790198
F	0.390332	5.268605	2.529830

42

B3LYP SCF energy: -3262.64417871 a.u.
B3LYP enthalpy: -3261.688840 a.u.
B3LYP free energy: -3261.847617 a.u.
M06-L SCF energy in solution: -3264.79047675 a.u.
M06-L enthalpy in solution: -3263.835138 a.u.
M06-L free energy in solution: -3263.993915 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.558891	-1.783655	-0.229503
P	-3.281974	0.643460	0.020721
O	-1.432587	-1.768507	-0.372269
C	0.371582	-2.606630	0.931423
C	0.797487	-3.274927	2.091038
C	-0.110978	-3.852975	2.981777
C	-1.479538	-3.765791	2.722944
C	-1.937118	-3.091134	1.589903
C	-1.022653	-2.504392	0.706393
C	-2.911191	-3.145357	-1.659469
C	-2.671442	-1.955418	-0.959918
C	-3.629338	-0.923501	-0.925811
C	-4.823720	-1.123598	-1.644919
C	-5.071553	-2.306132	-2.342395
C	-4.111931	-3.323397	-2.344157
C	3.229768	-2.459567	0.232735
C	4.304585	-1.574979	0.400373
C	5.592818	-2.056812	0.660327
C	5.821757	-3.430050	0.759278
C	4.759144	-4.323381	0.580468
C	3.477015	-3.843418	0.308659
C	1.334257	-2.715168	-1.816896
C	0.700681	-3.965718	-1.892076
C	0.660087	-4.669256	-3.100136
C	1.254129	-4.132816	-4.246048
C	1.890061	-2.889894	-4.177204
C	1.929489	-2.183895	-2.971730
C	-4.271473	1.866351	-0.969974
C	-3.682868	2.341242	-2.158265
C	-4.333724	3.291474	-2.947565
C	-5.576427	3.800511	-2.553876
C	-6.163407	3.347170	-1.370146
C	-5.518531	2.384928	-0.584168
C	-4.329692	0.427462	1.539201
C	-4.149073	1.377590	2.562722
C	-4.870541	1.296759	3.755494
C	-5.772648	0.247270	3.959557
C	-5.950187	-0.712054	2.959584
C	-5.238595	-0.621359	1.757706
H	1.864559	-3.349058	2.302855
H	0.254408	-4.366705	3.873575
H	-2.202563	-4.211057	3.410879
H	-5.572890	-0.329085	-1.654560
H	-6.009578	-2.430698	-2.888796
H	-4.289026	-4.250630	-2.894857
H	4.130231	-0.501804	0.313833
H	6.418809	-1.351405	0.781811
H	6.826758	-3.807376	0.965354
H	4.931722	-5.401019	0.642652
H	2.666652	-4.557063	0.146197
H	0.243260	-4.402354	-1.001293
H	0.164956	-5.643212	-3.143501
H	1.222109	-4.682819	-5.190095
H	2.355322	-2.460124	-5.067879
H	2.418973	-1.208409	-2.933269
H	-2.704683	1.962523	-2.469200
H	-3.862914	3.642341	-3.869680
H	-6.082429	4.551125	-3.166612
H	-7.133213	3.740878	-1.053696
H	-5.993676	2.038693	0.335980

H	-3.432173	2.191870	2.423336
H	-4.718623	2.049704	4.533330
H	-6.330869	0.175889	4.896612
H	-6.651678	-1.537131	3.110632
H	-5.401973	-1.373865	0.983718
H	-2.136113	-3.911950	-1.678760
H	-3.006396	-2.997308	1.397024
Pd	1.367289	0.521609	-0.164144
C	5.857596	3.282871	0.051669
C	4.769938	2.638009	0.619520
C	3.439403	2.992050	0.295975
C	3.224439	4.076124	-0.618177
C	4.357878	4.715011	-1.185758
C	5.648269	4.327631	-0.866027
H	6.873356	2.983399	0.322093
H	4.945403	1.843163	1.345236
C	2.292774	2.306877	0.914074
C	1.880537	4.515785	-0.942198
H	4.210158	5.533534	-1.891432
H	6.500772	4.839218	-1.320361
C	0.822573	3.857045	-0.368511
C	0.998827	2.756118	0.520308
H	-0.198052	4.177427	-0.595577
H	0.121802	2.400459	1.066534
C	1.652340	5.671131	-1.883154
H	2.129736	6.598314	-1.522476
H	2.063423	5.470926	-2.887721
H	0.577509	5.871823	-1.999059
C	2.388516	1.150555	1.765221
Si	1.447229	0.952413	3.391042
C	1.547392	2.577756	4.372554
H	1.050540	3.400672	3.832391
H	1.060003	2.479744	5.357858
H	2.594777	2.878297	4.541682
C	-0.380697	0.485367	3.246552
H	-0.963671	1.235328	2.689515
H	-0.517416	-0.479834	2.736641
H	-0.827349	0.401489	4.251999
C	2.340498	-0.393709	4.384185
H	3.392197	-0.119513	4.571351
H	1.855753	-0.547204	5.362915
H	2.334323	-1.358612	3.852875
H	3.408642	0.774689	1.900756
C	1.022494	1.460419	-2.985640
H	1.345744	2.460758	-2.669381
C	0.258720	0.692631	-1.987595
H	-0.095975	-0.273595	-2.368495
H	-0.595525	1.262815	-1.588187
C	1.366437	1.072752	-4.231408
H	1.051738	0.108248	-4.642439
H	1.958600	1.720285	-4.884903

43-ts

B3LYP SCF energy: -3262.62913864 a.u.
B3LYP enthalpy: -3261.674634 a.u.
B3LYP free energy: -3261.829433 a.u.
M06-L SCF energy in solution: -3264.77488981 a.u.
M06-L enthalpy in solution: -3263.820385 a.u.
M06-L free energy in solution: -3263.975184 a.u.
Imaginary frequency: -336.0902 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.721025	-1.649496	-0.374626
P	-3.353926	0.411298	0.024160
O	-1.323036	-1.773789	-0.637437
C	0.504703	-2.601417	0.660709
C	0.928619	-3.326805	1.788536
C	0.028873	-3.998816	2.618962
C	-1.335346	-3.956681	2.330887
C	-1.793151	-3.233181	1.229307
C	-0.887965	-2.547994	0.409062
C	-2.699555	-3.120241	-2.062974
C	-2.551085	-1.996986	-1.240369
C	-3.594151	-1.060985	-1.090241
C	-4.775505	-1.282616	-1.823984
C	-4.929188	-2.398547	-2.647776
C	-3.888551	-3.324744	-2.761686
C	3.358802	-2.424770	0.069402
C	4.425793	-1.599531	0.447546
C	5.690260	-2.137976	0.714770
C	5.901676	-3.513241	0.609640
C	4.844737	-4.348585	0.228280
C	3.587548	-3.809183	-0.046766
C	1.552814	-2.405339	-2.067150
C	0.910140	-3.629012	-2.310418
C	0.904700	-4.190012	-3.591752
C	1.544373	-3.536945	-4.648683
C	2.194980	-2.321832	-4.415126
C	2.197891	-1.760988	-3.135555
C	-4.613275	1.588513	-0.667347
C	-4.265975	2.269793	-1.850576
C	-5.128537	3.212914	-2.412020
C	-6.346674	3.509817	-1.790098
C	-6.694605	2.852780	-0.607717
C	-5.836703	1.896952	-0.050662
C	-4.162752	-0.156392	1.596813
C	-3.797752	0.524478	2.772057
C	-4.357071	0.178454	4.005234

C	-5.279897	-0.868520	4.086630
C	-5.642440	-1.562280	2.927959
C	-5.090933	-1.207874	1.692479
H	1.992270	-3.372714	2.023139
H	0.398406	-4.551510	3.485472
H	-2.054775	-4.475424	2.969218
H	-5.590642	-0.560501	-1.745147
H	-5.859844	-2.542223	-3.202120
H	-3.993708	-4.199737	-3.407926
H	4.255558	-0.526366	0.528010
H	6.509836	-1.476138	1.006274
H	6.887491	-3.936656	0.819042
H	5.003148	-5.426365	0.136817
H	2.780428	-4.475135	-0.358183
H	0.418980	-4.158733	-1.491131
H	0.401162	-5.145547	-3.762646
H	1.538785	-3.974970	-5.650048
H	2.702723	-1.804707	-5.233378
H	2.714315	-0.814193	-2.962134
H	-3.308365	2.061004	-2.336510
H	-4.843430	3.726047	-3.334291
H	-7.018595	4.254738	-2.224234
H	-7.642382	3.080898	-0.112504
H	-6.126433	1.390062	0.871933
H	-3.061387	1.330953	2.720269
H	-4.060957	0.721276	4.906586
H	-5.711805	-1.146745	5.051482
H	-6.362164	-2.383549	2.983896
H	-5.390431	-1.755575	0.796272
H	-1.865288	-3.813947	-2.163761
H	-2.860230	-3.177551	1.013280
Pd	1.551037	0.666377	-0.134537
C	5.258235	3.294895	-1.151124
C	4.436904	2.697062	-0.208904
C	3.102284	3.124151	0.004034
C	2.610097	4.213007	-0.780816
C	3.470416	4.803268	-1.740489
C	4.768861	4.358588	-1.929173
H	6.285164	2.943686	-1.281149
H	4.839405	1.886214	0.398232
C	2.239481	2.505122	1.036259
C	1.244970	4.697642	-0.593544
H	3.104261	5.634603	-2.344345
H	5.410188	4.839357	-2.672466
C	0.587376	4.286866	0.601882
C	1.021573	3.216216	1.336823
H	-0.349596	4.780343	0.877326
H	0.428810	2.883655	2.190077
C	0.850907	6.035593	-1.186771
H	1.465568	6.848368	-0.761312
H	0.968973	6.074219	-2.280059
H	-0.201678	6.262874	-0.960196
C	2.609988	1.329178	1.754931
Si	1.980595	0.805033	3.451156
C	2.236700	2.203654	4.716437
H	1.653536	3.103293	4.461096
H	1.932754	1.881735	5.727482
H	3.297448	2.501694	4.763301
C	0.156176	0.293937	3.506947
H	-0.516563	1.122849	3.235764
H	-0.051060	-0.536554	2.814504
H	-0.116114	-0.036169	4.524008
C	3.035166	-0.666005	4.017905
H	4.103390	-0.396001	4.066791
H	2.730092	-1.000358	5.023735
H	2.939637	-1.524019	3.334466
H	3.656222	1.029834	1.637088
C	-0.162468	2.109648	-1.696041
H	-1.055923	2.021693	-1.065738
C	0.473674	0.893785	-2.034276
H	1.227655	0.929655	-2.830075
H	-0.153569	0.000298	-2.047027
C	0.188284	3.402100	-2.108338
H	0.953323	3.524370	-2.880722
H	-0.603328	4.151668	-2.108142

44

B3LYP SCF energy: -3262.65652957 a.u.
B3LYP enthalpy: -3261.699689 a.u.
B3LYP free energy: -3261.853883 a.u.
M06-L SCF energy in solution: -3264.80003560 a.u.
M06-L enthalpy in solution: -3263.843195 a.u.
M06-L free energy in solution: -3263.997389 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.646697	-1.733109	-0.320377
P	-3.306625	0.484847	0.000499
O	-1.379807	-1.805604	-0.564729
C	0.431452	-2.695897	0.709656
C	0.843515	-3.452780	1.820664
C	-0.068698	-4.112234	2.648549
C	-1.434149	-4.022481	2.377925
C	-1.880700	-3.268341	1.292003
C	-0.961087	-2.603632	0.471517
C	-2.798998	-3.139301	-1.964662
C	-2.605748	-1.995778	-1.179255
C	-3.599914	-1.002172	-1.081022
C	-4.777835	-1.185427	-1.830716

C	-4.976612	-2.320437	-2.617761
C	-3.985387	-3.304896	-2.677590
C	3.285053	-2.521634	0.097986
C	4.366291	-1.691108	0.423762
C	5.634775	-2.228482	0.673517
C	5.837445	-3.607293	0.601291
C	4.768675	-4.447085	0.265561
C	3.507082	-3.908938	0.007917
C	1.455769	-2.473522	-2.018873
C	0.822258	-3.700674	-2.268399
C	0.793656	-4.240158	-3.558735
C	1.403046	-3.563051	-4.618473
C	2.043906	-2.343634	-4.379233
C	2.066994	-1.802792	-3.091083
C	-4.416350	1.732273	-0.812461
C	-3.916495	2.362256	-1.968846
C	-4.659194	3.345842	-2.624551
C	-5.906979	3.734655	-2.123953
C	-6.405539	3.128673	-0.968307
C	-5.668250	2.132248	-0.317663
C	-4.258482	0.044684	1.533691
C	-3.978769	0.807224	2.682757
C	-4.639282	0.558004	3.888314
C	-5.578876	-0.474262	3.972269
C	-5.855576	-1.249507	2.842599
C	-5.203282	-0.991287	1.632093
H	1.907391	-3.535363	2.043794
H	0.292616	-4.691322	3.501265
H	-2.162048	-4.528648	3.016793
H	-5.554133	-0.418365	-1.792178
H	-5.903116	-2.434446	-3.185762
H	-4.126541	-4.195761	-3.294682
H	4.209980	-0.612733	0.466506
H	6.465236	-1.562901	0.922719
H	6.826327	-4.029771	0.797802
H	4.921394	-5.527336	0.195390
H	2.690854	-4.578439	-0.271185
H	0.353917	-4.248522	-1.447432
H	0.295854	-5.197815	-3.734702
H	1.380735	-3.985003	-5.626512
H	2.527611	-1.807604	-5.200018
H	2.571118	-0.849535	-2.913118
H	-2.933176	2.079312	-2.356377
H	-4.257470	3.819020	-3.524547
H	-6.485086	4.511529	-2.631027
H	-7.377688	3.429031	-0.567962
H	-6.074005	1.665390	0.582238
H	-3.229225	1.601588	2.632795
H	-4.409648	1.164773	4.768096
H	-6.089629	-0.677424	4.917116
H	-6.586730	-2.060476	2.900488
H	-5.437935	-1.602334	0.758011
H	-2.001586	-3.879978	-2.024775
H	-2.947729	-3.175457	1.087077
Pd	1.488680	0.652930	-0.107056
C	5.589034	3.070441	-0.767987
C	4.639457	2.535292	0.099021
C	3.294758	2.955912	0.073244
C	2.916749	3.964132	-0.847324
C	3.886622	4.493469	-1.713346
C	5.211348	4.055270	-1.684293
H	6.625885	2.727163	-0.719606
H	4.954422	1.790082	0.830815
C	2.271661	2.420277	1.025483
C	1.453827	4.405873	-0.916368
H	3.608645	5.266912	-2.430933
H	5.945677	4.488720	-2.368216
C	0.842929	4.345848	0.463228
C	1.182427	3.370523	1.321923
H	0.044069	5.052388	0.708751
H	0.657072	3.273630	2.274734
C	1.295019	5.823245	-1.496474
H	1.913606	6.551049	-0.949166
H	1.567446	5.871632	-2.561909
H	0.243626	6.142138	-1.416098
C	2.502880	1.267247	1.809963
Si	1.710401	0.812662	3.462692
C	2.070764	2.164412	4.752354
H	1.608636	3.129560	4.489683
H	1.687587	1.868522	5.744215
H	3.156032	2.334341	4.849666
C	-0.159575	0.538876	3.380630
H	-0.693197	1.458529	3.093829
H	-0.418562	-0.234531	2.640998
H	-0.547593	0.217721	4.362118
C	2.555379	-0.770212	4.069630
H	3.642094	-0.620036	4.182906
H	2.155531	-1.075775	5.050956
H	2.403022	-1.605424	3.369853
H	3.504695	0.833404	1.731225
C	0.140934	2.109357	-1.342190
H	-0.633960	2.208514	-0.574295
C	0.240021	0.894444	-1.991909
H	0.836204	0.807354	-2.905441
H	-0.492998	0.106670	-1.816668
C	0.677032	3.406782	-1.882218
H	1.311219	3.222183	-2.765034
H	-0.203854	3.969106	-2.242437

45

B3LYP SCF energy: -3254.63869253 a.u.
B3LYP enthalpy: -3253.745562 a.u.
B3LYP free energy: -3253.896443 a.u.
M06-L SCF energy in solution: -3256.82858594 a.u.
M06-L enthalpy in solution: -3255.935455 a.u.
M06-L free energy in solution: -3256.086336 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.535149	-1.910569	-0.077940
P	2.288282	0.640342	0.099329
O	2.111918	-1.621017	-1.515057
C	0.081221	-2.889733	-1.536190
C	-0.672938	-3.912579	-2.141580
C	-0.200015	-4.595132	-3.265528
C	1.037646	-4.263466	-3.820718
C	1.815511	-3.267233	-3.228131
C	1.348103	-2.611624	-2.087426
C	3.838344	-3.077455	-0.564249
C	3.106096	-1.890408	-0.600574
C	3.365298	-0.839305	0.296739
C	4.400163	-0.993341	1.229315
C	5.145972	-2.175331	1.272380
C	4.859745	-3.212340	0.381219
C	-2.257811	-2.548524	0.147936
C	-3.193998	-2.438243	-0.897299
C	-4.498855	-2.904008	-0.734605
C	-4.897528	-3.474244	0.478835
C	-3.979206	-3.581077	1.524097
C	-2.666893	-3.124884	1.361841
C	0.345191	-2.633681	1.373679
C	0.823817	-3.953876	1.364556
C	1.391391	-4.506052	2.516082
C	1.479068	-3.752008	3.689948
C	0.998396	-2.439278	3.709602
C	0.439407	-1.882065	2.556253
C	2.816451	1.762300	1.471588
C	2.585941	1.347258	2.798604
C	2.898617	2.182948	3.872748
C	3.430337	3.456484	3.642093
C	3.650648	3.884541	2.331323
C	3.349234	3.044851	1.252389
C	2.984360	1.393165	-1.439236
C	2.133988	1.691582	-2.514677
C	2.650434	2.209870	-3.707320
C	4.023219	2.433007	-3.836644
C	4.881116	2.128050	-2.773626
C	4.367700	1.605428	-1.585146
H	-1.645225	-4.185514	-1.733409
H	-0.809520	-5.384738	-3.710298
H	1.401352	-4.780514	-4.711638
H	4.626780	-0.188568	1.930494
H	5.951179	-2.283286	2.002086
H	5.440009	-4.137608	0.412899
H	-2.909807	-1.987157	-1.847897
H	-5.208498	-2.814194	-1.560363
H	-5.921304	-3.833707	0.607305
H	-4.278999	-4.025256	2.476188
H	-1.968552	-3.225951	2.192588
H	0.750066	-4.559728	0.459381
H	1.762469	-5.533537	2.495970
H	1.918944	-4.188228	4.589994
H	1.056297	-1.847957	4.626791
H	0.062052	-0.856702	2.577166
H	2.170235	0.356657	2.996327
H	2.723500	1.839508	4.895207
H	3.671621	4.111448	4.482591
H	4.067084	4.876757	2.141059
H	3.542261	3.395492	0.237107
H	1.061528	1.501377	-2.426044
H	1.977422	2.431443	-4.539199
H	4.427948	2.836111	-4.768164
H	5.957043	2.290375	-2.873715
H	5.051809	1.354110	-0.771212
H	3.619305	-3.884527	-1.263897
H	2.786745	-2.984539	-3.638488
Pd	-0.250107	0.497159	-0.101195
C	-3.933238	0.718962	2.881218
C	-2.954744	0.628664	1.913257
C	-3.258482	0.711954	0.524160
C	-4.639933	0.876716	0.139208
C	-5.623352	0.965467	1.166225
C	-5.284346	0.893532	2.501777
H	-3.667786	0.652828	3.939213
H	-1.913018	0.481776	2.206471
C	-2.247292	0.634932	-0.487133
C	-4.992577	0.953743	-1.251969
H	-6.671018	1.093831	0.890508
H	-6.060356	0.967106	3.267578
C	-3.980921	0.867537	-2.190625
C	-2.621023	0.707568	-1.814813
H	-4.229896	0.922606	-3.254561
H	-1.873272	0.627679	-2.609890
C	-6.427725	1.126304	-1.683417
H	-7.064912	0.299170	-1.328368
H	-6.866293	2.057445	-1.287209
H	-6.507346	1.161875	-2.779242
N	-0.407677	2.920151	1.476561
N	-0.646568	3.041470	2.566409
C	-0.204184	2.769181	0.150037
Si	-1.198662	4.155023	-0.842875

C	-0.343635	5.761789	-0.335841
H	0.727744	5.761965	-0.594754
H	-0.809738	6.613087	-0.860478
H	-0.433184	5.959149	0.745258
C	-0.944914	3.860067	-2.679251
H	0.121596	3.887829	-2.950301
H	-1.374014	2.904751	-3.011424
H	-1.450273	4.668350	-3.234433
C	-2.999829	4.211754	-0.330383
H	-3.121179	4.269637	0.763243
H	-3.452960	5.122738	-0.757032
H	-3.568149	3.345103	-0.694107
H	0.860009	2.991426	-0.019613

46

B3LYP SCF energy: -5713.17686794 a.u.
B3LYP enthalpy: -5712.338354 a.u.
B3LYP free energy: -5712.495405 a.u.
M06-L SCF energy in solution: -5715.59228203 a.u.
M06-L enthalpy in solution: -5714.753768 a.u.
M06-L free energy in solution: -5714.910819 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.971230	-1.220700	-0.840856
P	-3.214535	-0.069318	0.472439
O	-0.993633	-1.820104	-0.464337
C	1.179392	-2.762209	-0.143337
C	1.939761	-3.861494	0.297198
C	1.342300	-5.023169	0.789648
C	-0.050665	-5.109162	0.859252
C	-0.832119	-4.040928	0.426006
C	-0.226018	-2.881177	-0.080152
C	-2.050286	-2.837537	-2.378964
C	-2.097852	-1.982482	-1.271068
C	-3.242958	-1.213480	-0.991699
C	-4.332978	-1.322074	-1.871561
C	-4.300491	-2.177587	-2.974616
C	-3.153891	-2.937323	-3.224945
C	3.754879	-1.461712	-0.362509
C	4.105281	-1.587665	0.995082
C	5.440967	-1.720720	1.379046
C	6.457211	-1.707195	0.418624
C	6.123753	-1.566409	-0.929878
C	4.784582	-1.449776	-1.318418
C	2.036366	-1.597428	-2.656089
C	1.959530	-2.906491	-3.158577
C	2.077973	-3.149767	-4.530881
C	2.283344	-2.087756	-5.416241
C	2.364386	-0.782436	-4.923599
C	2.231506	-0.535189	-3.554210
C	-4.452978	1.211806	-0.049032
C	-3.994134	2.194843	-0.948688
C	-4.834436	3.236520	-1.347482
C	-6.138269	3.324363	-0.846871
C	-6.599458	2.358258	0.050826
C	-5.764090	1.306916	0.446482
C	-4.167684	-1.046964	1.738784
C	-4.158788	-0.545107	3.055240
C	-4.808837	-1.222636	4.089444
C	-5.462544	-2.433361	3.834001
C	-5.464942	-2.952532	2.536800
C	-4.827145	-2.264345	1.497899
H	3.027365	-3.810609	0.247073
H	1.967364	-5.855810	1.121348
H	-0.532207	-6.005978	1.258021
H	-5.222764	-0.716314	-1.685976
H	-5.163100	-2.241331	-3.642739
H	-3.106575	-3.596686	-4.095759
H	3.331165	-1.584876	1.763372
H	5.685283	-1.818960	2.439682
H	7.503667	-1.801022	0.721606
H	6.907395	-1.550417	-1.692298
H	4.548051	-1.349888	-2.378346
H	1.811195	-3.747424	-2.478471
H	2.010856	-4.174701	-4.906428
H	2.373858	-2.276804	-6.489585
H	2.510738	0.056998	-5.607983
H	2.258420	0.489937	-3.183072
H	-2.973503	2.139691	-1.343063
H	-4.458365	3.991618	-2.042588
H	-6.789741	4.148382	-1.151066
H	-7.616564	2.419450	0.449155
H	-6.139376	0.559720	1.149244
H	-3.627752	0.386804	3.270676
H	-4.793104	-0.809521	5.101813
H	-5.962343	-2.971252	4.644328
H	-5.970699	-3.899577	2.326939
H	-4.847536	-2.678837	0.487795
H	-1.136942	-3.397090	-2.586891
H	-1.921312	-4.082584	0.482386
Pd	1.052442	0.923154	-0.220581
C	-0.261748	-0.782787	3.918344
C	0.265096	-0.238298	2.764002
C	1.551746	0.375856	2.740279
C	2.301559	0.430462	3.974595
C	1.723851	-0.140139	5.146557
C	0.477991	-0.734083	5.123081
H	-1.251400	-1.246071	3.899953

H	-0.310763	-0.260550	1.835768
C	2.099152	0.924656	1.527698
C	3.593382	1.054853	3.995302
H	2.279586	-0.104427	6.085907
H	0.060421	-1.164057	6.038379
C	4.081845	1.577286	2.812411
C	3.353699	1.507576	1.598594
H	5.064261	2.061134	2.807713
H	3.814813	1.929556	0.701556
Br	-0.439329	1.078616	-2.341512
C	4.395016	1.151977	5.270882
H	3.858793	1.716316	6.053879
H	4.623107	0.159288	5.698056
H	5.352131	1.664075	5.090852
C	1.220085	3.533025	-0.062339
H	2.104474	3.627655	0.578240
C	0.144069	2.816589	0.475003
H	-0.818687	2.858389	-0.038230
H	0.107318	2.680924	1.559411
C	1.246164	4.308521	-1.267515
H	0.446680	4.070027	-1.980289
H	2.235189	4.334995	-1.749711
B	1.048249	5.962591	-0.783825
F	1.117555	6.723494	-1.951159
F	-0.188484	6.116664	-0.159483
F	2.093900	6.295268	0.086711

47-ts

B3LYP SCF energy: -3024.28971445 a.u.
B3LYP enthalpy: -3023.404846 a.u.
B3LYP free energy: -3023.565630 a.u.
M06-L SCF energy in solution: -3026.24128944 a.u.
M06-L enthalpy in solution: -3025.356421 a.u.
M06-L free energy in solution: -3025.517205 a.u.
Imaginary frequency: -523.4720 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.878486	0.914401	0.784497
C	-2.265873	0.973402	2.600365
C	-1.197139	1.218222	3.484004
C	-3.541300	0.741046	3.139589
C	-1.403922	1.257694	4.864583
H	-0.191111	1.367193	3.081122
C	-3.745193	0.766250	4.524101
H	-4.383757	0.534247	2.476894
C	-2.680884	1.029305	5.389842
H	-0.562351	1.455598	5.533989
H	-4.744340	0.577072	4.926028
H	-2.842555	1.048846	6.470911
C	-3.401834	0.215789	0.012954
C	-4.584426	0.944494	-0.205770
C	-3.391595	-1.127515	-0.397392
C	-5.705849	0.361987	-0.790508
H	-4.635262	1.998210	0.079457
C	-4.503708	-1.728667	-0.980695
H	-2.476770	-1.711758	-0.264627
C	-5.700623	-0.999010	-1.192396
H	-6.592855	0.977274	-0.938409
H	-4.430925	-2.773141	-1.281868
C	-2.025632	2.703857	0.295050
C	-1.839901	3.025774	-1.062311
C	-2.284349	3.745563	1.200130
C	-1.933502	4.345316	-1.504661
H	-1.618814	2.232952	-1.781854
C	-2.365201	5.071687	0.757814
H	-2.432349	3.525290	2.258959
C	-2.196003	5.375874	-0.594424
H	-1.788005	4.572329	-2.563849
H	-2.569672	5.868788	1.478136
H	-2.263089	6.411110	-0.939318
N	-6.810549	-1.583795	-1.771440
C	-8.007660	-0.801814	-1.999428
H	-7.825230	0.059060	-2.669781
H	-8.772446	-1.433726	-2.469096
H	-8.432995	-0.403780	-1.059299
C	-6.769739	-2.973546	-2.176441
H	-6.555247	-3.648334	-1.327296
H	-7.744060	-3.261301	-2.592050
H	-6.003593	-3.164109	-2.951570
P	1.832154	0.337741	-0.798484
C	1.875767	-0.488779	-2.463182
C	0.645005	-0.693371	-3.115956
C	3.047648	-0.950665	-3.083440
C	0.591097	-1.319263	-4.363239
H	-0.278923	-0.369179	-2.628375
C	2.991701	-1.589785	-4.327857
H	4.013355	-0.817299	-2.592419
C	1.766463	-1.772085	-4.973497
H	-0.374215	-1.464320	-4.855707
H	3.914594	-1.947107	-4.792905
H	1.725012	-2.270922	-5.945394
C	3.556687	0.169129	-0.149934
C	4.647876	0.905368	-0.647508
C	3.813944	-0.710934	0.912675
C	5.931309	0.757569	-0.129576
H	4.496125	1.621524	-1.458766
C	5.090520	-0.872562	1.446136
H	2.982809	-1.277233	1.338550

C	6.193194	-0.143098	0.935421
H	6.735165	1.357097	-0.555434
H	5.223509	-1.567381	2.274580
C	1.845523	2.140426	-1.266906
C	1.770529	3.080912	-0.222946
C	1.923682	2.610785	-2.587428
C	1.795157	4.449905	-0.489268
H	1.690193	2.733222	0.810915
C	1.937155	3.985445	-2.855305
H	1.980910	1.903861	-3.417503
C	1.878404	4.908383	-1.809197
H	1.736373	5.163930	0.336256
H	2.000068	4.332552	-3.890543
H	1.890714	5.981131	-2.019129
N	7.464100	-0.293790	1.455874
C	8.562856	0.487520	0.927247
H	8.398961	1.575501	1.042629
H	9.484993	0.230115	1.464083
H	8.735303	0.291700	-0.147383
C	7.693407	-1.205852	2.557086
H	7.418855	-2.245753	2.300579
H	8.758792	-1.198713	2.821097
H	7.120773	-0.926348	3.461578
Pd	0.073230	-0.510352	0.504659
N	-1.068694	-2.783350	2.410824
N	-2.144669	-2.772973	2.712231
C	0.304194	-2.353808	1.369957
Si	0.507871	-3.988722	0.384469
C	0.417223	-5.528280	1.496429
H	-0.570471	-5.631404	1.975459
H	0.598803	-6.446147	0.910884
H	1.173851	-5.488939	2.298019
C	-0.832344	-4.139831	-0.941548
H	-1.839130	-4.179854	-0.493186
H	-0.798301	-3.282430	-1.631742
H	-0.695755	-5.061092	-1.532750
C	2.218435	-3.948674	-0.419211
H	3.017335	-3.825556	0.329746
H	2.398726	-4.900507	-0.947598
H	2.309272	-3.131465	-1.149893
H	1.025998	-2.362276	2.208246

48

B3LYP SCF energy: -2914.88247986 a.u.
B3LYP enthalpy: -2914.007157 a.u.
B3LYP free energy: -2914.161627 a.u.
M06-L SCF energy in solution: -2916.72038386 a.u.
M06-L enthalpy in solution: -2915.845061 a.u.
M06-L free energy in solution: -2915.999531 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.778282	0.851258	0.686030
C	-1.976367	1.216741	2.494947
C	-0.822976	1.260525	3.296649
C	-3.226837	1.434576	3.096395
C	-0.914801	1.538550	4.663299
H	0.150294	1.048238	2.845333
C	-3.318810	1.705440	4.465295
H	-4.136914	1.385363	2.494425
C	-2.163733	1.762102	5.251078
H	-0.007846	1.567052	5.272991
H	-4.299631	1.868640	4.920144
H	-2.237747	1.970728	6.321713
C	-3.401625	0.116851	0.199469
C	-4.496941	0.872104	-0.254334
C	-3.577713	-1.274486	0.299344
C	-5.710913	0.275125	-0.588130
H	-4.408671	1.955757	-0.357066
C	-4.785414	-1.885579	-0.022415
H	-2.738128	-1.889660	0.633918
C	-5.893949	-1.126576	-0.477737
H	-6.521801	0.912763	-0.938654
H	-4.858842	-2.968234	0.074425
C	-1.893022	2.537468	-0.086155
C	-1.734465	2.628623	-1.480898
C	-2.114018	3.717584	0.641559
C	-1.820602	3.859301	-2.132691
H	-1.544257	1.724030	-2.064487
C	-2.191042	4.953490	-0.011372
H	-2.233273	3.677331	1.725605
C	-2.050423	5.028429	-1.398559
H	-1.698416	3.907633	-3.217807
H	-2.365483	5.861683	0.572116
H	-2.112701	5.993909	-1.907390
N	-7.094695	-1.726580	-0.803218
C	-8.198625	-0.925471	-1.288852
H	-7.952747	-0.395344	-2.228341
H	-9.060717	-1.574891	-1.488311
H	-8.516999	-0.163290	-0.553496
C	-7.241423	-3.163523	-0.692675
H	-7.070784	-3.520826	0.339509
H	-8.261778	-3.448952	-0.979313
H	-6.540963	-3.709909	-1.351812
P	1.801348	0.352856	-0.720615
C	1.912753	-0.366517	-2.427932
C	0.715468	-0.631922	-3.115430
C	3.132410	-0.670557	-3.054356
C	0.736743	-1.165344	-4.406735

H	-0.240447	-0.438895	-2.621582
C	3.152840	-1.212779	-4.343730
H	4.073530	-0.489494	-2.531122
C	1.957060	-1.456867	-5.024934
H	-0.204042	-1.366962	-4.925547
H	4.110434	-1.448170	-4.815997
H	1.975140	-1.882411	-6.031753
C	3.452859	0.004270	0.030048
C	4.576628	0.826239	-0.170792
C	3.628263	-1.137781	0.829866
C	5.816099	0.522906	0.386936
H	4.490300	1.731359	-0.775836
C	4.860742	-1.458389	1.390632
H	2.768341	-1.785327	1.019833
C	5.997293	-0.635643	1.184876
H	6.648568	1.199967	0.198826
H	4.932198	-2.356079	2.003459
C	1.933487	2.178790	-1.038071
C	1.819530	3.042312	0.066576
C	2.135993	2.738089	-2.309669
C	1.927331	4.424292	-0.092091
H	1.646948	2.627002	1.063220
C	2.234715	4.125244	-2.469579
H	2.224895	2.091134	-3.184243
C	2.135184	4.971465	-1.363386
H	1.839326	5.078528	0.779113
H	2.394432	4.543272	-3.467325
H	2.213227	6.054455	-1.489590
N	7.222858	-0.943969	1.741845
C	8.358715	-0.072013	1.525931
H	8.184437	0.948755	1.914903
H	9.236023	-0.480620	2.043696
H	8.615899	0.022436	0.454415
C	7.371508	-2.131898	2.557608
H	7.127722	-3.054517	1.999285
H	8.412237	-2.213129	2.896778
H	6.726067	-2.108748	3.455636
Pd	0.028940	-0.696033	0.440161
C	0.165737	-2.519610	1.079986
Si	-0.106191	-4.180325	0.247242
C	-1.241354	-5.260374	1.332700
H	-2.229624	-4.791883	1.473593
H	-1.402577	-6.250291	0.871593
H	-0.803950	-5.419980	2.332254
C	-0.896942	-4.027717	-1.467988
H	-1.871106	-3.514785	-1.411364
H	-0.253980	-3.443666	-2.146361
H	-1.059565	-5.019842	-1.923257
C	1.562654	-5.079892	0.057543
H	2.038797	-5.249880	1.037526
H	1.427445	-6.061820	-0.428318
H	2.262059	-4.493069	-0.560343
H	0.574880	-2.680646	2.101263

49

B3LYP SCF energy: -4743.43963104 a.u.
B3LYP enthalpy: -4742.756602 a.u.
B3LYP free energy: -4742.884963 a.u.
M06-L SCF energy in solution: -4744.99603430 a.u.
M06-L enthalpy in solution: -4744.313005 a.u.
M06-L free energy in solution: -4744.441366 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.198526	1.100397	-0.046440
C	-1.446842	2.414110	1.239125
C	-0.348469	3.214325	1.592336
C	-2.687650	2.662004	1.853429
C	-0.485739	4.246170	2.524445
H	0.621153	3.015790	1.131627
C	-2.822078	3.689381	2.792442
H	-3.554807	2.047576	1.603170
C	-1.723211	4.485328	3.129099
H	0.381391	4.858416	2.785271
H	-3.793027	3.868099	3.262147
H	-1.830059	5.286671	3.864850
C	-2.618865	-0.040139	0.229423
C	-3.468091	-0.461930	-0.807109
C	-2.805903	-0.636290	1.491430
C	-4.460079	-1.418679	-0.600085
H	-3.359268	-0.038123	-1.807558
C	-3.797469	-1.585028	1.718128
H	-2.165900	-0.346573	2.329568
C	-4.658691	-2.010138	0.672276
H	-5.085883	-1.703260	-1.444982
H	-3.898369	-2.000954	2.719919
C	-1.655750	1.956111	-1.628280
C	-0.969351	1.616840	-2.805732
C	-2.675106	2.921905	-1.689495
C	-1.304418	2.221974	-4.021656
H	-0.161467	0.881485	-2.763697
C	-3.002179	3.531121	-2.903467
H	-3.214153	3.209782	-0.784692
C	-2.319179	3.180962	-4.073044
H	-0.762140	1.945949	-4.929687
H	-3.792576	4.285722	-2.934622
H	-2.575170	3.659993	-5.021797
N	-5.640508	-2.956274	0.885962
C	-6.482491	-3.386545	-0.211734

H	-5.900518	-3.848376	-1.031282
H	-7.201135	-4.132772	0.150365
H	-7.059324	-2.549262	-0.645683
C	-5.792414	-3.564429	2.191960
H	-6.029317	-2.819384	2.973802
H	-6.616737	-4.288362	2.163231
H	-4.881646	-4.104200	2.512763
Pd	0.998594	0.238988	-0.262495
C	2.321823	1.586933	-0.682310
Si	3.580425	2.420920	0.441276
C	5.274529	1.979890	-0.303019
H	5.372888	2.363107	-1.331844
H	6.084690	2.421937	0.302215
H	5.424393	0.888958	-0.330762
C	3.430498	4.320336	0.468291
H	4.226593	4.766937	1.089068
H	3.522191	4.736846	-0.548526
H	2.463288	4.656508	0.876481
C	3.498590	1.770626	2.217702
H	2.521408	1.978317	2.683160
H	3.644979	0.678372	2.226115
H	4.279153	2.227949	2.849274
H	2.312754	2.064883	-1.684107
C	5.048506	-2.957462	-0.656102
C	3.787771	-2.616730	-1.119068
C	2.707825	-2.417685	-0.229222
C	2.924716	-2.597007	1.178873
C	4.228469	-2.939569	1.616783
C	5.273614	-3.115701	0.723695
H	5.867506	-3.099516	-1.365719
H	3.617363	-2.483537	-2.187859
C	1.377243	-2.037298	-0.672869
C	1.826288	-2.442062	2.114247
H	4.414617	-3.069727	2.683812
H	6.268175	-3.380089	1.091732
C	0.574003	-2.158915	1.629153
C	0.306037	-1.967248	0.233727
H	-0.269813	-2.095276	2.320822
H	-0.723147	-2.005143	-0.120224
Br	0.922376	-2.269844	-2.545797
C	2.050176	-2.628685	3.593308
H	2.439359	-3.634240	3.827287
H	2.780745	-1.903089	3.989965
H	1.112153	-2.494076	4.151013

50-ts

B3LYP SCF energy: -4743.42051901 a.u.
B3LYP enthalpy: -4742.739234 a.u.
B3LYP free energy: -4742.867792 a.u.
M06-L SCF energy in solution: -4744.98039244 a.u.
M06-L enthalpy in solution: -4744.299107 a.u.
M06-L free energy in solution: -4744.427665 a.u.
Imaginary frequency: -198.0900 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.448642	0.739423	0.559289
C	2.092175	2.341473	-0.114102
C	1.540659	3.545411	0.361079
C	3.103321	2.395787	-1.084900
C	2.004771	4.773473	-0.109902
H	0.740321	3.522172	1.105345
C	3.556029	3.630010	-1.568348
H	3.544961	1.473300	-1.466481
C	3.013882	4.819889	-1.079960
H	1.569331	5.699842	0.273191
H	4.341495	3.655807	-2.328208
H	3.371016	5.782344	-1.455037
C	2.559134	-0.537160	-0.149840
C	3.789133	-0.903248	0.423134
C	2.173686	-1.195559	-1.331448
C	4.604236	-1.870557	-0.157233
H	4.123787	-0.430651	1.348939
C	2.981414	-2.156142	-1.930252
H	1.212586	-0.953832	-1.793161
C	4.226760	-2.525429	-1.358333
H	5.543160	-2.120043	0.335235
H	2.630585	-2.633112	-2.844236
C	1.937129	0.846305	2.343799
C	1.230937	0.082951	3.288707
C	3.003556	1.650974	2.782696
C	1.589331	0.115323	4.639071
H	0.394607	-0.539116	2.964295
C	3.358404	1.683115	4.134602
H	3.557994	2.263453	2.068992
C	2.653256	0.915221	5.065863
H	1.028011	-0.483562	5.360795
H	4.188942	2.314925	4.460386
H	2.929200	0.944892	6.123162
N	5.030160	-3.482743	-1.940270
C	6.284782	-3.855454	-1.317900
H	6.141906	-4.266083	-0.301119
H	6.776719	-4.627071	-1.923559
H	6.980033	-2.999670	-1.236058
C	4.609353	-4.139892	-3.161940
H	4.461762	-3.422373	-3.989779
H	5.380374	-4.855404	-3.474694
H	3.663661	-4.698447	-3.033312
Pd	-0.831269	0.247419	0.208820

C	-1.581994	1.903633	-0.449035
Si	-1.666821	2.464083	-2.241226
C	-3.524558	2.504249	-2.650826
H	-4.067864	3.191627	-1.981785
H	-3.681628	2.847077	-3.688302
H	-3.969026	1.502925	-2.539608
C	-0.967347	4.199976	-2.585975
H	-1.137598	4.489672	-3.637824
H	-1.452810	4.958152	-1.948574
H	0.116571	4.247576	-2.394999
C	-0.803221	1.236795	-3.400153
H	0.282317	1.206343	-3.210098
H	-1.203780	0.220123	-3.262185
H	-0.949775	1.524260	-4.455180
H	-1.649411	2.728949	0.288224
C	-4.785504	-0.545451	2.869297
C	-3.627916	-0.850754	2.179754
C	-3.649569	-1.153817	0.795884
C	-4.909305	-1.138865	0.097517
C	-6.078747	-0.815495	0.842919
C	-6.024347	-0.527272	2.192295
H	-4.740865	-0.316403	3.936958
H	-2.669097	-0.862966	2.699694
C	-2.460626	-1.431183	0.032639
C	-4.969066	-1.449650	-1.305482
H	-7.043149	-0.797070	0.332880
H	-6.941125	-0.284814	2.736125
C	-3.795303	-1.807014	-1.950067
C	-2.550182	-1.845841	-1.290573
H	-3.827223	-2.075636	-3.010246
H	-1.656825	-2.157946	-1.833315
Br	-0.836849	-2.318220	1.070918
C	-6.279417	-1.432374	-2.050845
H	-7.005010	-2.150776	-1.630898
H	-6.759739	-0.439387	-2.017516
H	-6.130595	-1.692541	-3.109057

51

B3LYP SCF energy: -4743.57313384 a.u.
B3LYP enthalpy: -4742.886541 a.u.
B3LYP free energy: -4743.011671 a.u.
M06-L SCF energy in solution: -4745.13207676 a.u.
M06-L enthalpy in solution: -4744.445484 a.u.
M06-L free energy in solution: -4744.570614 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.961364	0.585274	0.656689
C	-0.942887	-0.021163	2.408279
C	0.206709	0.205410	3.188445
C	-2.019273	-0.715155	2.979655
C	0.273509	-0.246792	4.507298
H	1.052824	0.751991	2.763256
C	-1.948346	-1.174191	4.300679
H	-2.919937	-0.901671	2.392250
C	-0.804931	-0.942506	5.067693
H	1.170890	-0.055192	5.101659
H	-2.795806	-1.715394	4.729337
H	-0.751886	-1.299528	6.099392
C	-2.659236	0.250837	0.062863
C	-3.769131	1.013363	0.466165
C	-2.888473	-0.806485	-0.832842
C	-5.052760	0.724292	0.015566
H	-3.635176	1.863023	1.139812
C	-4.166867	-1.114070	-1.286815
H	-2.042660	-1.390407	-1.202576
C	-5.292613	-0.356459	-0.873713
H	-5.874145	1.355249	0.353084
H	-4.281515	-1.939052	-1.988426
C	-0.888263	2.425319	0.891036
C	-0.515734	3.244422	-0.189130
C	-1.233571	3.028334	2.114600
C	-0.490755	4.634176	-0.043497
H	-0.253149	2.791908	-1.148889
C	-1.205061	4.419137	2.253877
H	-1.523884	2.415723	2.969612
C	-0.832375	5.226230	1.175678
H	-0.198341	5.255718	-0.893768
H	-1.474985	4.870814	3.212259
H	-0.807175	6.313533	1.286599
N	-6.563001	-0.648981	-1.323160
C	-7.683512	0.179290	-0.925559
H	-7.572656	1.227975	-1.260195
H	-8.605672	-0.218164	-1.368259
H	-7.818936	0.193140	0.171233
C	-6.767502	-1.723858	-2.274026
H	-6.431460	-2.698045	-1.875035
H	-7.837678	-1.809904	-2.501440
H	-6.231879	-1.551653	-3.226280
Pd	0.736164	-0.234823	-0.729310
C	1.762142	-1.604835	0.539322
Si	1.121334	-3.396443	0.412715
C	0.758665	-4.015618	-1.340770
H	1.670428	-4.109161	-1.951862
H	0.305836	-5.019718	-1.275917
H	0.051091	-3.363940	-1.877826
C	2.471689	-4.501090	1.162414
H	2.157421	-5.558845	1.165098
H	3.410090	-4.429221	0.588304

H	2.693826	-4.215833	2.203997
C	-0.447419	-3.581411	1.446587
H	-0.303424	-3.225449	2.478541
H	-1.290146	-3.019815	1.014465
H	-0.739811	-4.644094	1.494640
H	1.800809	-1.318072	1.597194
C	5.177700	0.714545	2.119384
C	4.154526	-0.082441	1.631049
C	3.896710	-0.190250	0.244470
C	4.734362	0.526432	-0.670130
C	5.770740	1.337179	-0.139472
C	5.989434	1.435011	1.224508
H	5.356342	0.777359	3.195707
H	3.542233	-0.651094	2.332278
C	2.824916	-1.046019	-0.268963
C	4.523371	0.417449	-2.101964
H	6.412960	1.896511	-0.820826
H	6.796895	2.066619	1.603602
C	3.530067	-0.407776	-2.561709
C	2.688047	-1.149198	-1.679315
H	3.361165	-0.508062	-3.635945
H	2.051591	-1.920489	-2.112000
Br	-0.049684	0.855891	-2.882356
C	5.387078	1.189555	-3.065250
H	5.305534	2.277292	-2.900499
H	6.454208	0.928364	-2.963047
H	5.088661	0.987208	-4.103516

52

B3LYP SCF energy: -1854.72455282 a.u.
B3LYP enthalpy: -1854.206661 a.u.
B3LYP free energy: -1854.316673 a.u.
M06-L SCF energy in solution: -1855.86700598 a.u.
M06-L enthalpy in solution: -1855.349114 a.u.
M06-L free energy in solution: -1855.459126 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.430662	-0.916609	-0.038143
C	-1.078626	-2.134162	-1.284220
C	-0.212679	-3.158711	-1.707913
C	-2.367543	-2.070202	-1.836560
C	-0.632201	-4.107089	-2.642659
H	0.803312	-3.200170	-1.304637
C	-2.783355	-3.013981	-2.783195
H	-3.052513	-1.276323	-1.531772
C	-1.920322	-4.036068	-3.185660
H	0.052887	-4.898928	-2.957455
H	-3.788952	-2.947040	-3.207452
H	-2.246398	-4.771997	-3.925474
C	-1.719738	0.402077	-0.004752
C	-2.887552	0.351050	0.774263
C	-1.532619	1.540749	-0.807527
C	-3.828029	1.379173	0.752762
H	-3.072993	-0.507970	1.423399
C	-2.464908	2.573104	-0.849264
H	-0.623856	1.618399	-1.411920
C	-3.645961	2.523379	-0.064803
H	-4.710753	1.287410	1.384718
H	-2.263751	3.429259	-1.492245
C	-0.721048	-1.805178	1.569009
C	-0.076743	-1.306759	2.715447
C	-1.537335	-2.940662	1.696162
C	-0.256823	-1.916181	3.958601
H	0.580158	-0.437514	2.621606
C	-1.708711	-3.558261	2.940577
H	-2.041010	-3.352315	0.819144
C	-1.072813	-3.047164	4.074548
H	0.251221	-1.513893	4.839230
H	-2.343358	-4.445022	3.020892
H	-1.206027	-3.531959	5.045336
N	-4.573467	3.547170	-0.092062
C	-5.767671	3.467852	0.723198
H	-5.535735	3.409055	1.803188
H	-6.379470	4.364752	0.562016
H	-6.388945	2.588328	0.470645
C	-4.351124	4.704715	-0.933152
H	-4.275518	4.436323	-2.003401
H	-5.191467	5.402220	-0.823697
H	-3.426470	5.248354	-0.662882
Pd	1.691795	-0.207333	-0.419718
C	3.691557	0.537196	-0.893963
N	4.548039	-0.456397	-0.649617
N	5.296494	-1.267208	-0.400193
Si	3.936799	2.143655	0.127625
C	5.642817	2.860585	-0.286283
H	5.725316	3.114724	-1.355989
H	5.829233	3.781674	0.292117
H	6.451381	2.150043	-0.045999
C	2.598954	3.360300	-0.396960
H	2.759672	4.336760	0.091039
H	2.614559	3.523779	-1.487121
H	1.599693	2.989007	-0.122235
C	3.866077	1.741803	1.967558
H	2.870779	1.359959	2.242470
H	4.611213	0.977765	2.244970
H	4.076193	2.643481	2.567593
H	3.544670	0.646776	-1.981846

53-ts

B3LYP SCF energy: -1854.68989856 a.u.
B3LYP enthalpy: -1854.174480 a.u.
B3LYP free energy: -1854.285653 a.u.
M06-L SCF energy in solution: -1855.83052113 a.u.
M06-L enthalpy in solution: -1855.315103 a.u.
M06-L free energy in solution: -1855.426276 a.u.
Imaginary frequency: -422.6797 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.471895	0.672215	-0.060089
C	0.833848	2.054160	-1.244004
C	-0.232784	2.896282	-1.610310
C	2.094761	2.270959	-1.820978
C	-0.036098	3.943114	-2.512629
H	-1.226262	2.720011	-1.187894
C	2.287612	3.314145	-2.734251
H	2.931891	1.620355	-1.560219
C	1.226214	4.154192	-3.079251
H	-0.874327	4.590459	-2.783750
H	3.275088	3.468276	-3.177681
H	1.378639	4.967907	-3.793195
C	2.028640	-0.304692	0.004393
C	3.155176	0.057768	0.762318
C	2.107958	-1.492180	-0.743036
C	4.312492	-0.716421	0.767092
H	3.133227	0.962937	1.374244
C	3.258796	-2.274600	-0.755484
H	1.236105	-1.814519	-1.320219
C	4.401768	-1.906858	-0.000042
H	5.151882	-0.390559	1.380309
H	3.259686	-3.186613	-1.351230
C	0.451253	1.529328	1.584605
C	-0.085778	0.827540	2.678937
C	0.942102	2.828476	1.790151
C	-0.117701	1.405434	3.949593
H	-0.487981	-0.177542	2.524282
C	0.899957	3.410639	3.062417
H	1.356013	3.394972	0.953269
C	0.373313	2.701362	4.144585
H	-0.536614	0.845380	4.789894
H	1.281762	4.425171	3.205450
H	0.340155	3.158181	5.137210
N	5.547995	-2.677581	-0.003788
C	6.679317	-2.301873	0.819070
H	6.431307	-2.286899	1.897424
H	7.492521	-3.024390	0.672670
H	7.070015	-1.302074	0.555550
C	5.590760	-3.911673	-0.761268
H	5.409682	-3.742816	-1.838254
H	6.584138	-4.367327	-0.659647
H	4.843549	-4.649008	-0.411128
Pd	-1.468945	-0.518418	-0.589414
C	-3.065183	-1.699584	-0.507638
N	-3.902163	-1.609880	-2.182993
N	-4.229145	-1.166769	-3.146789
Si	-4.539481	-1.325487	0.653277
C	-6.015815	-2.481326	0.355660
H	-5.725233	-3.539563	0.464518
H	-6.825755	-2.281208	1.077988
H	-6.436768	-2.352106	-0.655376
C	-3.859451	-1.633608	2.392346
H	-4.664089	-1.517483	3.138414
H	-3.451089	-2.652449	2.492866
H	-3.057675	-0.919221	2.633243
C	-5.101586	0.465486	0.457908
H	-4.261159	1.152716	0.643153
H	-5.480253	0.662685	-0.558752
H	-5.912036	0.704614	1.166989
H	-2.884868	-2.785878	-0.607754

54

B3LYP SCF energy: -1745.26662837 a.u.
B3LYP enthalpy: -1744.761188 a.u.
B3LYP free energy: -1744.865926 a.u.
M06-L SCF energy in solution: -1746.30185416 a.u.
M06-L enthalpy in solution: -1745.796414 a.u.
M06-L free energy in solution: -1745.901152 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.209190	0.694573	-0.105335
C	0.669212	2.335663	-0.829393
C	-0.366119	3.260824	-1.066531
C	1.976645	2.666934	-1.219138
C	-0.093968	4.495789	-1.657601
H	-1.393371	3.008583	-0.787319
C	2.244822	3.902537	-1.818758
H	2.790101	1.957421	-1.054976
C	1.213796	4.819891	-2.036483
H	-0.907716	5.204634	-1.831293
H	3.267751	4.147120	-2.117190
H	1.426139	5.783738	-2.506266
C	1.773659	-0.257309	-0.024631
C	2.747635	-0.073643	0.972273

C	2.027404	-1.229139	-1.007893
C	3.926643	-0.812610	0.983854
H	2.584827	0.657404	1.768067
C	3.203651	-1.972127	-1.015004
H	1.274731	-1.416217	-1.779592
C	4.194105	-1.784339	-0.016390
H	4.642637	-0.632954	1.785010
H	3.342767	-2.713831	-1.800501
C	-0.165424	1.083816	1.663114
C	-0.869153	0.125276	2.413459
C	0.232198	2.277056	2.287606
C	-1.156160	0.349981	3.761463
H	-1.199976	-0.797800	1.930084
C	-0.064728	2.503955	3.636055
H	0.771632	3.038501	1.720265
C	-0.756282	1.541634	4.376086
H	-1.703581	-0.404844	4.331973
H	0.246853	3.439519	4.108093
H	-0.989317	1.721394	5.428821
N	5.361487	-2.518867	-0.012174
C	6.331443	-2.337518	1.048940
H	5.916316	-2.581272	2.044993
H	7.190585	-2.997502	0.873986
H	6.710381	-1.300152	1.092013
C	5.587708	-3.528527	-1.027072
H	5.579024	-3.100340	-2.045745
H	6.570687	-3.990176	-0.869166
H	4.828433	-4.332450	-0.997933
Pd	-1.535248	-0.330667	-1.290366
C	-2.811827	-1.748211	-1.121356
Si	-4.419326	-1.760477	-0.140479
C	-5.719780	-2.586250	-1.257002
H	-5.437704	-3.621482	-1.509220
H	-6.698156	-2.615301	-0.747342
H	-5.847314	-2.030309	-2.199874
C	-4.240833	-2.783579	1.454608
H	-5.197083	-2.817869	2.004657
H	-3.937347	-3.820526	1.235936
H	-3.486135	-2.346946	2.129521
C	-5.001730	-0.020265	0.314250
H	-4.259223	0.487859	0.951047
H	-5.136409	0.592552	-0.591858
H	-5.960773	-0.043988	0.859386
H	-2.462542	-2.782937	-1.323539

55

B3LYP SCF energy: -4852.92384007 a.u.
B3LYP enthalpy: -4852.227664 a.u.
B3LYP free energy: -4852.359732 a.u.

M06-L SCF energy in solution: -4854.59698824 a.u.
M06-L enthalpy in solution: -4853.900812 a.u.
M06-L free energy in solution: -4854.032880 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.074396	1.300116	0.054704
C	0.320374	1.980229	1.731183
C	1.455901	1.521638	2.416380
C	-0.501771	2.939414	2.350788
C	1.778206	2.021841	3.681589
H	2.081787	0.753599	1.959622
C	-0.178151	3.440467	3.614289
H	-1.407710	3.286429	1.849440
C	0.963499	2.985252	4.281764
H	2.663614	1.648898	4.202753
H	-0.826328	4.185526	4.082918
H	1.211143	3.373908	5.272846
C	-1.908671	1.333273	0.033031
C	-2.652001	2.037878	-0.925865
C	-2.622297	0.595578	0.995771
C	-4.045220	2.017264	-0.927397
H	-2.143685	2.620496	-1.696154
C	-4.010729	0.569135	1.009330
H	-2.087121	0.022240	1.756024
C	-4.769225	1.281354	0.043161
H	-4.568592	2.581491	-1.698100
H	-4.506982	-0.023962	1.775973
C	0.387948	2.637929	-1.141199
C	0.595673	2.271398	-2.483560
C	0.518297	3.988204	-0.779879
C	0.913588	3.235985	-3.443691
H	0.516028	1.220620	-2.776660
C	0.843273	4.950363	-1.740695
H	0.378029	4.297196	0.257242
C	1.039263	4.578448	-3.073552
H	1.069939	2.934280	-4.482467
H	0.949358	5.996344	-1.441879
H	1.296153	5.332622	-3.821815
N	-6.148593	1.256405	0.050899
C	-6.892306	1.962205	-0.972483
H	-6.679274	1.581085	-1.989367
H	-7.967805	1.844025	-0.788592
H	-6.670845	3.044946	-0.971425
C	-6.855211	0.438722	1.016769
H	-6.629658	0.737437	2.056482
H	-7.936587	0.551029	0.866755
H	-6.609790	-0.635458	0.918890
Pd	1.082200	-0.646966	-0.576818
C	-0.871289	-3.224653	2.751978

C	-0.414177	-2.482913	1.682112
C	-1.116393	-2.437703	0.443510
C	-2.334736	-3.202266	0.321229
C	-2.772036	-3.960356	1.446243
C	-2.065431	-3.973458	2.631706
H	-0.307980	-3.240723	3.688669
H	0.512283	-1.911516	1.767087
C	-0.657192	-1.662600	-0.668830
C	-3.070728	-3.182785	-0.910207
H	-3.689562	-4.546424	1.367235
H	-2.425896	-4.566266	3.476761
C	-2.582489	-2.417152	-1.951652
C	-1.387114	-1.663923	-1.838575
H	-3.127322	-2.393385	-2.900625
H	-1.048135	-1.095782	-2.708023
C	-4.342691	-3.978864	-1.071577
H	-4.175563	-5.058894	-0.918974
H	-5.118455	-3.672892	-0.348073
H	-4.760178	-3.847892	-2.080777
Br	2.152701	-2.688198	-1.593314
C	3.405811	0.215542	-0.580192
N	3.523546	1.533764	-0.556215
N	3.611456	2.656494	-0.461207
Si	4.605823	-0.731591	0.608545
C	5.799797	-1.700647	-0.476711
H	6.377819	-1.035665	-1.138873
H	6.512474	-2.268109	0.145344
H	5.237728	-2.413216	-1.100100
C	5.531375	0.599874	1.589627
H	6.247367	0.118832	2.277122
H	6.106288	1.276097	0.935700
H	4.855187	1.218914	2.202427
C	3.711653	-1.873346	1.807065
H	3.033233	-1.326715	2.480904
H	3.127245	-2.626661	1.258584
H	4.456511	-2.393574	2.433783
H	3.370304	-0.155614	-1.614333

56-ts

B3LYP SCF energy: -4852.88814772 a.u.
B3LYP enthalpy: -4852.194444 a.u.
B3LYP free energy: -4852.327006 a.u.
M06-L SCF energy in solution: -4854.56045872 a.u.
M06-L enthalpy in solution: -4853.866755 a.u.
M06-L free energy in solution: -4853.999317 a.u.
Imaginary frequency: -445.4533 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-0.098410	1.322522	0.058106
C	0.299281	1.956198	1.752777
C	1.437026	1.480196	2.422757
C	-0.526116	2.892630	2.402428
C	1.759034	1.943878	3.702019
H	2.063483	0.727285	1.941703
C	-0.202080	3.357525	3.679581
H	-1.436453	3.248143	1.915152
C	0.942483	2.887005	4.331306
H	2.645709	1.557414	4.211024
H	-0.852902	4.085002	4.171584
H	1.190090	3.246739	5.333282
C	-1.933109	1.321153	0.051260
C	-2.696727	2.014156	-0.900236
C	-2.625570	0.557577	1.009445
C	-4.088924	1.956948	-0.899596
H	-2.206136	2.615892	-1.667330
C	-4.012517	0.494492	1.025079
H	-2.074459	-0.009559	1.762803
C	-4.791304	1.193242	0.065233
H	-4.628402	2.513427	-1.664805
H	-4.491457	-0.118800	1.786787
C	0.317860	2.704576	-1.105257
C	0.553455	2.375128	-2.452145
C	0.382425	4.051958	-0.716136
C	0.833529	3.372378	-3.390340
H	0.527780	1.327297	-2.763902
C	0.672347	5.047513	-1.654535
H	0.217188	4.333183	0.325153
C	0.895317	4.711671	-2.992780
H	1.011421	3.099302	-4.433569
H	0.727376	6.091152	-1.334330
H	1.122743	5.491723	-3.723897
N	-6.169348	1.129244	0.073516
C	-6.933544	1.821770	-0.943711
H	-6.708118	1.457124	-1.963930
H	-8.005057	1.668739	-0.762219
H	-6.745524	2.910806	-0.932066
C	-6.851539	0.283806	1.033209
H	-6.636009	0.582267	2.075144
H	-7.935707	0.364041	0.882737
H	-6.573053	-0.781499	0.928244
Pd	1.099764	-0.569312	-0.573679
C	-0.891356	-3.262384	2.691848
C	-0.440485	-2.485064	1.644405
C	-1.113447	-2.446907	0.388812
C	-2.295323	-3.259370	0.226775
C	-2.728943	-4.053109	1.328483
C	-2.050745	-4.057003	2.530774
H	-0.350371	-3.271154	3.641860

H	0.459848	-1.877589	1.760941
C	-0.649437	-1.629417	-0.693729
C	-3.000103	-3.249718	-1.023038
H	-3.619585	-4.674753	1.218237
H	-2.406655	-4.677774	3.357634
C	-2.514902	-2.449607	-2.039956
C	-1.354708	-1.650605	-1.881057
H	-3.036583	-2.433140	-3.002340
H	-1.022328	-1.052118	-2.734219
C	-4.235572	-4.091881	-1.228709
H	-4.030487	-5.167144	-1.088447
H	-5.040285	-3.828291	-0.520162
H	-4.633166	-3.960634	-2.245964
Br	2.320077	-2.590677	-1.486310
C	3.180412	-0.060859	-0.665140
N	3.554604	1.767094	-0.532859
N	3.457092	2.854852	-0.356064
Si	4.558428	-0.804289	0.499229
C	5.858894	-1.718522	-0.518506
H	6.321739	-1.052262	-1.265625
H	6.661523	-2.097000	0.137315
H	5.409918	-2.569552	-1.051017
C	5.446829	0.603669	1.423453
H	6.179000	0.157510	2.118016
H	6.004032	1.271037	0.746006
H	4.761721	1.222799	2.025327
C	3.797810	-1.923898	1.813536
H	3.091439	-1.375850	2.458144
H	3.259785	-2.766961	1.357198
H	4.596916	-2.323592	2.461052
H	3.509424	-0.042036	-1.714233

57

B3LYP SCF energy: -4743.48947369 a.u.
B3LYP enthalpy: -4742.805256 a.u.
B3LYP free energy: -4742.933272 a.u.
M06-L SCF energy in solution: -4745.04719301 a.u.
M06-L enthalpy in solution: -4744.362975 a.u.
M06-L free energy in solution: -4744.490991 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.001052	-1.185275	0.267452
C	-0.137999	-1.286710	2.108206
C	-1.186478	-0.615716	2.756976
C	0.768106	-2.037148	2.877650
C	-1.336230	-0.700328	4.143743
H	-1.884136	-0.018122	2.167785
C	0.618537	-2.118622	4.265149
H	1.598652	-2.553798	2.392598
C	-0.433319	-1.452004	4.900955
H	-2.156460	-0.169278	4.633265
H	1.331876	-2.702936	4.852148
H	-0.544636	-1.512776	5.986617
C	1.780768	-1.498421	-0.051400
C	2.244089	-2.558990	-0.845939
C	2.744552	-0.632303	0.500062
C	3.603208	-2.753972	-1.083550
H	1.538163	-3.259463	-1.294991
C	4.102512	-0.821305	0.282457
H	2.430767	0.212958	1.115261
C	4.576794	-1.888136	-0.526313
H	3.901861	-3.593060	-1.710374
H	4.799522	-0.118261	0.735984
C	-0.815209	-2.729439	-0.349861
C	-1.132580	-2.813660	-1.717127
C	-1.113099	-3.818880	0.483116
C	-1.721471	-3.966430	-2.241375
H	-0.921425	-1.965975	-2.374122
C	-1.715536	-4.967735	-0.041416
H	-0.883343	-3.775725	1.549069
C	-2.018047	-5.046560	-1.402810
H	-1.957626	-4.017448	-3.307382
H	-1.949671	-5.804267	0.622028
H	-2.488596	-5.945023	-1.810247
N	5.923664	-2.070133	-0.758650
C	6.374305	-3.160617	-1.599252
H	5.977493	-3.088375	-2.629247
H	7.469854	-3.144636	-1.661368
H	6.075765	-4.146588	-1.197731
C	6.889777	-1.145309	-0.199097
H	6.862635	-1.131941	0.906020
H	7.900308	-1.446018	-0.503704
H	6.726238	-0.109161	-0.548093
Pd	-0.963304	0.673182	-0.619450
C	0.500911	3.870368	2.528404
C	0.247536	2.918145	1.562330
C	1.066978	2.776495	0.404209
C	2.192228	3.670218	0.259935
C	2.424717	4.641970	1.276861
C	1.604490	4.743249	2.382559
H	-0.148727	3.952176	3.403937
H	-0.605718	2.243923	1.669425
C	0.785320	1.780931	-0.594517
C	3.037538	3.564601	-0.895269
H	3.270659	5.325214	1.179005
H	1.807035	5.499578	3.145926
C	2.739327	2.595023	-1.834900
C	1.638707	1.713983	-1.683784

H	3.372464	2.501406	-2.723501
H	1.477172	0.962782	-2.464201
C	4.216420	4.487181	-1.086953
H	3.908330	5.546034	-1.135094
H	4.945012	4.408043	-0.261405
H	4.747508	4.254656	-2.021983
Br	-2.797109	2.018437	-1.922404
C	-2.951499	0.142826	-1.092396
Si	-4.510315	0.032844	-0.021948
C	-6.071698	0.225433	-1.081139
H	-6.114047	-0.542712	-1.871307
H	-6.983750	0.126671	-0.467936
H	-6.100674	1.212313	-1.571069
C	-4.529569	-1.692322	0.763414
H	-5.464630	-1.840795	1.330028
H	-4.473333	-2.482657	-0.002861
H	-3.687365	-1.840471	1.456832
C	-4.534798	1.364122	1.323072
H	-3.667897	1.295727	1.999113
H	-4.529501	2.372994	0.880653
H	-5.446369	1.269841	1.936934
H	-3.015359	-0.515909	-1.973096

58

B3LYP SCF energy: -4852.92078356 a.u.
B3LYP enthalpy: -4852.224338 a.u.
B3LYP free energy: -4852.357035 a.u.
M06-L SCF energy in solution: -4854.58455891 a.u.
M06-L enthalpy in solution: -4853.888113 a.u.
M06-L free energy in solution: -4854.020810 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.620396	-0.783925	-0.364308
C	-2.219975	-1.434587	-1.990578
C	-1.291796	-2.023393	-2.864740
C	-3.570731	-1.378298	-2.370718
C	-1.709720	-2.567284	-4.082992
H	-0.231795	-2.034824	-2.601529
C	-3.985643	-1.915121	-3.592161
H	-4.304873	-0.903590	-1.717107
C	-3.057146	-2.514537	-4.449156
H	-0.974388	-3.017613	-4.754533
H	-5.039500	-1.859597	-3.877466
H	-3.382692	-2.930198	-5.406388
C	-2.765653	0.578765	0.090642
C	-4.047870	0.365428	0.631766
C	-2.374775	1.912266	-0.132773
C	-4.898050	1.422356	0.942831
H	-4.400215	-0.649902	0.827422
C	-3.215766	2.978310	0.169973
H	-1.399755	2.120615	-0.579530
C	-4.505599	2.768137	0.720742
H	-5.877597	1.193138	1.360880
H	-2.858316	3.987319	-0.031324
C	-2.107159	-2.145349	0.805366
C	-2.250240	-1.872727	2.180291
C	-2.216758	-3.480252	0.377432
C	-2.508362	-2.899186	3.093206
H	-2.176709	-0.843366	2.539776
C	-2.468671	-4.507715	1.293284
H	-2.114288	-3.721797	-0.682434
C	-2.617085	-4.222574	2.653093
H	-2.629576	-2.661802	4.153542
H	-2.555951	-5.537314	0.936446
H	-2.819814	-5.025551	3.366178
N	-5.340799	3.821848	1.026443
C	-6.660496	3.570021	1.568066
H	-6.618703	3.021854	2.527250
H	-7.167167	4.525631	1.753783
H	-7.293746	2.982160	0.877256
C	-4.919973	5.183391	0.759736
H	-4.718679	5.356733	-0.313613
H	-5.712939	5.876442	1.068412
H	-4.003772	5.451902	1.316566
Pd	0.841617	-0.280408	-0.403659
C	3.286782	3.567211	0.818101
C	2.687578	2.404458	0.378734
C	3.435552	1.352099	-0.223574
C	4.855342	1.543518	-0.399963
C	5.441123	2.753646	0.074593
C	4.683165	3.739426	0.673013
H	2.682239	4.359460	1.267641
H	1.606193	2.280034	0.457877
C	2.818605	0.131373	-0.661208
C	5.638926	0.531404	-1.051356
H	6.515057	2.907375	-0.044966
H	5.160064	4.658864	1.023347
C	4.993902	-0.603707	-1.501653
C	3.600944	-0.800341	-1.314812
H	5.568845	-1.377403	-2.020375
H	3.157996	-1.717097	-1.716776
C	7.123559	0.706170	-1.258031
H	7.353125	1.599464	-1.863854
H	7.663589	0.822831	-0.302513
H	7.550985	-0.164700	-1.776437
Br	0.475639	1.205737	-2.371893
C	1.261703	-1.631138	1.310327
N	2.107419	-2.570958	0.851852

N	2.866455	-3.294641	0.446252
Si	1.878198	-0.840039	2.981797
C	1.500403	-2.127936	4.317164
H	2.059063	-3.063753	4.149287
H	1.788348	-1.745655	5.311392
H	0.427129	-2.376475	4.349827
C	3.729572	-0.533822	2.908283
H	4.074180	-0.153177	3.884574
H	4.288890	-1.460709	2.700371
H	3.993019	0.205313	2.138145
C	0.881489	0.718970	3.307117
H	1.125902	1.509836	2.584033
H	-0.201413	0.526344	3.256507
H	1.110575	1.095320	4.318512
H	0.291504	-2.126318	1.471727

59-ts

B3LYP SCF energy: -4852.88978826 a.u.
B3LYP enthalpy: -4852.195868 a.u.
B3LYP free energy: -4852.328666 a.u.
M06-L SCF energy in solution: -4854.55562199 a.u.
M06-L enthalpy in solution: -4853.861702 a.u.
M06-L free energy in solution: -4853.994500 a.u.
Imaginary frequency: -358.3450 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.575913	-0.828856	-0.342383
C	-2.019178	-1.570826	-1.977850
C	-1.041877	-2.307719	-2.667135
C	-3.297025	-1.440264	-2.542989
C	-1.344177	-2.924520	-3.883738
H	-0.030684	-2.379137	-2.259744
C	-3.594815	-2.050001	-3.765164
H	-4.063723	-0.849265	-2.039003
C	-2.622163	-2.797090	-4.435530
H	-0.571693	-3.490740	-4.410123
H	-4.592074	-1.934047	-4.197663
H	-2.856317	-3.269391	-5.393142
C	-2.745517	0.553052	-0.050072
C	-4.087313	0.351707	0.327180
C	-2.316230	1.881833	-0.222703
C	-4.960692	1.416554	0.523912
H	-4.467838	-0.660407	0.482850
C	-3.178513	2.956028	-0.029185
H	-1.291600	2.079730	-0.544332
C	-4.530488	2.758453	0.350997
H	-5.986755	1.197499	0.817043
H	-2.788969	3.961279	-0.184051
C	-2.157830	-2.130376	0.852920
C	-2.455092	-1.781398	2.184184
C	-2.209612	-3.488190	0.493366
C	-2.803960	-2.757378	3.121399
H	-2.431923	-0.732927	2.489870
C	-2.553442	-4.465252	1.434192
H	-1.990261	-3.789826	-0.532589
C	-2.853209	-4.105097	2.750158
H	-3.043001	-2.461271	4.146306
H	-2.593045	-5.514498	1.130081
H	-3.127248	-4.868683	3.482441
N	-5.388232	3.819828	0.544356
C	-6.770325	3.581725	0.908517
H	-6.860741	3.040909	1.868534
H	-7.289152	4.542469	1.017983
H	-7.310488	2.993126	0.143587
C	-4.921635	5.177489	0.339989
H	-4.579625	5.351229	-0.696967
H	-5.740891	5.878420	0.544370
H	-4.083947	5.434438	1.013555
Pd	0.877781	-0.334150	-0.275949
C	3.455487	3.513008	0.681818
C	2.823978	2.334123	0.342432
C	3.529212	1.240080	-0.235515
C	4.939960	1.402051	-0.491626
C	5.561368	2.628926	-0.117755
C	4.844205	3.658444	0.457190
H	2.882937	4.336838	1.116187
H	1.748322	2.224875	0.491243
C	2.877826	0.005740	-0.570890
C	5.680244	0.344034	-1.121505
H	6.629780	2.760425	-0.297696
H	5.347409	4.590198	0.729390
C	5.004138	-0.808392	-1.467944
C	3.621355	-0.978071	-1.196716
H	5.544953	-1.618277	-1.967716
H	3.148071	-1.909832	-1.521182
C	7.153603	0.489261	-1.413076
H	7.359964	1.346902	-2.075960
H	7.743209	0.649152	-0.493791
H	7.545147	-0.412842	-1.905727
Br	0.524061	1.039636	-2.369963
C	1.047880	-1.245796	1.481156
N	2.503700	-2.488571	1.460494
N	3.442870	-2.895434	1.038957
Si	1.407044	-0.400910	3.187436
C	0.977895	-1.619038	4.572151
H	1.633879	-2.504993	4.543775
H	1.105236	-1.145522	5.560549
H	-0.063853	-1.970399	4.496553

C	3.209909	0.116446	3.353855
H	3.346142	0.658408	4.304981
H	3.885912	-0.753385	3.370625
H	3.523014	0.779338	2.534340
C	0.266093	1.101513	3.274050
H	0.499230	1.824547	2.478561
H	-0.795603	0.826625	3.182594
H	0.400895	1.606476	4.245586
H	0.346635	-2.085343	1.615614

60

B3LYP SCF energy: -4743.55416062 a.u.
B3LYP enthalpy: -4742.867684 a.u.
B3LYP free energy: -4742.994511 a.u.
M06-L SCF energy in solution: -4745.11598262 a.u.
M06-L enthalpy in solution: -4744.429506 a.u.
M06-L free energy in solution: -4744.556333 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.279149	0.732323	0.483706
C	-1.704826	1.100526	2.252415
C	-0.678049	1.444646	3.146142
C	-3.029452	1.078211	2.716974
C	-0.972316	1.783237	4.469911
H	0.360412	1.423282	2.808457
C	-3.320742	1.406701	4.043453
H	-3.843211	0.789708	2.050347
C	-2.294101	1.765446	4.921823
H	-0.160485	2.043942	5.153800
H	-4.356550	1.376483	4.392246
H	-2.523441	2.019558	5.960211
C	-2.516912	-0.478874	-0.118320
C	-3.859850	-0.144943	-0.383531
C	-2.140646	-1.822520	-0.295372
C	-4.782095	-1.097826	-0.803368
H	-4.204851	0.885587	-0.273498
C	-3.051982	-2.785611	-0.714577
H	-1.114974	-2.126366	-0.075523
C	-4.404855	-2.454869	-0.981493
H	-5.805556	-0.777535	-0.995163
H	-2.699567	-3.810072	-0.827445
C	-1.752529	2.324201	-0.348628
C	-2.303117	2.345871	-1.641988
C	-1.522773	3.550020	0.301859
C	-2.637922	3.556610	-2.255977
H	-2.488846	1.411247	-2.173169
C	-1.848762	4.759507	-0.317258
H	-1.099568	3.563399	1.308260
C	-2.414798	4.767957	-1.595662
H	-3.074314	3.549929	-3.258077
H	-1.666966	5.700290	0.208736
H	-2.677591	5.713677	-2.075674
N	-5.311646	-3.405983	-1.396937
C	-6.691092	-3.038155	-1.643585
H	-6.784057	-2.277649	-2.440843
H	-7.253288	-3.924881	-1.962734
H	-7.184964	-2.634620	-0.739876
C	-4.894676	-4.785334	-1.558842
H	-4.520616	-5.222236	-0.614915
H	-5.749791	-5.387184	-1.891015
H	-4.094596	-4.891661	-2.314300
Pd	0.906479	0.025990	0.372001
C	3.309157	-2.716770	-2.099382
C	2.877298	-1.454560	-1.748824
C	3.478532	-0.721973	-0.685992
C	4.555200	-1.350489	0.039452
C	4.974811	-2.654735	-0.353276
C	4.374501	-3.323736	-1.397303
H	2.818275	-3.250574	-2.916575
H	2.035175	-1.021111	-2.281914
C	3.036619	0.617201	-0.313036
C	5.176875	-0.676906	1.139703
H	5.785648	-3.138246	0.192625
H	4.713434	-4.325138	-1.674747
C	4.712150	0.581677	1.497052
C	3.669737	1.204668	0.801398
H	5.167949	1.100451	2.344548
H	3.347602	2.202610	1.110079
C	6.298820	-1.316234	1.914950
H	5.976579	-2.260078	2.385508
H	7.158775	-1.556920	1.267611
H	6.654853	-0.649255	2.712802
Br	0.680233	-1.820419	2.078257
C	1.915439	1.334382	-0.946462
Si	1.674976	1.622037	-2.819775
C	1.136132	3.428863	-2.996098
H	1.918679	4.104538	-2.611198
H	0.965965	3.686447	-4.054848
H	0.207845	3.640431	-2.444701
C	3.326945	1.449550	-3.739259
H	3.204722	1.759365	-4.791356
H	4.095683	2.098301	-3.287662
H	3.713839	0.419299	-3.734444
C	0.384997	0.523061	-3.675577
H	0.724359	-0.514761	-3.818696
H	-0.556929	0.487467	-3.108329
H	0.163207	0.933489	-4.675669
H	1.825767	2.333652	-0.492008

61-ts

B3LYP SCF energy: -2286.82096571 a.u.
B3LYP enthalpy: -2286.065309 a.u.
B3LYP free energy: -2286.196464 a.u.
M06-L SCF energy in solution: -2288.32667100 a.u.
M06-L enthalpy in solution: -2287.571014 a.u.
M06-L free energy in solution: -2287.702169 a.u.
Imaginary frequency: -438.7240 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.898117	-0.774646	0.127562
C	2.674016	-1.507999	1.642340
C	2.274822	-2.803279	2.022784
C	3.580304	-0.815517	2.460647
C	2.790052	-3.399959	3.174557
H	1.549533	-3.346062	1.409778
C	4.086554	-1.410079	3.622652
H	3.894455	0.194875	2.191718
C	3.698119	-2.703059	3.980265
H	2.473787	-4.409305	3.450681
H	4.789935	-0.855885	4.249914
H	4.094839	-3.165802	4.887621
C	2.629610	0.909437	0.000305
C	3.945535	1.159866	-0.427412
C	1.836793	2.021673	0.331911
C	4.453768	2.452684	-0.509163
H	4.593083	0.327283	-0.713453
C	2.329539	3.321756	0.260700
H	0.800274	1.863295	0.643959
C	3.659242	3.577042	-0.161689
H	5.478561	2.586831	-0.853499
H	1.665714	4.143220	0.526870
C	2.747966	-1.682877	-1.251284
C	2.213136	-1.545435	-2.545097
C	3.886794	-2.485958	-1.075881
C	2.807943	-2.181567	-3.636242
H	1.316921	-0.936484	-2.695649
C	4.476287	-3.131907	-2.168696
H	4.318257	-2.613809	-0.081051
C	3.941567	-2.980326	-3.450341
H	2.378211	-2.061770	-4.634168
H	5.360343	-3.756375	-2.014078
H	4.402698	-3.486812	-4.302211
N	4.157082	4.861678	-0.239565
C	5.510072	5.090737	-0.704334
H	5.666311	4.730029	-1.738357
H	5.722653	6.167307	-0.690469
H	6.260566	4.593152	-0.062918
C	3.312202	5.989231	0.098945
H	2.948249	5.937149	1.141325
H	3.885442	6.919056	-0.007195
H	2.425532	6.062892	-0.558364
Pd	-0.466369	-0.803583	0.056103
C	-2.419594	3.551671	-1.427914
C	-2.388439	2.189422	-1.164690
C	-3.440425	1.530774	-0.485391
C	-4.554716	2.319402	-0.046729
C	-4.566373	3.704722	-0.337717
C	-3.522494	4.317268	-1.016254
H	-1.581223	4.024534	-1.946043
H	-1.511290	1.616200	-1.467906
C	-3.425104	0.080199	-0.244716
C	-5.660735	1.696576	0.673648
H	-5.414244	4.310467	-0.014325
H	-3.557051	5.390865	-1.219612
C	-5.547983	0.385392	1.021643
C	-4.368299	-0.406602	0.728879
H	-6.357935	-0.094746	1.580810
H	-4.534600	-1.484762	0.717147
C	-6.888926	2.494623	1.031390
H	-6.653581	3.336191	1.706095
H	-7.371504	2.929271	0.139294
H	-7.631108	1.861172	1.538999
C	-2.492237	-0.796087	-0.842246
Si	-2.843128	-2.623078	-1.239014
C	-1.568996	-3.191857	-2.522404
H	-0.543561	-3.160995	-2.119749
H	-1.776430	-4.226195	-2.845229
H	-1.596838	-2.552477	-3.420934
C	-2.765591	-3.820849	0.232403
H	-1.750065	-3.860267	0.657412
H	-3.458902	-3.552135	1.045730
H	-3.031443	-4.837720	-0.103857
C	-4.561100	-2.791948	-2.038594
H	-4.635071	-2.158290	-2.937971
H	-4.745787	-3.835939	-2.345128
H	-5.374155	-2.492757	-1.358141
H	-1.948895	-0.331882	-1.686957
C	-2.023399	-0.152941	2.519504
H	-1.770228	0.903969	2.668745
C	-0.972606	-1.026785	2.238714
H	-1.178266	-2.103662	2.256553
H	0.027825	-0.746457	2.577124
C	-3.396693	-0.492546	2.543559
H	-3.634150	-1.545685	2.723603
H	-4.055075	0.204984	3.064541

62

B3LYP SCF energy: -2286.86013761 a.u.
B3LYP enthalpy: -2286.101532 a.u.
B3LYP free energy: -2286.228325 a.u.
M06-L SCF energy in solution: -2288.37064835 a.u.
M06-L enthalpy in solution: -2287.612043 a.u.
M06-L free energy in solution: -2287.738836 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.427545	-0.827868	-0.063835
C	-2.104741	-2.019045	-1.313370
C	-1.481100	-3.274356	-1.450284
C	-3.141806	-1.687719	-2.199610
C	-1.897693	-4.178555	-2.428841
H	-0.660572	-3.548893	-0.782371
C	-3.550808	-2.590354	-3.188636
H	-3.635208	-0.717255	-2.120762
C	-2.935222	-3.838344	-3.304585
H	-1.404469	-5.150590	-2.512877
H	-4.358975	-2.312537	-3.870652
H	-3.257579	-4.542853	-4.075643
C	-2.638514	0.563248	-0.048615
C	-3.967203	0.417539	0.390746
C	-2.237803	1.843325	-0.463587
C	-4.858117	1.485573	0.397240
H	-4.321557	-0.554102	0.743914
C	-3.114288	2.925993	-0.461989
H	-1.204943	1.995696	-0.786687
C	-4.458256	2.777438	-0.036573
H	-5.873996	1.311812	0.750280
H	-2.741416	3.895246	-0.790631
C	-1.831356	-1.648709	1.557449
C	-1.306937	-1.055130	2.719715
C	-2.631050	-2.794737	1.693136
C	-1.582855	-1.582914	3.981764
H	-0.672994	-0.169143	2.631440
C	-2.896924	-3.332361	2.958482
H	-3.052549	-3.276902	0.809164
C	-2.376906	-2.728672	4.105352
H	-1.168683	-1.103563	4.872740
H	-3.518395	-4.227893	3.044230
H	-2.585720	-3.149684	5.092243
N	-5.337881	3.840928	-0.037364
C	-6.695602	3.663203	0.435908
H	-6.734906	3.350440	1.496337
H	-7.239309	4.612444	0.347531
H	-7.245910	2.906747	-0.153181
C	-4.889961	5.152041	-0.460935
H	-4.515539	5.146054	-1.500883
H	-5.729692	5.857101	-0.413828
H	-4.080194	5.548375	0.180290
Pd	0.765476	-0.109089	-0.591333
C	1.914917	3.539466	1.940160
C	1.882870	2.246772	1.416690
C	2.913058	1.747683	0.597460
C	4.007664	2.606396	0.297863
C	4.026314	3.905773	0.840559
C	2.995511	4.376537	1.653029
H	1.091303	3.891398	2.566874
H	1.022816	1.608346	1.625376
C	2.890320	0.334704	0.092591
C	5.114690	2.125725	-0.557225
H	4.866628	4.566109	0.621375
H	3.035497	5.392134	2.055107
C	5.011300	0.935946	-1.178282
C	3.817295	0.020817	-1.108970
H	5.833240	0.600638	-1.821112
H	4.215920	-0.995612	-0.968525
C	6.341555	2.985141	-0.732669
H	6.099651	3.950070	-1.210609
H	6.815834	3.220759	0.235196
H	7.087394	2.478590	-1.362031
C	2.363456	-0.684337	0.908275
Si	2.786237	-2.528213	0.927190
C	1.617245	-3.391476	2.137748
H	0.568778	-3.342859	1.805692
H	1.893040	-4.454045	2.246039
H	1.665237	-2.931307	3.138367
C	2.678676	-3.416817	-0.746898
H	1.706140	-3.247942	-1.235116
H	3.464917	-3.094305	-1.447704
H	2.801711	-4.503164	-0.596208
C	4.557574	-2.739555	1.587247
H	4.659564	-2.293098	2.590269
H	4.822696	-3.808019	1.665649
H	5.302336	-2.255829	0.934277
H	2.002863	-0.350352	1.890367
C	1.765206	0.835149	-2.377684
H	1.905928	1.895225	-2.135286
C	0.525650	0.431066	-2.830552
H	0.384317	-0.545558	-3.303996
H	-0.280156	1.155274	-2.973581
C	3.032961	0.008212	-2.462038
H	2.763691	-1.028171	-2.718932
H	3.677674	0.377822	-3.282860

63-ts

B3LYP SCF energy: -2286.80942569 a.u.
B3LYP enthalpy: -2286.053567 a.u.
B3LYP free energy: -2286.185064 a.u.
M06-L SCF energy in solution: -2288.31630200 a.u.
M06-L enthalpy in solution: -2287.560443 a.u.
M06-L free energy in solution: -2287.691940 a.u.
Imaginary frequency: -301.2849 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	-1.841986	-0.786882	0.016667
C	-2.746779	-1.706370	-1.317487
C	-2.367743	-3.037532	-1.573106
C	-3.750689	-1.127017	-2.109088
C	-2.995209	-3.776349	-2.577677
H	-1.567402	-3.493850	-0.984380
C	-4.369177	-1.865137	-3.125465
H	-4.053434	-0.092730	-1.934507
C	-3.997853	-3.190884	-3.359817
H	-2.693170	-4.811517	-2.757875
H	-5.147097	-1.397625	-3.735132
H	-4.482631	-3.766392	-4.152725
C	-2.587245	0.896953	-0.010483
C	-3.831958	1.212515	0.561679
C	-1.881705	1.941452	-0.632080
C	-4.356268	2.500958	0.507969
H	-4.410663	0.438781	1.071647
C	-2.393144	3.234449	-0.701476
H	-0.897968	1.736322	-1.063911
C	-3.652771	3.553924	-0.132732
H	-5.322212	2.687163	0.976097
H	-1.797184	4.001458	-1.194400
C	-2.557011	-1.529533	1.562838
C	-1.851833	-1.350756	2.765999
C	-3.763789	-2.247945	1.589884
C	-2.347415	-1.861941	3.967577
H	-0.899799	-0.812492	2.753038
C	-4.255461	-2.767651	2.792486
H	-4.323470	-2.410899	0.666368
C	-3.551523	-2.573932	3.983844
H	-1.785570	-1.712591	4.893374
H	-5.194049	-3.328444	2.795277
H	-3.935670	-2.982805	4.922053
N	-4.168289	4.833135	-0.192927
C	-5.442530	5.133628	0.427145
H	-5.432069	4.954729	1.518875
H	-5.686817	6.191129	0.264170
H	-6.265203	4.530889	0.000508
C	-3.411773	5.891800	-0.830127
H	-3.200773	5.669979	-1.892208
H	-3.988560	6.824845	-0.793395
H	-2.441551	6.075390	-0.331219
Pd	0.459956	-0.853218	-0.128208
C	1.679130	3.453092	1.028121
C	1.995345	2.136079	0.758545
C	3.263992	1.752986	0.238170
C	4.222011	2.800554	-0.021253
C	3.865124	4.146813	0.279124
C	2.627376	4.472320	0.793503
H	0.688953	3.701947	1.418475
H	1.235230	1.371226	0.928442
C	3.610358	0.369905	-0.037743
C	5.508607	2.489425	-0.578737
H	4.589629	4.941011	0.093737
H	2.380959	5.514567	1.013246
C	5.790458	1.167305	-0.857831
C	4.864143	0.136357	-0.592830
H	6.760084	0.903530	-1.290001
H	5.159978	-0.884243	-0.833984
C	6.525699	3.566732	-0.859819
H	6.144629	4.317876	-1.572511
H	6.811032	4.112767	0.055568
H	7.441720	3.135395	-1.288916
C	2.695583	-0.777512	0.244260
Si	3.411294	-2.417708	0.931227
C	4.631757	-3.353165	-0.188116
H	5.631568	-2.891509	-0.202606
H	4.754100	-4.374792	0.210653
H	4.287108	-3.449717	-1.229226
C	4.324002	-2.000005	2.541082
H	5.155973	-1.299821	2.363013
H	3.647173	-1.536402	3.277747
H	4.741273	-2.913601	2.998126
C	1.982554	-3.591645	1.323385
H	1.458368	-3.904423	0.406478
H	2.366134	-4.496580	1.825502
H	1.239798	-3.123700	1.988657
C	2.065566	-1.111485	-1.778423
H	3.110463	-1.407306	-1.888253
H	1.935798	-0.079393	-2.123987
C	1.148816	-2.081171	-2.418349
H	0.189159	-1.685931	-2.767420
C	1.418592	-3.381272	-2.660275
H	2.355321	-3.849870	-2.344468
H	0.697839	-4.017227	-3.180605
H	1.991324	-0.473583	1.065388

64

B3LYP SCF energy: -989.31800656 a.u.
B3LYP enthalpy: -988.930588 a.u.
B3LYP free energy: -989.002339 a.u.
M06-L SCF energy in solution: -989.98092189 a.u.
M06-L enthalpy in solution: -989.593503 a.u.
M06-L free energy in solution: -989.665254 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.637957	-2.316028	-1.310031
C	-1.437959	-1.661466	-1.121952
C	-1.351878	-0.414742	-0.434279
C	-2.581283	0.156007	0.064349
C	-3.800885	-0.550123	-0.146874
C	-3.836273	-1.755921	-0.814719
H	-2.659605	-3.269467	-1.844121
H	-0.532675	-2.122110	-1.516758
C	-0.101352	0.279925	-0.226097
C	-2.567841	1.413400	0.756058
H	-4.731712	-0.123889	0.229794
H	-4.786694	-2.275266	-0.961982
C	-1.353264	2.047200	0.926711
C	-0.145999	1.489558	0.450208
H	-1.317424	3.007724	1.448924
H	0.777952	2.042981	0.619954
C	-3.837887	2.032141	1.284956
H	-4.566397	2.230044	0.480349
H	-4.341529	1.378179	2.017040
H	-3.626600	2.988910	1.784218
C	1.229707	-0.271102	-0.711930
Si	2.301417	-0.995790	0.724449
C	2.641048	0.217021	2.137558
H	1.705071	0.564329	2.602298
H	3.234620	-0.287760	2.918778
H	3.207069	1.103770	1.811452
C	1.369041	-2.483400	1.429875
H	0.384745	-2.188381	1.827987
H	1.201369	-3.259947	0.665489
H	1.940861	-2.943104	2.253441
C	3.951856	-1.586575	-0.000675
H	4.573149	-0.749498	-0.358522
H	4.535779	-2.126937	0.763380
H	3.798187	-2.276492	-0.847366
C	1.973583	0.645408	-1.734964
H	1.263590	0.939804	-2.526970
H	2.737844	0.014931	-2.226281
C	2.673179	1.875005	-1.223724
H	3.460409	1.710197	-0.476644
C	2.446638	3.125370	-1.638830
H	1.675153	3.349490	-2.383300
H	3.021149	3.971495	-1.251004
H	1.031005	-1.188020	-1.286287

65-ts

B3LYP SCF energy: -2286.79784194 a.u.
B3LYP enthalpy: -2286.042327 a.u.
B3LYP free energy: -2286.170714 a.u.
M06-L SCF energy in solution: -2288.30763289 a.u.
M06-L enthalpy in solution: -2287.552118 a.u.
M06-L free energy in solution: -2287.680505 a.u.
Imaginary frequency: -323.6633 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	1.397702	-0.889836	0.062255
C	1.986989	-1.849633	1.534705
C	1.521867	-3.166215	1.718796
C	2.780299	-1.271817	2.539382
C	1.859491	-3.889300	2.864030
H	0.887681	-3.630515	0.959298
C	3.108678	-1.994470	3.692127
H	3.146184	-0.249742	2.423107
C	2.654033	-3.304637	3.857197
H	1.493929	-4.912378	2.985376
H	3.726147	-1.527202	4.463910
H	2.913259	-3.868554	4.756909
C	2.538833	0.553613	-0.026659
C	3.920187	0.436963	-0.263526
C	2.022601	1.849818	0.136365
C	4.749729	1.551990	-0.320048
H	4.368964	-0.547562	-0.415703
C	2.836977	2.978283	0.083695
H	0.948017	1.978357	0.298594
C	4.231545	2.862460	-0.143347
H	5.811469	1.399235	-0.510429
H	2.375549	3.956282	0.214166
C	1.956585	-1.944721	-1.362166
C	1.306993	-1.771383	-2.595628
C	3.014099	-2.866640	-1.279650
C	1.713754	-2.489100	-3.723630
H	0.466764	-1.074653	-2.657693
C	3.414195	-3.592119	-2.406619
H	3.525614	-3.030111	-0.328636
C	2.767918	-3.403461	-3.631564
H	1.197660	-2.340667	-4.675836
H	4.235651	-4.309042	-2.324823
H	3.080979	-3.972170	-4.511098
N	5.049202	3.972815	-0.195887

C	6.467322	3.821130	-0.449931
H	6.671351	3.354582	-1.431950
H	6.946431	4.808522	-0.443859
H	6.964515	3.203168	0.320279
C	4.484857	5.297389	-0.033442
H	3.987035	5.419889	0.945981
H	5.285669	6.045229	-0.096099
H	3.739822	5.535155	-0.815598
Pd	-0.819841	-0.224292	0.102261
C	-2.105604	3.834905	-2.161906
C	-2.066256	2.482167	-1.836144
C	-2.793336	1.961969	-0.747498
C	-3.579288	2.858401	0.036834
C	-3.612217	4.225389	-0.319106
C	-2.887787	4.713245	-1.401207
H	-1.521967	4.207147	-3.007818
H	-1.441037	1.810174	-2.425752
C	-2.793500	0.506726	-0.426431
C	-4.347216	2.353949	1.179276
H	-4.215602	4.918293	0.269239
H	-2.927368	5.776593	-1.651098
C	-4.168058	1.063232	1.577887
C	-3.258744	0.158333	0.913273
H	-4.712920	0.692267	2.450683
H	-3.399711	-0.902317	1.123495
C	-5.298900	3.263851	1.910647
H	-4.775923	4.119140	2.372924
H	-6.058874	3.687481	1.232255
H	-5.823428	2.722311	2.711000
C	-2.464701	-0.479434	-1.399862
Si	-3.087997	-2.259817	-1.508866
C	-2.404089	-3.448140	-0.200610
H	-2.585636	-3.101370	0.829040
H	-2.868967	-4.443263	-0.310785
H	-1.315564	-3.564973	-0.322200
C	-4.985348	-2.272360	-1.390232
H	-5.334331	-1.887451	-0.418105
H	-5.434122	-1.642030	-2.175669
H	-5.382456	-3.295177	-1.507889
C	-2.592269	-2.909659	-3.218691
H	-1.496462	-2.945838	-3.331164
H	-2.977527	-3.930870	-3.377782
H	-2.996077	-2.271922	-4.022894
H	-2.253518	-0.070802	-2.395118
C	-1.586999	0.358635	2.500696
H	-1.899169	1.396772	2.621226
H	-0.503199	0.270133	2.337327
C	-2.112255	-0.606615	3.452443
H	-3.086709	-0.362102	3.896123
C	-1.536277	-1.772277	3.817078
H	-0.572061	-2.090396	3.410077
H	-2.019983	-2.439691	4.535283

66

B3LYP SCF energy: -2286.85731869 a.u.
B3LYP enthalpy: -2286.098781 a.u.
B3LYP free energy: -2286.232393 a.u.
M06-L SCF energy in solution: -2288.35511535 a.u.
M06-L enthalpy in solution: -2287.596578 a.u.
M06-L free energy in solution: -2287.730190 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.620667	-0.810427	0.114965
C	1.979183	-1.605971	1.753043
C	1.039044	-2.521320	2.260802
C	3.122006	-1.318910	2.516153
C	1.248806	-3.151359	3.489628
H	0.131112	-2.731227	1.688962
C	3.324866	-1.941293	3.753085
H	3.857040	-0.601181	2.146817
C	2.392851	-2.860526	4.241215
H	0.510461	-3.864088	3.866453
H	4.217526	-1.703155	4.337748
H	2.552644	-3.344572	5.208232
C	2.840569	0.561819	0.002593
C	4.174705	0.392349	-0.405360
C	2.431763	1.861068	0.349385
C	5.064970	1.461904	-0.455315
H	4.533254	-0.597051	-0.699954
C	3.309512	2.940108	0.313142
H	1.393213	2.033696	0.647284
C	4.659645	2.771701	-0.089419
H	6.085180	1.272253	-0.786960
H	2.933620	3.923880	0.591214
C	2.272859	-2.043759	-1.106362
C	2.011055	-1.813645	-2.469709
C	3.001186	-3.186888	-0.741717
C	2.480622	-2.696278	-3.443762
H	1.427230	-0.937178	-2.764168
C	3.460813	-4.077555	-1.719422
H	3.211329	-3.389835	0.310259
C	3.205457	-3.834374	-3.070654
H	2.270742	-2.500810	-4.498626
H	4.022948	-4.965719	-1.418571
H	3.564739	-4.531146	-3.832434
N	5.537320	3.836088	-0.131227
C	6.900308	3.637160	-0.580137
H	6.950681	3.266412	-1.621188

H	7.440454	4.591622	-0.539105
H	7.446801	2.915924	0.055098
C	5.084504	5.165494	0.225283
H	4.699143	5.208967	1.260283
H	5.924706	5.867911	0.153780
H	4.281876	5.530875	-0.442790
Pd	-0.612521	-0.248095	-0.235076
C	-1.895894	4.054567	-1.447860
C	-1.798264	2.684868	-1.190839
C	-2.834218	1.984256	-0.553896
C	-4.009424	2.690995	-0.170215
C	-4.092439	4.067981	-0.445918
C	-3.047609	4.749617	-1.072300
H	-1.069552	4.575902	-1.938043
H	-0.893523	2.137543	-1.469857
C	-2.790449	0.503488	-0.332189
C	-5.126182	1.957123	0.467796
H	-4.990766	4.620466	-0.164498
H	-3.135621	5.821747	-1.266631
C	-4.912277	0.712251	0.941065
C	-3.556142	0.043631	0.908301
H	-5.732946	0.171486	1.423650
H	-3.702189	-1.044793	0.847582
C	-6.473730	2.622207	0.588745
H	-6.431354	3.514396	1.237216
H	-6.849196	2.960727	-0.391823
H	-7.214366	1.933188	1.019952
C	-2.468903	-0.359112	-1.384714
Si	-2.959100	-2.166089	-1.698153
C	-2.485141	-3.405418	-0.346552
H	-2.910166	-3.155253	0.638036
H	-2.846695	-4.411477	-0.621244
H	-1.389984	-3.453211	-0.241792
C	-4.838575	-2.239147	-1.964347
H	-5.388382	-1.932147	-1.059716
H	-5.148102	-1.567822	-2.782297
H	-5.160904	-3.261685	-2.225372
C	-2.098670	-2.681737	-3.303343
H	-1.002840	-2.667571	-3.187097
H	-2.393393	-3.703558	-3.595795
H	-2.361170	-2.006973	-4.135254
H	-2.194826	0.151221	-2.321118
C	-2.773287	0.312517	2.232194
H	-2.621280	1.403195	2.321574
H	-1.773413	-0.145276	2.137266
C	-3.459119	-0.204007	3.465039
H	-4.434214	0.240546	3.703103
C	-2.971115	-1.148366	4.276397
H	-1.998143	-1.616033	4.089887
H	-3.519282	-1.481396	5.162677

67-ts

B3LYP SCF energy: -5713.16256407 a.u.
B3LYP enthalpy: -5712.325408 a.u.
B3LYP free energy: -5712.484826 a.u.
M06-L SCF energy in solution: -5715.55968557 a.u.
M06-L enthalpy in solution: -5714.722529 a.u.
M06-L free energy in solution: -5714.881947 a.u.
Imaginary frequency: -38.6015 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	2.084626	-1.302940	-0.657804
P	-3.117155	-0.261505	0.559345
O	-0.728030	-1.986625	0.144437
C	1.541700	-2.509520	0.665544
C	2.433903	-3.245729	1.464390
C	1.986194	-4.156505	2.424732
C	0.615618	-4.351304	2.610384
C	-0.295617	-3.638681	1.832960
C	0.162833	-2.730833	0.868003
C	-1.706704	-3.749115	-1.175817
C	-1.825097	-2.550705	-0.460096
C	-3.047061	-1.853309	-0.400792
C	-4.140310	-2.392436	-1.100046
C	-4.035777	-3.589425	-1.811941
C	-2.813811	-4.268284	-1.845508
C	3.929835	-1.254216	-0.399737
C	4.457522	-0.818072	0.831102
C	5.837228	-0.707410	1.020211
C	6.720657	-1.004225	-0.021707
C	6.210087	-1.416545	-1.254656
C	4.829573	-1.544540	-1.440581
C	1.990177	-2.396481	-2.164132
C	2.147728	-3.792204	-2.089872
C	2.128753	-4.576060	-3.246922
C	1.956821	-3.974555	-4.498320
C	1.803271	-2.588855	-4.581776
C	1.813851	-1.802582	-3.423796
C	-4.542368	0.587274	-0.277973
C	-4.250511	1.232251	-1.496878
C	-5.243981	1.940746	-2.176206
C	-6.536046	2.035177	-1.646527
C	-6.830041	1.410142	-0.432084
C	-5.841302	0.688572	0.247483
C	-3.889311	-0.825273	2.159762
C	-3.841554	0.089127	3.230127
C	-4.369088	-0.237686	4.482024
C	-4.935456	-1.498864	4.697666

C	-4.972140	-2.424064	3.650968
C	-4.457872	-2.089447	2.392844
H	3.507065	-3.110626	1.328910
H	2.711441	-4.709614	3.026852
H	0.251368	-5.051173	3.367294
H	-5.092344	-1.857356	-1.084861
H	-4.903213	-3.984826	-2.346807
H	-2.712303	-5.197052	-2.413496
H	3.789319	-0.559681	1.653221
H	6.217616	-0.367878	1.987014
H	7.800181	-0.908414	0.125365
H	6.887525	-1.646551	-2.082009
H	4.455122	-1.874992	-2.410390
H	2.293652	-4.274255	-1.121006
H	2.251289	-5.660350	-3.169336
H	1.938655	-4.586870	-5.404642
H	1.655538	-2.108491	-5.552701
H	1.650448	-0.726191	-3.495400
H	-3.237724	1.174161	-1.913652
H	-4.998606	2.433368	-3.120987
H	-7.308613	2.600629	-2.175550
H	-7.835712	1.481301	-0.006892
H	-6.088337	0.204752	1.195121
H	-3.374595	1.066776	3.078745
H	-4.324132	0.491085	5.296107
H	-5.338551	-1.761124	5.679855
H	-5.407614	-3.414886	3.810948
H	-4.502763	-2.821405	1.583696
H	-0.737880	-4.248461	-1.226370
H	-1.371061	-3.764700	1.972113
Pd	1.021061	0.928515	-0.639846
C	0.152610	0.444409	3.923394
C	0.544280	0.672333	2.618701
C	1.763528	1.340062	2.301128
C	2.591313	1.793755	3.395431
C	2.156648	1.539510	4.729872
C	0.971455	0.881166	4.991161
H	-0.789073	-0.071537	4.128890
H	-0.084141	0.345738	1.785870
C	2.158196	1.550507	0.929851
C	3.816068	2.487594	3.117487
H	2.774374	1.876493	5.565522
H	0.663595	0.700496	6.025769
C	4.157515	2.692201	1.792737
C	3.350558	2.232379	0.722669
H	5.086689	3.224779	1.559854
H	3.700321	2.419153	-0.296756
Br	-0.616816	0.451195	-2.635012
C	4.700601	2.992093	4.232536
H	4.175900	3.711662	4.886114
H	5.056435	2.176369	4.887317
H	5.587835	3.501516	3.826130
C	0.968804	3.748051	-1.375497
H	1.924506	4.082039	-0.949101
C	0.174140	2.869334	-0.516022
H	-0.858208	2.735271	-0.860906
H	0.207196	3.187134	0.534504
C	0.656363	4.189435	-2.621275
H	-0.252751	3.847405	-3.124571
H	1.373081	4.769624	-3.208937
B	-0.497827	6.301476	-1.549025
F	-1.694874	5.738416	-1.504444
F	0.165234	6.510375	-0.419254
F	-0.164048	7.023463	-2.616974

68

B3LYP SCF energy: -5388.83565713 a.u.
B3LYP enthalpy: -5388.016423 a.u.
B3LYP free energy: -5388.162893 a.u.
M06-L SCF energy in solution: -5390.93519594 a.u.
M06-L enthalpy in solution: -5390.115962 a.u.
M06-L free energy in solution: -5390.262432 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-2.027678	-1.148165	-0.386305
P	3.149655	0.530252	-0.000783
O	0.824207	-0.823752	-1.272599
C	-1.411118	-0.728873	-2.103732
C	-2.256906	-0.499261	-3.202903
C	-1.753610	-0.214846	-4.475137
C	-0.372868	-0.151091	-4.676913
C	0.493309	-0.373866	-3.607677
C	-0.020761	-0.662440	-2.336122
C	1.852955	-2.904049	-1.917658
C	1.933779	-1.629173	-1.342180
C	3.128947	-1.168795	-0.756332
C	4.231631	-2.039928	-0.750607
C	4.164057	-3.310068	-1.327048
C	2.969239	-3.738767	-1.913560
C	-3.867988	-0.928377	-0.586604
C	-4.387314	0.342443	-0.901838
C	-5.765648	0.551176	-0.991019
C	-6.657750	-0.496615	-0.743782
C	-6.156710	-1.757289	-0.411044
C	-4.776412	-1.972191	-0.337107
C	-1.912302	-3.007346	-0.431284
C	-1.955149	-3.744355	-1.627832
C	-1.925362	-5.142135	-1.607706

C	-1.857473	-5.824235	-0.388322
C	-1.816068	-5.100160	0.805601
C	-1.835661	-3.701061	0.787392
C	4.499967	0.334439	1.261616
C	4.147769	-0.329365	2.454454
C	5.081106	-0.472207	3.483507
C	6.370080	0.057858	3.352497
C	6.722698	0.728347	2.178684
C	5.795426	0.863796	1.138372
C	4.006989	1.521577	-1.327825
C	3.918589	2.922488	-1.212220
C	4.500945	3.763392	-2.164225
C	5.166108	3.218891	-3.268053
C	5.247028	1.830408	-3.405899
C	4.675707	0.989577	-2.443724
H	-3.336965	-0.551936	-3.063176
H	-2.443578	-0.042219	-5.305056
H	0.034092	0.082114	-5.664575
H	5.160494	-1.711731	-0.278779
H	5.037830	-3.966662	-1.307674
H	2.895557	-4.737943	-2.351519
H	-3.712116	1.179725	-1.081140
H	-6.139675	1.547928	-1.238719
H	-7.736887	-0.329094	-0.804486
H	-6.841399	-2.586261	-0.209751
H	-4.408486	-2.966796	-0.081460
H	-2.021538	-3.225982	-2.586734
H	-1.958946	-5.698881	-2.548838
H	-1.831873	-6.917763	-0.370923
H	-1.748047	-5.622000	1.763919
H	-1.758506	-3.142603	1.721448
H	3.136549	-0.738334	2.572034
H	4.790619	-0.993451	4.399853
H	7.094881	-0.047444	4.165060
H	7.726754	1.148494	2.066052
H	6.087942	1.387233	0.225364
H	3.375423	3.356398	-0.367451
H	4.421614	4.848146	-2.050339
H	5.612315	3.874598	-4.021046
H	5.760682	1.394884	-4.268120
H	4.753785	-0.093175	-2.562306
H	0.903208	-3.242563	-2.334499
H	1.575496	-0.313158	-3.738490
Pd	-1.047668	0.129608	1.492316
C	-0.104864	3.740582	-1.341291
C	-0.520213	2.756169	-0.465868
C	-1.767367	2.831826	0.221535
C	-2.600098	3.989622	-0.015263
C	-2.140815	4.985320	-0.927689
C	-0.927536	4.867455	-1.576129
H	0.857924	3.648188	-1.851165
H	0.110184	1.884722	-0.269609
C	-2.180341	1.783501	1.123225
C	-3.853680	4.113459	0.670821
H	-2.762799	5.863614	-1.115582
H	-0.601422	5.647844	-2.270920
C	-4.214901	3.102522	1.543881
C	-3.400290	1.964890	1.764834
H	-5.166723	3.181215	2.082172
H	-3.761666	1.206834	2.465853
Br	0.572598	-1.811273	2.246542
C	-4.748001	5.311874	0.460474
H	-4.251803	6.258087	0.742138
H	-5.058581	5.424207	-0.593949
H	-5.662850	5.225958	1.066977
C	-1.072521	1.201773	4.265642
H	-1.990290	1.806783	4.261805
C	-0.240098	1.306143	3.052367
H	0.763925	0.885948	3.189659
H	-0.178184	2.342541	2.690751
C	-0.828047	0.449053	5.356146
H	0.054595	-0.196011	5.414261
H	-1.523808	0.427340	6.201798

69-ts

B3LYP SCF energy: -3254.60454383 a.u.
B3LYP enthalpy: -3253.713996 a.u.
B3LYP free energy: -3253.866183 a.u.
M06-L SCF energy in solution: -3256.79226578 a.u.
M06-L enthalpy in solution: -3255.901718 a.u.
M06-L free energy in solution: -3256.053905 a.u.
Imaginary frequency: -265.8837 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.565082	1.940018	-0.069634
P	-2.318071	-0.614310	0.072841
O	-2.100636	1.704160	-1.468101
C	-0.063781	2.962511	-1.492373
C	0.690962	3.989545	-2.089134
C	0.207109	4.697723	-3.192430
C	-1.041536	4.386786	-3.735518
C	-1.818538	3.384300	-3.152206
C	-1.338711	2.703180	-2.031876
C	-3.762551	3.172883	-0.428285
C	-3.068896	1.965804	-0.525154
C	-3.344295	0.889873	0.337587
C	-4.356582	1.040662	1.295925
C	-5.063666	2.242335	1.398569

C	-4.760907	3.303363	0.541787
C	2.315592	2.513381	0.093374
C	3.202814	2.353018	-0.987101
C	4.532289	2.762497	-0.880554
C	5.002653	3.324655	0.310751
C	4.132361	3.480121	1.390819
C	2.796090	3.080257	1.284859
C	-0.239445	2.676311	1.419553
C	-0.654983	4.017367	1.456300
C	-1.179248	4.561428	2.631817
C	-1.286198	3.778025	3.784916
C	-0.868931	2.444111	3.759428
C	-0.353522	1.895656	2.581566
C	-2.846439	-1.753330	1.429869
C	-2.560107	-1.379707	2.758233
C	-2.872251	-2.229038	3.821620
C	-3.459994	-3.475715	3.577426
C	-3.735902	-3.862617	2.264589
C	-3.433551	-3.008770	1.196569
C	-3.059128	-1.309117	-1.470301
C	-2.234851	-1.613039	-2.564364
C	-2.784379	-2.096209	-3.756918
C	-4.165094	-2.275769	-3.868385
C	-4.997241	-1.962856	-2.787354
C	-4.450303	-1.476809	-1.598230
H	1.673501	4.242193	-1.691703
H	0.816522	5.490449	-3.631789
H	-1.413925	4.924308	-4.610606
H	-4.595034	0.217634	1.971526
H	-5.850852	2.347203	2.148095
H	-5.310012	4.244695	0.620347
H	2.859519	1.909200	-1.922161
H	5.204263	2.635558	-1.732509
H	6.045179	3.640713	0.395212
H	4.489477	3.918790	2.325606
H	2.134105	3.217354	2.140293
H	-0.566373	4.644736	0.567051
H	-1.501152	5.605486	2.647588
H	-1.692332	4.207882	4.703707
H	-0.943451	1.829316	4.659867
H	-0.026643	0.852688	2.566688
H	-2.100889	-0.410162	2.965430
H	-2.655975	-1.916939	4.846378
H	-3.702814	-4.140801	4.409537
H	-4.196166	-4.833185	2.063975
H	-3.667301	-3.326988	0.179223
H	-1.156236	-1.452058	-2.491165
H	-2.130927	-2.323526	-4.602675
H	-4.595894	-2.650613	-4.800016
H	-6.079027	-2.090775	-2.873384
H	-5.113971	-1.219864	-0.769274
H	-3.530531	3.999073	-1.100891
H	-2.797726	3.116948	-3.554036
Pd	0.227989	-0.566630	-0.130500
C	3.945136	-0.739869	2.837855
C	2.959640	-0.680873	1.874609
C	3.251828	-0.799912	0.485720
C	4.632541	-0.960808	0.095627
C	5.623716	-1.020110	1.117473
C	5.294481	-0.918266	2.453413
H	3.687843	-0.643844	3.895722
H	1.919013	-0.529182	2.168863
C	2.231349	-0.755580	-0.518275
C	4.978542	-1.057321	-1.295602
H	6.670194	-1.147661	0.836956
H	6.076463	-0.968366	3.214993
C	3.960229	-0.995694	-2.228934
C	2.600469	-0.855146	-1.846267
H	4.203198	-1.064576	-3.293497
H	1.846748	-0.817314	-2.638595
C	6.412651	-1.223506	-1.733050
H	7.044434	-0.385193	-1.394919
H	6.862133	-2.144486	-1.325556
H	6.485832	-1.275203	-2.828700
N	0.538693	-3.041915	1.837489
N	0.811127	-3.158990	2.898579
C	0.132587	-2.603943	-0.083843
Si	1.052386	-4.138181	-0.867027
C	0.166029	-5.676243	-0.216023
H	-0.916707	-5.648805	-0.420635
H	0.571994	-6.575693	-0.709152
H	0.303561	-5.814248	0.868856
C	0.719129	-3.979690	-2.719280
H	-0.358170	-3.962624	-2.944435
H	1.189836	-3.087556	-3.155954
H	1.148747	-4.866285	-3.216181
C	2.880019	-4.251847	-0.463175
H	3.065386	-4.233680	0.622113
H	3.259734	-5.214184	-0.846360
H	3.463509	-3.443946	-0.924211
H	-0.891892	-2.953552	0.132246

70

B3LYP SCF energy: -3145.29493242 a.u.
B3LYP enthalpy: -3144.411710 a.u.
B3LYP free energy: -3144.555958 a.u.
M06-L SCF energy in solution: -3147.37103813 a.u.
M06-L enthalpy in solution: -3146.487816 a.u.
M06-L free energy in solution: -3146.632064 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.840057	1.054481	-0.196774
P	-2.001558	0.720034	0.375977
O	-0.401534	3.037790	0.168207
C	1.867261	2.877768	-0.555924
C	2.991224	3.523002	-1.104343
C	2.977209	4.894586	-1.369800
C	1.831179	5.649991	-1.105823
C	0.700963	5.032076	-0.567817
C	0.733301	3.664166	-0.288109
C	-0.251979	3.769156	2.492397
C	-0.707032	2.903341	1.497282
C	-1.568327	1.828390	1.789467
C	-1.997952	1.664159	3.114776
C	-1.557549	2.530830	4.119643
C	-0.679916	3.572013	3.808319
C	3.265050	0.498004	-1.235540
C	3.074923	0.432394	-2.628300
C	4.112198	0.023707	-3.468374
C	5.353764	-0.333098	-2.927157
C	5.549599	-0.272076	-1.545339
C	4.511814	0.142362	-0.700988
C	2.451083	0.931032	1.540024
C	3.227175	1.934410	2.145098
C	3.691728	1.774339	3.453566
C	3.388352	0.613595	4.171652
C	2.613806	-0.387990	3.578825
C	2.142926	-0.228575	2.272833
C	-3.272831	-0.404925	1.102521
C	-2.859416	-1.337207	2.073324
C	-3.779072	-2.208783	2.660017
C	-5.122692	-2.179735	2.269625
C	-5.537083	-1.275115	1.289905
C	-4.620755	-0.389973	0.710152
C	-2.907292	1.834737	-0.775857
C	-2.577348	1.849792	-2.138194
C	-3.236850	2.713205	-3.018060
C	-4.229154	3.573522	-2.540850
C	-4.554760	3.574645	-1.179988
C	-3.895066	2.714499	-0.299137
H	3.888873	2.947317	-1.333491
H	3.863768	5.371257	-1.793754
H	1.812592	6.719715	-1.326749
H	-2.683002	0.855517	3.370792
H	-1.902354	2.389515	5.146017
H	-0.329561	4.247218	4.592592
H	2.110126	0.709358	-3.063632
H	3.953049	-0.016239	-4.548744
H	6.166053	-0.653889	-3.583761
H	6.517529	-0.543768	-1.116743
H	4.682630	0.187012	0.376059
H	3.471657	2.847009	1.597873
H	4.293352	2.561983	3.913772
H	3.751609	0.492279	5.195104
H	2.368355	-1.295627	4.135514
H	1.529716	-1.012820	1.821007
H	-1.809048	-1.387492	2.372187
H	-3.443334	-2.916946	3.421567
H	-5.842067	-2.864017	2.725707
H	-6.582261	-1.251007	0.972241
H	-4.966839	0.308470	-0.052298
H	-1.786829	1.193708	-2.508322
H	-2.970035	2.717017	-4.077599
H	-4.745012	4.249329	-3.227257
H	-5.323491	4.252355	-0.800766
H	-4.148010	2.735706	0.763599
H	0.420876	4.589824	2.240362
H	-0.216049	5.590873	-0.371484
Pd	-0.129418	-0.457027	-0.533132
C	-0.536336	-5.029178	2.293456
C	-0.775018	-4.183578	1.222468
C	0.285791	-3.647649	0.453965
C	1.630072	-4.022525	0.781617
C	1.842111	-4.884409	1.889255
C	0.784422	-5.375504	2.635027
H	-1.374093	-5.434969	2.865466
H	-1.804464	-3.939384	0.961219
C	0.037637	-2.776120	-0.694594
C	2.741214	-3.552209	-0.022987
H	2.858617	-5.176566	2.154070
H	0.974812	-6.042798	3.478936
C	2.484202	-2.738414	-1.099834
C	1.160930	-2.337715	-1.441144
H	3.307602	-2.404400	-1.732225
H	1.007065	-1.843482	-2.402074
C	4.151879	-3.970633	0.296253
H	4.449203	-3.651562	1.309271
H	4.270136	-5.066152	0.258230
H	4.861327	-3.529122	-0.416736
C	-1.247871	-2.206723	-1.040634
Si	-1.982826	-2.322120	-2.813781
C	-2.009402	-4.167176	-3.231451
H	-2.587711	-4.742354	-2.490148
H	-2.477864	-4.328911	-4.216958
H	-0.992741	-4.590907	-3.267974
C	-3.754523	-1.677501	-2.776426
H	-4.344460	-2.176612	-1.990854
H	-3.812426	-0.591773	-2.607995
H	-4.241930	-1.890894	-3.742418
C	-0.990695	-1.413219	-4.147500

H	-0.022345	-1.897394	-4.351552	H	-0.799947	-0.357340	-3.898149
H	-1.561564	-1.431557	-5.091147	H	-2.041318	-2.432735	-0.319253