Supplementary Information

Understanding the Reactivity of Geminal P/B and P/Al Frustrated Lewis Pairs in CO_2 Addition and H_2 Activation

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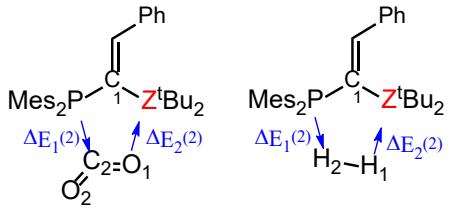
Table S1. Solvent-corrected relative energies (in kcal/mol) for the reactions of **1PZ[b]** (Z = B, Al) in the CO_2 addition and the H_2 activation calculated by ωB97XD/BS2 and PBE0/BS2 on the gas-phase geometries optimized by ωB97XD/BS1.

CO_2 addition	ωB97XD/BS2	PBE0/BS2
1PB[b]	0.0	0.0
TS14_PB[b]	13.1	12.3
4PB[b]	-12.4	-13.1
1PAl[b]	0.0	0.0
TS14_PAl[b]	5.1	8.3
4PAl[b]	-25.6	-24.9

H_2 activation	ωB97XD/BS2	PBE0/BS2
1PB[b]	0.0	0.0
TS13_PB[b]	25.3	21.0
3PB[b]	-4.4	-5.0
1PAl[b]	0.0	0.0
TS13_PAl[b]	18.5	15.2
3PAl[b]	-5.3	-3.7

BS1 (basis set 1) is the 6-31++G(d,p) for P, Al, B, and C, O, and H of the substrates involved in the reaction (H_2 and CO_2) and 6-31G(d) for all other atoms. Quasi-harmonic correction was applied for all free energies.
BS2 (basis set 2) is the 6-311++G(d,p) basis set for all atoms.

Table S2. Second-order perturbative energy ($\Delta E^{(2)}$) (kcal/mol) from donor orbital to acceptor orbital of CO_2 addition and H_2 activation transition states (**TS14_PZ[a]** and **TS13_PZ[a]**) (Z = B, Al).



TS14_PZ[a] **TS13_PZ[a]**

CO_2 addition	Donor	Acceptor	**TS14_PB[a]**	**TS14_PAl[a]**
	LP(P)	π*(C2-O1)	2.1	0.3
$\Delta E_1^{(2)}$	LP(P)	π*(C2-O2)	58.8	18.9
$\Delta E_2^{(2)}$	LP(O1)	LV(Z)	22.0	0.9
H_2 activation	Donor	Acceptor	**TS13_PB[a]**	**TS13_PAl[a]**
$\Delta E_1^{(2)}$	LP(P)	σ*(H1-H2)	157.7	273.9
$\Delta E_2^{(2)}$	σ(H1-H2)	LV(Z)	249.4	77.7

Table S3. Distortion-interaction energies (in kcal/mol) and natural energy decomposition analysis (NEDA) of CO_2 addition and H_2 activation transition states (**TS14_PZ[a]** and **TS13_PZ[a]**).

	CO_2		H_2	
	TS14_PB[a]	**TS14_PAl[a]**	**TS13_PB[a]**	**TS13_PAl[a]**
Distortion-interaction energy				
$\Delta E^{\ddagger}$	9.5	-4.0	17.4	13.0
ΔE_{dist_PZ}	7.5	5.4	16.3	14.1
ΔE_{dist_sub}	16.9	5.1	16.2	25.1
ΔE_{int}	-14.8	-14.4	-15.2	-26.2
NEDA				
ΔE_{el}	-77.1	-58.5	-53.8	-52.5
ΔE_{ct}	-115.7	-93.8	-298.6	-233.6
ΔE_{core}	184.0	143.4	335.9	260.1
ΔE_{int}	-8.8	-9.0	-16.4	-26.0

Table S4. Absolute electronic energies, enthalpies, entropies, Gibbs free energies in gas phase and solvent phase for intermediates and transition states of all complexes involved in CO_2 addition and H_2 activation. Geometry structure of complexes in gas phase were optimized using ωB97XD/BS1, and the solvent correction is in dichloromethane using ωB97XD/BS2).*

Complex	ωB97XD/BS1						ωB97XD/BS2
	Imaginary Frequency	**E_{elec} (hartree)**	**H_{gas} (hartree)**	**S (cal/mol)**	**G_{gas} (hartree)**	**G_{qhHS} (hartree)**	**G_{solv} (hartree)**
H_2	-	-1.175283845	-1.161841845	31.134	-1.176634845	-1.168695	-1.175807497
CO_2	-	-188.524613	-188.509236	51.075	-188.533503	-188.39679	-188.5803889
$PtBu_3$	-	-814.7348546	-814.3407566	123.532	-814.3994506	-814.400078	-814.9015096
BPh_3	-	-719.5729459	-719.2754899	124.267	-719.3345339	-719.334631	-719.7669945
TS14_$^tBu_3P/BPh_3$	-157.8i	-1722.840505	-1722.131659	225.433	-1722.23877	-1722.237858	-1723.252557
4_$^tBu_3P/BPh_3$	-	-1722.856847	-1722.14609	216.163	-1722.248796	-1722.24821	-1723.280594
1PB[b]	-	-1184.247574	-1183.754931	167.099	-1183.834325	-1183.833644	-1184.508885
TS14_PB[b]	-178.3i	-1372.769215	-1372.26047	180.093	-1372.346038	-1372.345522	-1373.087088
4PB[b]	-	-1372.80594	-1372.296144	178.934	-1372.381162	-1372.380055	-1373.129846
1PB[c]	-	-1222.312631	-1221.813285	167.163	-1221.892709	-1221.892734	-1222.582424
TS14_PB[c]	-184.0i	-1410.832493	-1410.317439	181.604	-1410.403725	-1410.403495	-1411.156984
4PB[c]	-	-1410.86927	-1410.353	180.669	-1410.438842	-1410.4382	-1411.20018
1PB[d]	-	-1567.607673	-1567.001198	200.74	-1567.096576	-1567.096255	-1567.962299
TS14_PB[d]	-166.9i	-1756.121279	-1755.499969	216.76	-1755.602959	-1755.602227	-1756.531533
4PB[d]	-	-1756.147302	-1755.523795	211.229	-1755.624156	-1755.62317	-1756.560627

Complex	ωB97XD/BS1						ωB97XD/BS2
	Imaginary Frequency	E_{elec} (hartree)	H_{gas} (hartree)	S (cal/mol)	G_{gas} (hartree)	G_{qhHS} (hartree)	G_{solv} (hartree)
1PB[e]	-	-1420.062624	-1419.391238	205.004	-1419.488642	-1419.488083	-1420.38343
TS14_PB[e]	-198.6i	-1608.576912	-1607.889396	214.717	-1607.991415	-1607.991545	-1608.952349
4PB[e]	-	-1608.60568	-1607.916862	209.648	-1608.016472	-1608.016335	-1608.982294
1PB[f]	-	-1458.123441	-1457.445975	204.792	-1457.543279	-1457.543565	-1458.449982
TS14_PB[f]	-182.8i	-1646.636903	-1645.943482	217.532	-1646.046839	-1646.047068	-1647.018856
4PB[f]	-	-1646.665839	-1645.971041	210.043	-1646.07084	-1646.071252	-1647.050146
1PB[a]	-	-1689.097998	-1688.332399	225.505	-1688.439544	-1688.43951	-1689.487151
TS14_PB[a]	-181.6i	-1877.610703	-1876.829335	236.183	-1876.941553	-1876.941367	-1878.054218
4PB[a]	-	-1877.635023	-1876.852737	235.07	-1876.964426	-1876.964033	-1878.078921
TS14_PAl[b]	-82.6i	-1590.347069	-1589.84331	188.542	-1589.932893	-1589.932035	-1590.681049
4PAl[b]	-	-1590.392740	-1589.88702	189.379	-1589.977001	-1589.975011	-1590.732649
TS14_PAl[a]	-129.0i	-2095.213617	-2094.438613	248.571	-2094.556717	-2094.556823	-2095.672329
4PAl[a]	-	-2095.243544	-2094.466159	244.953	-2094.582544	-2094.582116	-2095.704105
TS13_$^{t}Bu_3P/BPh_3$	-351.4i	-1535.483652	-1534.774756	207.121	-1534.873166	-1534.872536	-1535.843462
3_$^{t}Bu_3P/BPh_3$	-	-1535.494825	-1534.782448	208.6	-1534.88156	-1534.881408	-1535.872679
TS13_PB[b]	-916.4i	-1185.394208	-1184.88701	165.689	-1184.965735	-1184.96535	-1185.660693
3PB[b]	-	-1185.436319	-1184.923694	165.012	-1185.002097	-1185.001955	-1185.713529
TS13_PB[c]	-907.4i	-1223.458882	-1222.945307	168.801	-1223.02551	-1223.025295	-1223.733552
3PB[c]	-	-1223.499883	-1222.981354	171.376	-1223.06278	-1223.062268	-1223.783842
TS13_PB[d]	-820.8i	-1568.748101	-1568.127854	207.474	-1568.226432	-1568.225033	-1569.106728
3PB[d]	-	-1568.784568	-1568.159476	210.497	-1568.25949	-1568.257353	-1569.152755
TS13_PB[e]	-973.3i	-1421.209264	-1420.523345	201.219	-1420.618951	-1420.619075	-1421.531247
3PB[e]	-	-1421.242934	-1420.552164	204.465	-1420.649311	-1420.648775	-1421.573719
TS13_PB[f]	-924.5i	-1459.270492	-1458.579165	204.882	-1458.676511	-1458.676726	-1459.600673
3PB[f]	-	-1459.298664	-1458.601515	203.611	-1458.698258	-1458.698462	-1459.637056
TS13_PB[a]	-923.3i	-1690.246029	-1689.466572	226.571	-1689.574223	-1689.574002	-1690.636674
3PB[a]	-	-1690.27211	-1689.487944	229.968	-1689.597209	-1689.596807	-1690.670004
1PAl[b]	-	-1401.811416	-1401.323141	175.092	-1401.406333	-1401.405311	-1402.09101
TS13_PAl[b]	-940.7i	-1402.966609	-1402.464942	176.524	-1402.548815	-1402.547779	-1403.25143
3PAl[b]	-	-1402.999787	-1402.494324	177.665	-1402.578738	-1402.577776	-1403.292477
1PAl[c]	-	-1439.869591	-1439.374859	180.246	-1439.4605	-1439.459478	-1440.157414
TS13_PAl[c]	-894.9i	-1441.027718	-1440.519558	184.078	-1440.607019	-1440.605346	-1441.318966
3PAl[c]	-	-1441.059594	-1440.547433	180.824	-1440.633348	-1440.632596	-1441.359337
pre_1PAl[d]	-	-1785.174096	-1784.572152	208.36	-1784.67115	-1784.670414	-1785.545646
1PAl[d]	-	-1785.161567	-1784.560581	215.694	-1784.663064	-1784.661328	-1785.534093

Complex	ωB97XD/BS1						ωB97XD/BS2
	Imaginary Frequency	E_{elec} (hartree)	H_{gas} (hartree)	S (cal/mol)	G_{gas} (hartree)	G_{qhHS} (hartree)	G_{solv} (hartree)
TS13_PAl[d]	-823.6i	-1786.323045	-1785.708501	213.795	-1785.810082	-1785.80856	-1786.697943
3PAl[d]	-	-1786.354235	-1785.735326	215.715	-1785.837819	-1785.836317	-1786.73595
1PAl[e]	-	-1637.629605	-1636.964086	215.76	-1637.0666	-1637.065879	-1637.967181
TS13_PAl[e]	-888.1i	-1638.785424	-1638.106783	214.799	-1638.208841	-1638.208379	-1639.124339
3PAl[e]	-	-1638.808351	-1638.12584	216.292	-1638.228607	-1638.228218	-1639.15587
1PAl[f]	-	-1675.69179	-1675.020004	219.745	-1675.124413	-1675.124034	-1676.036217
TS13_PAl[f]	-968.2i	-1676.849017	-1676.16418	219.323	-1676.268387	-1676.268047	-1677.195937
3PAl[f]	-	-1676.869229	-1676.179273	218.644	-1676.283158	-1676.282659	-1677.224426
1PAl[a]	-	-1906.681708	-1905.922279	236.352	-1906.034578	-1906.03429	-1907.085163
TS13_PAl[a]	-1010.7i	-1907.835889	-1907.06329	240.331	-1907.177479	-1907.176558	-1908.24341
3PAl[a]	-	-1907.852144	-1907.07521	242.219	-1907.190296	-1907.189422	-1908.2681

*BS1 (basis set 1) is the 6-31++G(d,p) for P, Al, B, and C, O, and H of the substrates involved in the reaction (H_2 and CO_2) and 6-31G(d) for all other atoms. Quasi-harmonic correction was applied to all free energies (G_{qhHS}).
BS2 (basis set 2) is the 6-311++G(d,p) basis set for all atoms.

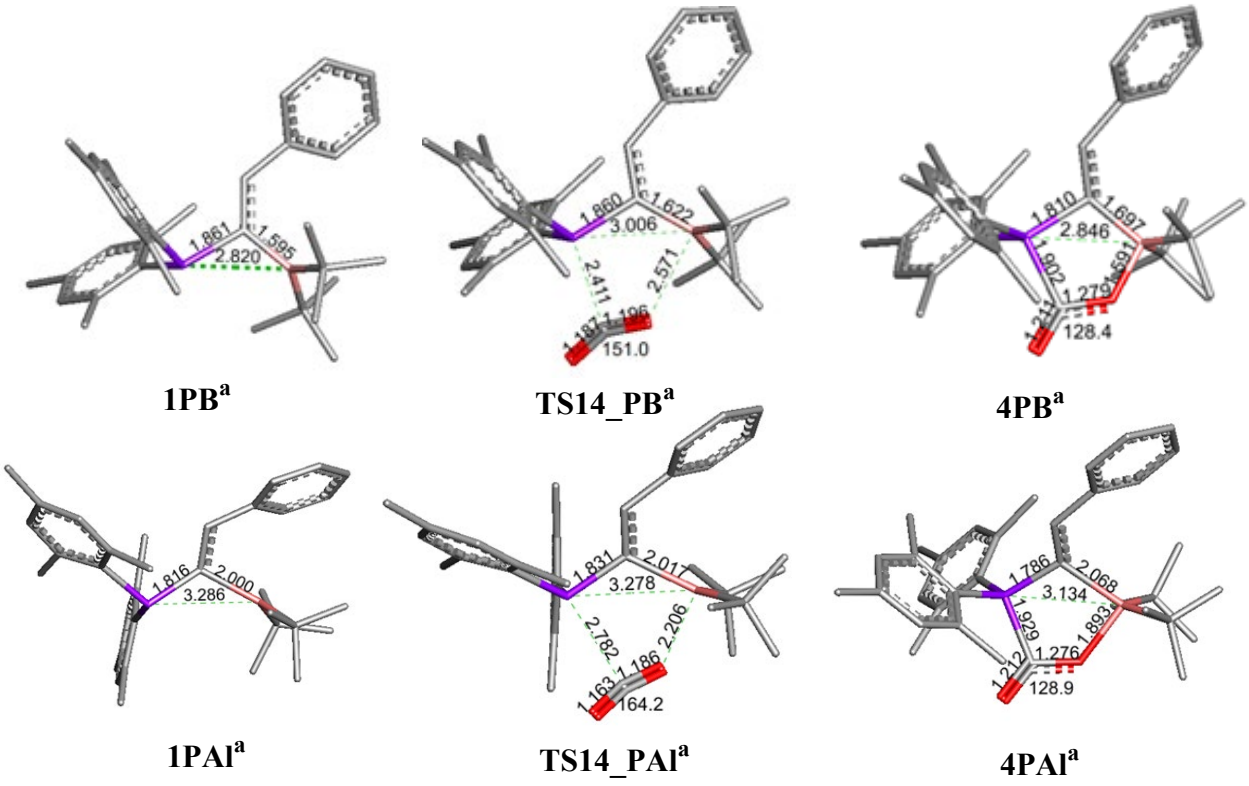


Fig. S1 Optimized geometries of transition states and products from the CO_2 addition to **1PZ[a]** (Z = B, Al). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity.

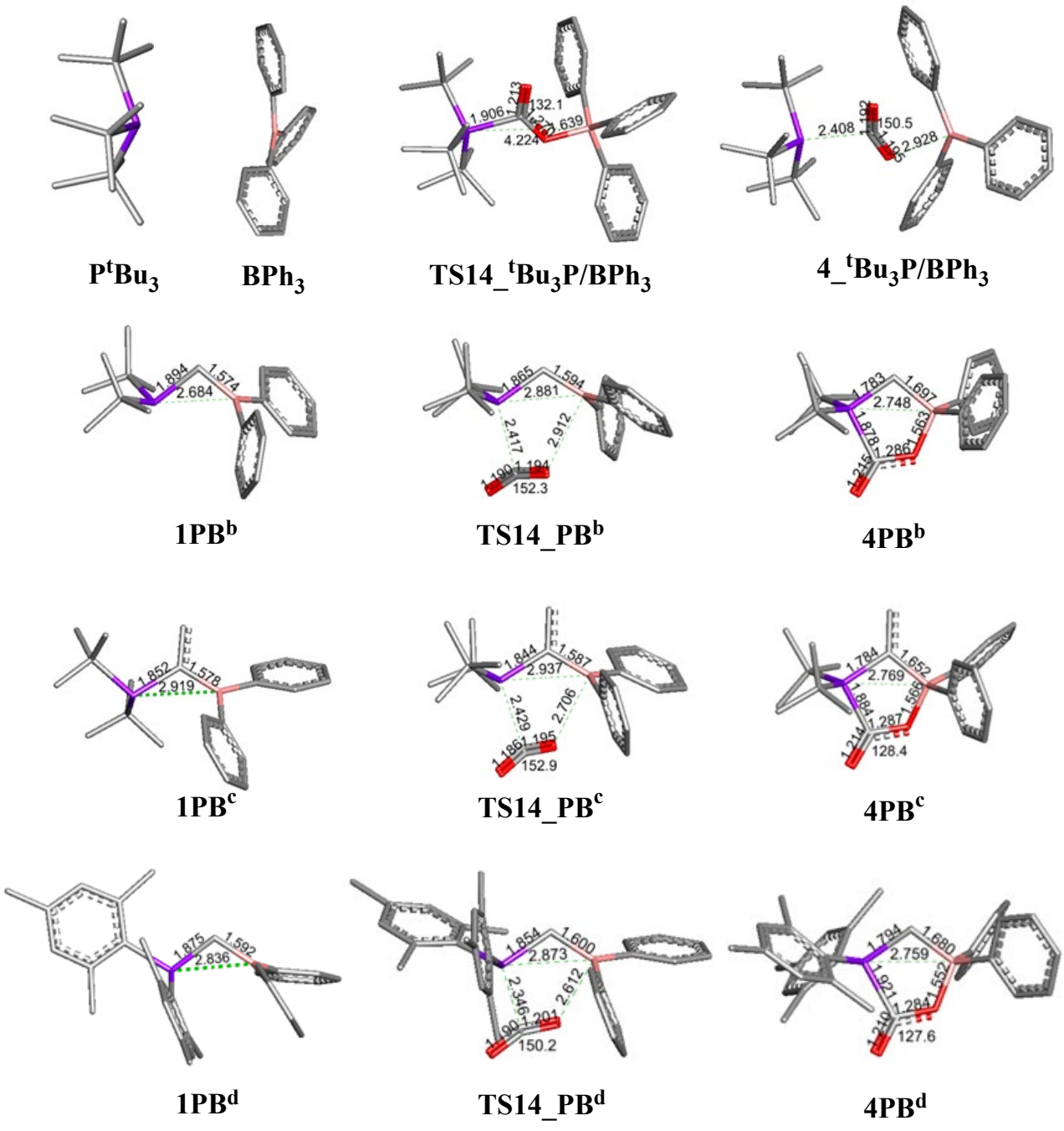


Fig. S2 Optimized geometries of ^{t}**Bu$_3$P/BPh$_3$**, **1PB^b**, **1PB^c**, and **1PB^d** compounds The transition states, and products from CO_2 addition (**TS14_PB** and **4PB**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity.

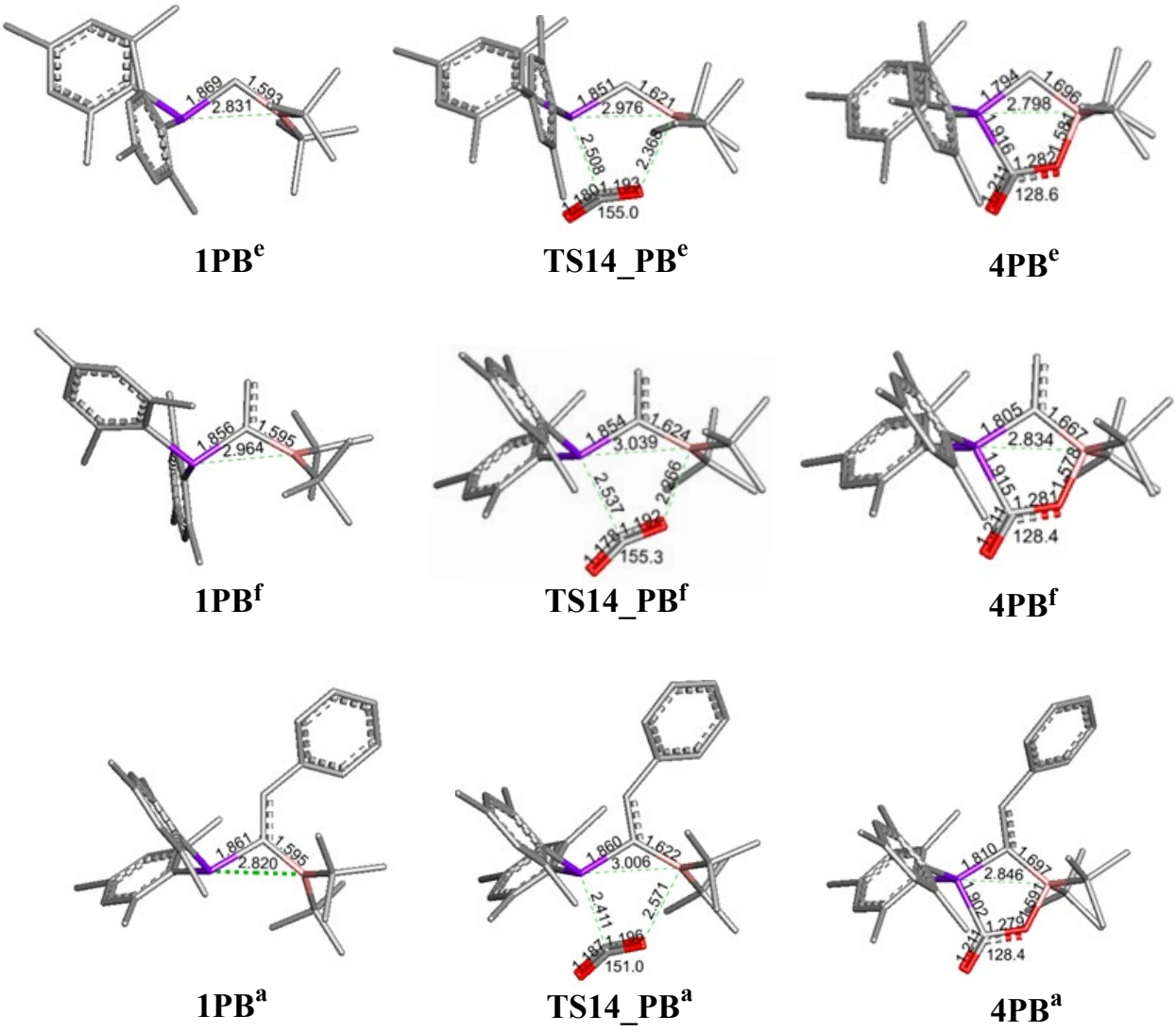


Fig. S3 Optimized geometries of **1PB^{e}**, **1PB^{f}** and **1PB^{a}** compounds The transition states, and products from CO_2 addition (**TS14_PB** and **4PB**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity.

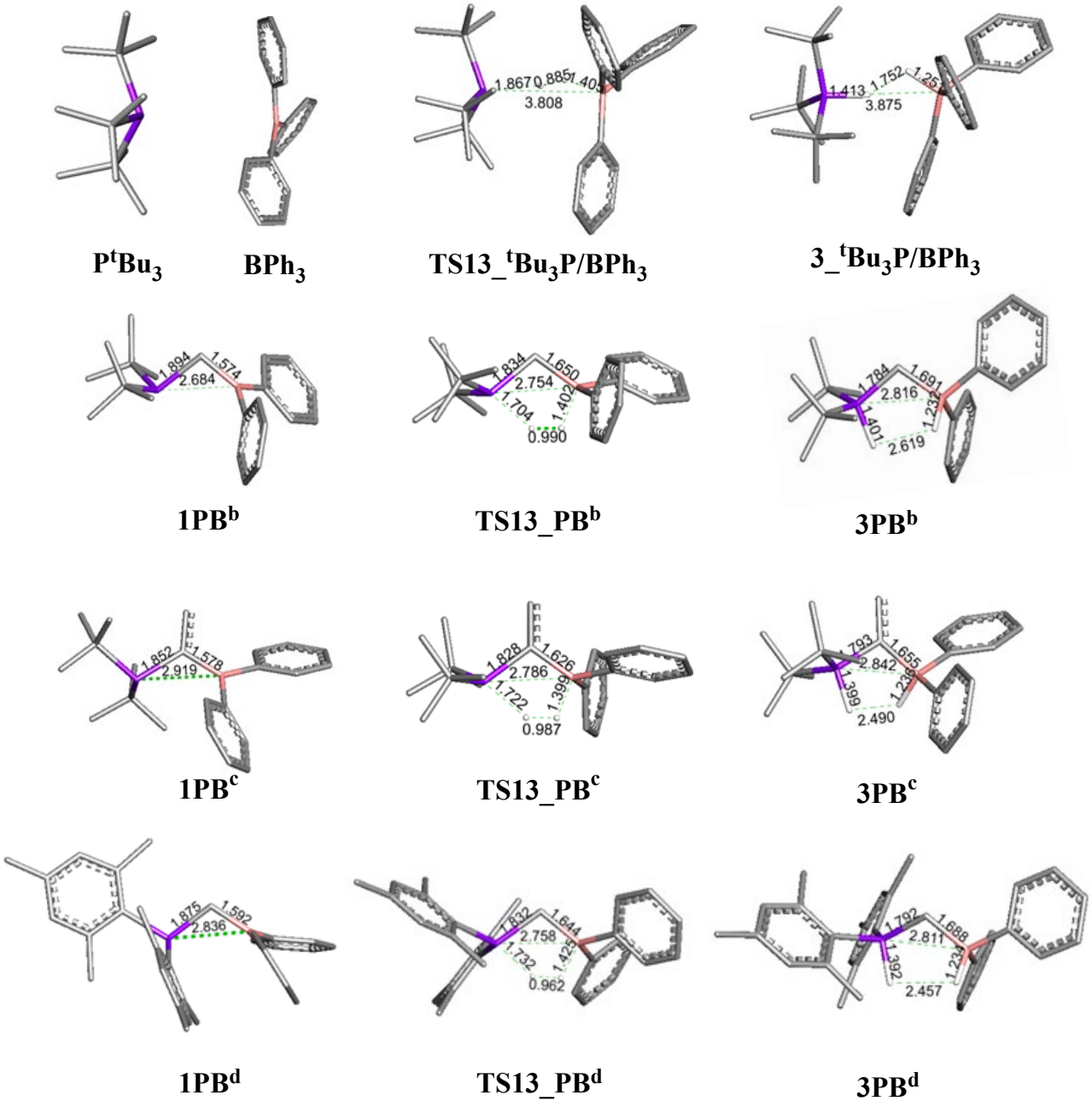


Fig. S4 Optimized geometries of **^{t}Bu$_3$P/BPh$_3$**, **1PB^b**, **1PB^c**, and **1PB^d** compounds The transition states, and products from H_2 activation (**TS13_PB** and **3PB**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity except for those of H_2.

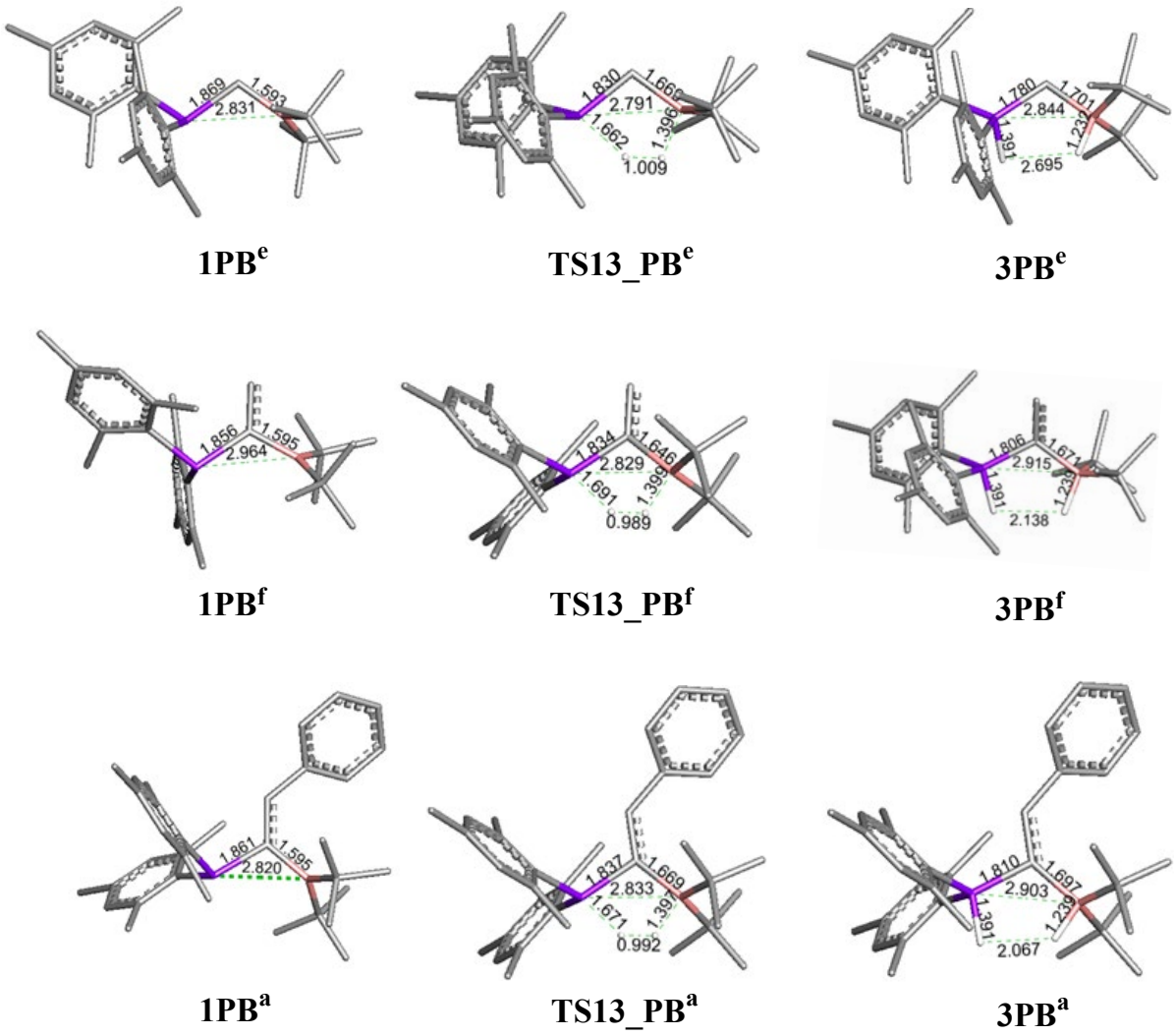


Fig. S5 Optimized geometries of **1PB^{e}**, **1PB^{f}** and **1PB^{a}** compounds The transition states, and products from H_2 activation (**TS13_PB** and **3PB**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity except for those of H_2.

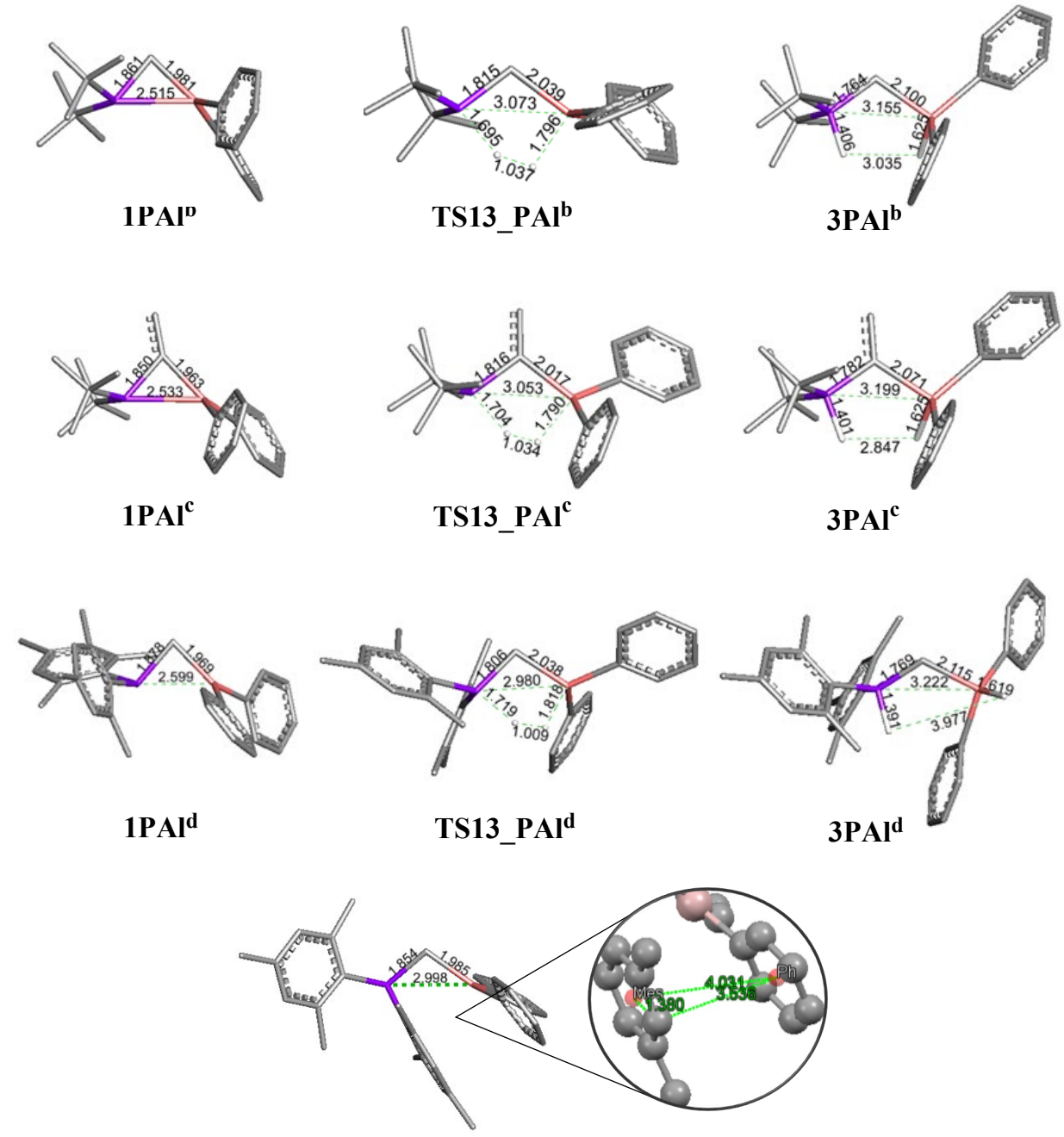


Fig. S6 Optimized geometries of **1PAl^{b}**, **1PAl^{c}**, and **1PAl^{d}** compounds The transition states, and products from H_2 activation (**TS13_PAl** and **3PAl**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity except for those of H_2.

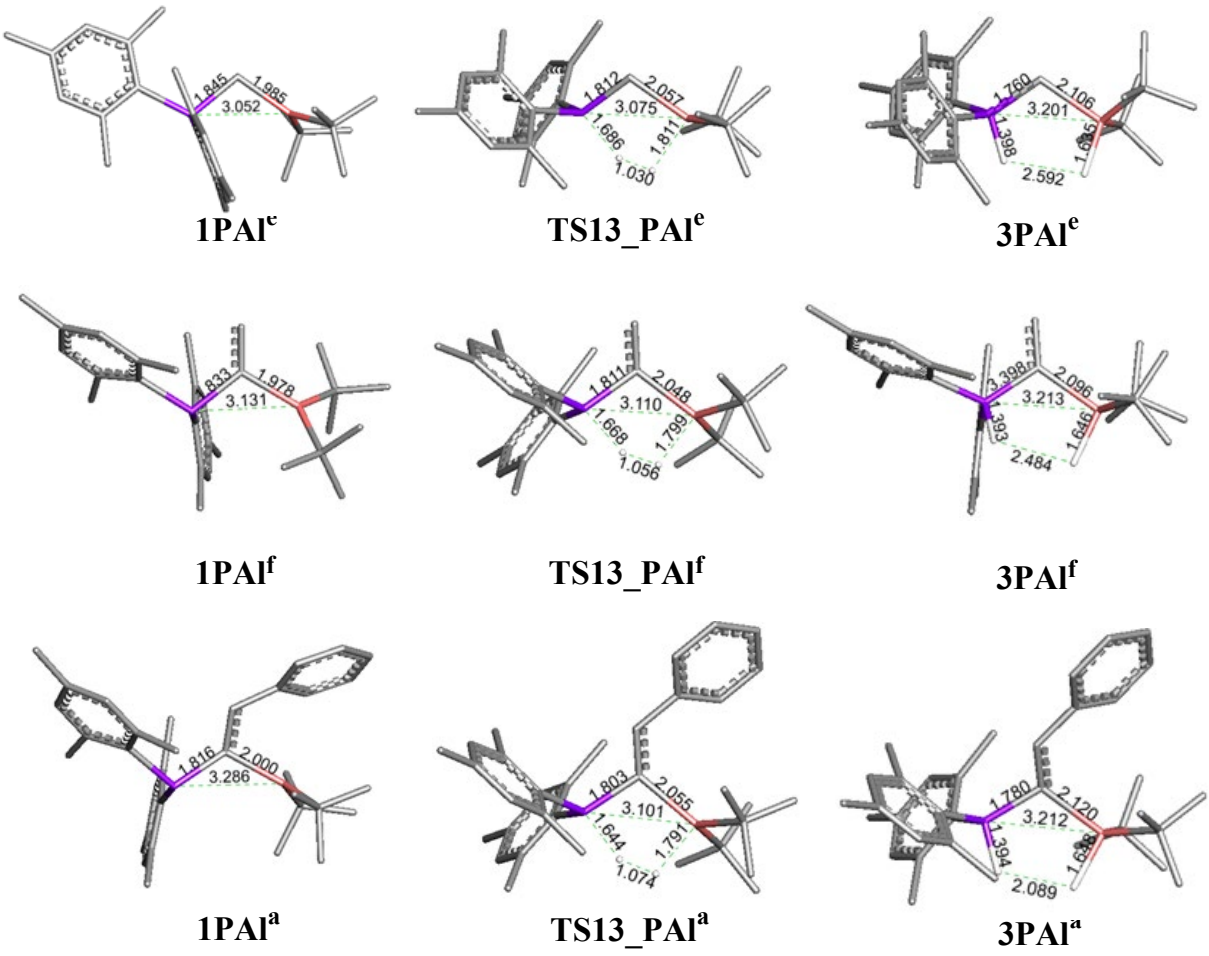


Fig. S7 Optimized geometries of **1PAl^{e}**, **1PAl^{f}** and **1PAl^{a}** compounds The transition states, and products from H_2 activation (**TS13_PAl** and **3PAl**). The selected bond distances are shown in Å. Hydrogen atoms are omitted for clarity except for those of H_2.

$H_2 + B(C_6F_5)_3 + P^tBu_3 \rightarrow [HB(C_6F_5)_3]^- + [HP^tBu_3]^+$ ΔG_{HH}

$(Ph_3B{-}P^tBu_3 \rightarrow BPh_3 + P^tBu_3)$ ΔG_{prep}

$P^tBu_3 + [HP^tBu_3]^+ \rightarrow [HP^tBu_3]^+ + P^tBu_3$ ΔG_{pa}

$BPh_3 + [HB(C_6F_5)_3]^- \rightarrow [Ph_3BH]^- + B(C_6F_5)_3$ ΔG_{ha}

$[Ph_3BH]^- + [HP^tBu_3]^+ \rightarrow [HBPh_3]^-[HP^tBu_3]^+$ ΔG_{stab}

$BPh_3 + P^tBu_3 + H_2 \rightarrow [HBPh_3]^-[HP^tBu_3]^+$ ΔG

$(Ph_3B{-}P^tBu_3 + H_2 \rightarrow [HBPh_3]^-[HP^tBu_3]^+)$

$$\Delta G = \Delta G_{HH} + \Delta G_{prep} + \Delta G_{pa} + \Delta G_{ha} + \Delta G_{stab}$$

Scheme S1. Five partitioning steps contributed to the reaction energy of H_2 activation by BPh_3/P^tBu_3.

Cartesian coordinates of optimized geometries

P^{t}Bu3

Total number of atoms = 40

C	2.306330577	-1.574188998	-0.222751920
C	1.783411179	-0.141191438	-0.006159922
P	0.000155125	0.000401520	-0.713445089
C	-0.769586863	1.615121162	-0.006718344
C	-1.995740556	1.953566477	-0.883630730
C	1.994573530	0.226703383	1.470806529
C	2.691410214	0.750269273	-0.882812839
C	-1.014068653	-1.473221539	-0.006505165
C	-2.517407397	-1.209131725	-0.217201133
C	-0.796958406	-1.842429840	1.469244684
C	-0.698154096	-2.703331984	-0.886613896
C	0.209767468	2.784646338	-0.222536096
C	-1.194005619	1.613358288	1.470236436
H	3.384605466	-1.588942707	-0.018803181
H	3.043289201	0.045459524	1.743683809
H	3.738911275	0.583747965	-0.598640774
H	1.845824670	-2.303417701	0.446848908
H	2.163535047	-1.906428745	-1.256717210
H	1.371466533	-0.369349345	2.142379847
H	0.218380968	-2.195855713	1.664265925
H	1.791035710	1.281730899	1.669309035
H	2.585224530	0.498570981	-1.943324489
H	0.325805056	-3.061731824	-0.781300588
H	2.493070208	1.815779153	-0.768115412
H	-1.478994130	-2.658988682	1.743414405
H	-0.997980408	-1.005498589	2.142736386
H	-1.361499273	-3.529783933	-0.598577828
H	1.068444596	2.751274822	0.451295913
H	-0.872375103	-2.484710037	-1.945459433
H	-0.366022047	1.372870313	2.141943377
H	0.574242438	2.824793605	-1.254656595
H	-0.317577665	3.726272756	-0.023076774
H	-2.004647023	0.907937999	1.668606901
H	-1.562939330	2.611558495	1.743349089
H	-3.068173792	-2.136512227	-0.014052867
H	-2.915715099	-0.447988836	0.456954720
H	-2.738423177	-0.915439803	-1.249035312
H	-1.722395934	1.994144722	-1.943347419
H	-2.815041365	1.243148879	-0.774851968
H	-2.381806473	2.940318876	-0.595297735

BPh_3

Total number of atoms = 34

C	-2.129831558	-1.338858424	0.637524747
C	-1.553232324	-0.227494658	-0.003641395
C	-2.425262478	0.672692739	-0.642780105
C	-3.801203144	0.469145239	-0.653278907
C	-4.344541826	-0.632852744	0.003061956
C	-3.506772004	-1.534892668	0.654825168
B	-0.001499019	-0.000935193	-0.003696875
C	0.578424947	1.456195545	-0.003367257
C	1.786702893	1.763525084	-0.655028472
C	2.297975041	3.057159433	-0.667318788
C	1.623744424	4.076258818	0.001342150
C	0.432561818	3.798916385	0.668017709
C	-0.086818678	2.508555684	0.651561485
C	0.971513228	-1.230494278	-0.002216796
C	0.634215359	-2.433949733	-0.647985624
C	1.501853936	-3.521250265	-0.658768288
C	2.723895966	-3.440966558	0.005122334
C	3.078794496	-2.267048519	0.665625374
C	2.218014671	-1.174478559	0.647481800
H	-1.023747364	2.306677505	1.163916974
H	-0.094120921	4.590572120	1.193364045
H	2.026461011	5.085531255	0.003028077
H	2.328810048	0.973400417	-1.167917404
H	3.225719305	3.270307023	-1.190757260
H	2.511205215	-0.259192554	1.154948726
H	4.029452033	-2.201879504	1.187367379
H	3.399207063	-4.292229668	0.007746838
H	1.223482884	-4.434051512	-1.177893105
H	-0.322256219	-2.512686937	-1.158253145
H	-1.484854284	-2.055782037	1.138595082
H	-3.927629626	-2.394001521	1.169550773
H	-5.419825278	-0.788501221	0.006196886
H	-4.451350467	1.172845148	-1.165309678
H	-2.013266904	1.542692341	-1.147162357

TS14_^{t}Bu$_3$P/BPh$_3$

Total number of atoms = 77

B	-2.733096497	-0.042312381	-0.273040379
C	0.563042587	-1.014886274	1.188752727
O	0.849737747	-2.166247852	1.305095958
P	2.592627124	0.006395779	0.390377282
C	3.005967067	-0.955649629	-1.206544780
O	-0.237592568	-0.130911401	1.255634398

C	1.691595567	-1.203944066	-1.974666892
C	3.539441280	-2.357391289	-0.850805478
C	4.012005142	-0.268598482	-2.143706298
C	2.333418528	1.852457771	-0.013777758
C	1.351499383	1.956446603	-1.197661020
C	1.638208212	2.528541995	1.191257745
C	3.603004524	2.649691423	-0.352696413
C	4.028061451	-0.183602102	1.633522736
C	3.902545991	-1.559379874	2.322935199
C	5.435497595	-0.038421986	1.031657729
C	3.879118854	0.857444581	2.758418326
C	-2.125441797	-1.071691589	-1.293355023
C	-1.836912821	-0.710195323	-2.621151495
C	-1.345010287	-1.634223324	-3.538192777
C	-1.095299577	-2.944780410	-3.137873499
C	-1.329137517	-3.321551746	-1.817100752
C	-1.841116333	-2.396869380	-0.912361808
C	-3.534647974	-0.532232913	0.984467143
C	-4.347543212	-1.677462107	0.929381786
C	-5.094948060	-2.093964909	2.028093131
C	-5.024747815	-1.385376004	3.223687577
C	-4.226582526	-0.245659355	3.305922842
C	-3.511897808	0.183738017	2.193823657
C	-2.681934188	1.504394372	-0.588883983
C	-1.896128950	2.412372038	0.134760846
C	-1.894308284	3.771787904	-0.166087775
C	-2.692559920	4.264154458	-1.194689474
C	-3.492751428	3.384263739	-1.918350298
C	-3.482624890	2.023949357	-1.619249229
H	1.917122804	-1.807201025	-2.863062310
H	1.200901547	-0.296053704	-2.320196242
H	0.972474378	-1.769046072	-1.376273736
H	2.864814235	-2.885800379	-0.171480056
H	4.542943110	-2.339819374	-0.420297381
H	3.599260295	-2.940822251	-1.777943146
H	4.956062911	-0.027159106	-1.648477061
H	3.608796123	0.648445754	-2.580649250
H	4.238666330	-0.947937599	-2.975689856
H	1.041393332	3.002661155	-1.304190721
H	0.441959919	1.370166557	-1.035344252
H	1.806759511	1.657140588	-2.144496767
H	1.210208198	3.480472378	0.853867286
H	2.329084050	2.758556589	2.002543370
H	0.825582484	1.917535641	1.588616025
H	4.148741028	2.237091254	-1.204271970
H	4.290672782	2.713137851	0.494995302
H	3.313534783	3.676927196	-0.610534217

H	4.704974303	-1.646757416	3.066713343
H	3.995975439	-2.402113238	1.639587247
H	2.946127150	-1.661547564	2.842726366
H	5.570457945	0.914323329	0.512636757
H	5.677079014	-0.843187658	0.333888304
H	6.174304995	-0.081510667	1.842664144
H	4.575385418	0.595356564	3.564445571
H	2.870714305	0.864358659	3.184678099
H	4.131763289	1.868753454	2.433017651
H	-0.704771063	-3.667029856	-3.849618951
H	-1.109584001	-4.333763914	-1.490344707
H	-2.005545084	-2.701436022	0.117070470
H	-1.147096194	-1.330447008	-4.562374315
H	-2.005768079	0.313872901	-2.942697135
H	-4.117370532	1.354905653	-2.197573442
H	-4.126284529	3.756164514	-2.718935228
H	-2.695146299	5.325083174	-1.428059939
H	-1.268689369	4.448968795	0.410008018
H	-1.260538318	2.045812416	0.933271925
H	-4.172493614	0.314919413	4.234866913
H	-5.595762977	-1.714610867	4.087426210
H	-5.725525010	-2.975395003	1.952531296
H	-4.409021133	-2.246187420	0.005095233
H	-2.912125919	1.085902574	2.268400895

4_^{t}Bu$_3$P/BPh$_3$

Total number of atoms = 77

B	-1.889991909	0.168692074	-0.041874099
C	0.562251864	-0.142755030	-0.730455330
O	0.532593033	0.219560712	-1.887881991
P	2.302403454	-0.339348547	0.021244600
C	3.186448778	1.247868138	-0.540977076
O	-0.359768834	-0.400217373	0.104826449
C	2.242986815	2.454537550	-0.332005823
C	3.510344658	1.197555687	-2.047554075
C	4.500678331	1.481438055	0.224948708
C	2.236863125	-0.480289189	1.916342416
C	1.861113710	0.885605618	2.523121540
C	1.146112396	-1.462068880	2.401129117
C	3.594396730	-0.938948517	2.484114221
C	3.017230150	-1.899556937	-0.787678313
C	2.598091813	-1.979487996	-2.271679786
C	4.552263986	-1.943422451	-0.687034156
C	2.432769790	-3.154450312	-0.112108242

C	-1.631413257	1.772840858	-0.073798916
C	-1.296094414	2.469196208	1.099445885
C	-0.910143630	3.808347674	1.084665019
C	-0.850201042	4.500759824	-0.123027131
C	-1.183487141	3.839918295	-1.302876701
C	-1.563931531	2.498211168	-1.272806213
C	-2.568568557	-0.488682739	-1.349859104
C	-3.729516960	0.070273169	-1.902784102
C	-4.388700377	-0.516344193	-2.981117423
C	-3.902622848	-1.695388470	-3.540446701
C	-2.759602137	-2.280522562	-3.002474991
C	-2.112032615	-1.682532940	-1.924186888
C	-2.601672516	-0.410739031	1.292528518
C	-2.367265398	-1.730160458	1.710229133
C	-2.999264998	-2.279685404	2.821306509
C	-3.911802831	-1.518841730	3.549511910
C	-4.184099678	-0.215373110	3.145106116
C	-3.536721020	0.324334029	2.033381456
H	2.769720832	3.346750456	-0.689951874
H	1.977121347	2.631541689	0.708173009
H	1.318807326	2.366829304	-0.907731181
H	2.613867606	1.031111455	-2.646747215
H	4.266790109	0.449916087	-2.297141434
H	3.923469464	2.174965366	-2.321645700
H	5.205429110	0.650989010	0.124708852
H	4.343500681	1.679229727	1.286893174
H	4.981030064	2.370245781	-0.199527608
H	1.677544092	0.728067821	3.591862221
H	0.939864570	1.286089709	2.090609514
H	2.654434802	1.630690591	2.438394809
H	1.277639107	-1.571007395	3.484315558
H	1.214665244	-2.457232632	1.966223063
H	0.145198674	-1.077124548	2.213870448
H	4.440225246	-0.337887951	2.143192579
H	3.800089825	-1.988927577	2.259990478
H	3.547830096	-0.847290219	3.575329234
H	3.071091711	-2.874115352	-2.693511147
H	2.913057053	-1.124519260	-2.866382536
H	1.517043740	-2.082906232	-2.386982650
H	4.915078607	-1.870158498	0.340896364
H	5.029830968	-1.158913373	-1.278170284
H	4.894028041	-2.904492488	-1.088701110
H	2.745385733	-4.024667273	-0.700408094
H	1.338212707	-3.144941785	-0.100844370
H	2.800132946	-3.303001203	0.905109193
H	-0.555159622	5.546734887	-0.143163162
H	-1.140649654	4.367419132	-2.252543159

H	-1.794915593	1.993107096	-2.206738635
H	-0.664874662	4.313752567	2.016019190
H	-1.346040584	1.946841855	2.053312326
H	-3.762177463	1.347326854	1.739121139
H	-4.900429453	0.387056730	3.698404924
H	-4.410582978	-1.941384373	4.417646433
H	-2.788587839	-3.305332116	3.115136885
H	-1.675245406	-2.347628000	1.139497641
H	-2.370150530	-3.203571813	-3.425678460
H	-4.410685580	-2.154997628	-4.383935228
H	-5.284532616	-0.051656046	-3.385533013
H	-4.128958413	0.989666508	-1.477772319
H	-1.223252284	-2.164373666	-1.518209448

1PB[b]

Total number of atoms = 53

C	-0.306341470	-0.280606763	-1.194271879
B	1.072843004	0.154006687	-0.572141447
C	2.221319011	-0.880315642	-0.293803692
C	3.335088744	-0.544277351	0.496530578
C	2.204029709	-2.169136830	-0.856746665
C	4.356544243	-1.456378920	0.743236336
C	3.226049633	-3.083706597	-0.629072319
C	4.302169152	-2.729608517	0.181347656
C	1.267965090	1.678429490	-0.220942073
C	1.298597744	2.635609393	-1.244742771
C	1.361345891	2.136751732	1.101628926
C	1.427584955	3.993247865	-0.965164057
C	1.468137731	3.495287783	1.389696998
C	1.505839502	4.427459433	0.355950496
P	-1.396909533	-0.346578084	0.352667582
C	-2.051371728	-2.135898604	0.302610516
C	-3.290146911	-2.260160624	1.202900380
C	-2.381624436	-2.724149373	-1.077191066
C	-0.924936281	-2.974408147	0.936870661
C	-2.788815321	0.881736578	-0.067577057
C	-3.655298552	1.080321518	1.189564919
C	-3.673944987	0.491342531	-1.256120934
C	-2.122486756	2.239221969	-0.363603391
H	-0.308828363	-1.248924052	-1.696472399
H	-0.717327433	0.457345068	-1.890123410
H	-4.181352725	-1.827579790	0.737908381
H	-3.499745835	-3.322240110	1.384590276
H	-3.137008956	-1.781012574	2.176513193
H	-3.097463860	-2.116541383	-1.635510986
H	-1.488880797	-2.850027077	-1.697540310

H	-2.820089550	-3.722647327	-0.948020670
H	0.019491341	-2.879930086	0.392286694
H	-0.740041795	-2.673168758	1.973261244
H	-1.207145862	-4.035934287	0.933174307
H	-4.382047547	1.882710794	1.006928002
H	-4.219999992	0.186388941	1.462317096
H	-3.041188485	1.371035624	2.049004571
H	-4.288999673	-0.387095582	-1.036237370
H	-4.358186978	1.315733998	-1.498180781
H	-3.081853747	0.280019640	-2.154135192
H	-1.430480691	2.541412294	0.429446873
H	-1.566917894	2.242608628	-1.305242302
H	-2.903159014	3.006520808	-0.443726100
H	1.211140846	2.316349850	-2.282062012
H	1.453983865	4.714724829	-1.777027156
H	1.594666089	5.487111086	0.577547921
H	1.522116690	3.826198783	2.423205080
H	1.317800249	1.420377369	1.918506252
H	3.403113733	0.451757153	0.924499091
H	5.199435234	-1.171768236	1.366552945
H	5.100205312	-3.442755388	0.368347133
H	3.183949988	-4.070671233	-1.080505482
H	1.376014069	-2.465926677	-1.495220708

TS14_PB[b]

Total number of atoms = 56

C	0.653961435	-0.046008267	2.268886324
O	-0.446028739	-0.488263488	2.131242862
C	0.192589511	-0.301041896	-1.238687716
O	1.524852937	0.425138019	2.928143837
B	-1.230760258	0.059966703	-0.619373076
P	1.552296400	-0.287834746	0.037824111
C	2.308452185	-2.014979342	-0.102754759
C	3.631807596	-2.068115221	0.676225054
C	1.301173100	-2.955983034	0.588435950
C	2.547250154	-2.517794617	-1.534926874
C	2.745084621	1.074521230	-0.488617258
C	3.430776112	0.834589812	-1.838499378
C	1.908166086	2.366043174	-0.560903685
C	3.806519357	1.277821620	0.609471651
C	-2.344866897	-1.023005617	-0.437858798
C	-3.546835778	-0.714667324	0.224233262
C	-2.206212167	-2.331820948	-0.933142620
C	-4.541781048	-1.667947378	0.410823523
C	-3.200495226	-3.289051351	-0.765259142
C	-4.369411108	-2.958525317	-0.084160491

C	-1.524128287	1.585934706	-0.354229481
C	-1.811851162	2.128881368	0.907226568
C	-1.493221292	2.468207112	-1.446528867
C	-2.028931236	3.495268664	1.072434659
C	-1.736881191	3.829495820	-1.292014041
C	-1.994216055	4.349604198	-0.026064144
H	0.203158514	-1.274700439	-1.731995379
H	0.456457345	0.441246991	-2.001857149
H	3.548227026	-1.601987449	1.664026107
H	3.917546994	-3.116915491	0.824271877
H	4.445238229	-1.582659815	0.128384614
H	0.295068836	-2.880054771	0.164141269
H	1.638949383	-3.993189994	0.469151291
H	1.220363740	-2.749481542	1.659723126
H	3.197480626	-1.856832917	-2.112213308
H	3.030372223	-3.502006268	-1.487436572
H	1.614324248	-2.648034612	-2.091877110
H	3.966719635	1.743130872	-2.141930587
H	4.167288005	0.027079251	-1.779891152
H	2.714099080	0.592672943	-2.631646805
H	1.347897238	2.546904093	0.362903249
H	2.584805718	3.215474597	-0.714884022
H	1.193103621	2.362598168	-1.386919465
H	4.510388131	0.445626007	0.674444786
H	4.387564731	2.177976563	0.371955137
H	3.347879889	1.417054709	1.592356586
H	-3.701042993	0.290540763	0.604911754
H	-1.306722976	-2.615006443	-1.473214020
H	-5.455159378	-1.404279466	0.936005129
H	-3.064859562	-4.290477510	-1.163440265
H	-5.147540496	-3.704006914	0.054225807
H	-1.846721783	1.475767516	1.774167950
H	-1.275868015	2.085444879	-2.442918834
H	-2.228378037	3.892263859	2.063733308
H	-1.715354456	4.486118613	-2.157397039
H	-2.168215967	5.413860818	0.103091399

4PB[b]

Total number of atoms = 56

C	-0.939689450	0.037482772	1.580606375
O	0.342964500	0.047885136	1.494619219
C	-0.143798069	0.086903082	-1.074585129
O	-1.629668359	0.055481463	2.580697156
B	1.069290136	0.033042155	0.110596968
P	-1.666403144	-0.004191254	-0.151102680
C	-2.674874576	1.546761045	-0.350383294

C	-3.991921636	1.476300884	0.435743926
C	-1.801581498	2.685513309	0.217940374
C	-2.954134799	1.806022458	-1.839594579
C	-2.507297116	-1.655734935	-0.331845164
C	-3.107239982	-1.787328529	-1.739247152
C	-1.407062958	-2.718250198	-0.125171488
C	-3.594013309	-1.858353237	0.737431878
C	1.940814127	1.390388823	0.028090778
C	2.721530937	1.666420956	-1.105158510
C	1.907913780	2.370193657	1.028973871
C	3.421513133	2.861364747	-1.242948374
C	2.605543075	3.571786166	0.902405686
C	3.362431823	3.824607003	-0.236650207
C	1.908545760	-1.343181652	0.036990689
C	2.275101974	-2.033852625	1.201529404
C	2.317353196	-1.901829213	-1.182787299
C	2.999088766	-3.223043627	1.152550877
C	3.046816753	-3.087525271	-1.245321468
C	3.387880156	-3.757204405	-0.073168532
H	-0.103168586	1.025561568	-1.632906705
H	-0.077435356	-0.733453149	-1.793767845
H	-3.834271198	1.159104676	1.471081368
H	-4.440184314	2.476376944	0.451372622
H	-4.712204120	0.803498970	-0.039369040
H	-0.805611879	2.731510098	-0.235184513
H	-2.303989789	3.638312415	0.015871301
H	-1.678614453	2.595190076	1.301445256
H	-3.560555215	1.017099329	-2.293822785
H	-3.510293836	2.746109155	-1.930287203
H	-2.032228517	1.910662018	-2.419634982
H	-3.473858332	-2.811579272	-1.872535556
H	-3.957401759	-1.112967649	-1.883234203
H	-2.368579419	-1.593566227	-2.524892214
H	-0.942943444	-2.647846643	0.863844257
H	-1.872228544	-3.707230633	-0.205701968
H	-0.608260264	-2.662732011	-0.869299193
H	-4.452445525	-1.200208388	0.589276886
H	-3.954101827	-2.891086011	0.664116161
H	-3.207790767	-1.700340805	1.747897354
H	2.788198566	0.924944139	-1.900286556
H	1.329720241	2.187203187	1.931454123
H	4.016265784	3.041892560	-2.134865238
H	2.557250207	4.311418738	1.697655861
H	3.904866125	4.760307506	-0.340348935
H	1.982192154	-1.630160139	2.167479019
H	2.064262696	-1.402257380	-2.117891324
H	3.260695613	-3.734070697	2.075652945

H	3.347105338	-3.490363569	-2.209381001
H	3.951317319	-4.685250855	-0.115129471

1PB[c]

Total number of atoms = 54

C	0.302991420	-0.468767938	0.804963774
B	-1.116623114	0.089926295	0.400945295
C	-2.358909863	-0.869083109	0.373983172
C	-3.655922685	-0.373298495	0.604071437
C	-2.232311341	-2.250349746	0.139765478
C	-4.766383013	-1.210990703	0.607652811
C	-3.339344878	-3.091807117	0.119304631
C	-4.609573062	-2.572270045	0.358105560
C	-1.303069200	1.610682690	0.070084856
C	-0.597522078	2.597512385	0.778868411
C	-2.176170307	2.040531944	-0.942532638
C	-0.771510797	3.949924197	0.508650466
C	-2.328819181	3.391103066	-1.244844817
C	-1.632574091	4.348724414	-0.512389420
P	1.749315977	0.197873454	-0.141316202
C	1.769787645	-1.052374893	-1.579434835
C	2.993530185	-0.777383387	-2.466459579
C	1.741690066	-2.538223193	-1.199453337
C	0.503376521	-0.731677374	-2.399401344
C	3.312210766	0.003813163	0.926348776
C	4.391286586	0.869844886	0.242555968
C	3.889639374	-1.400737795	1.147008923
C	3.012426916	0.670981672	2.282698066
C	0.358946691	-1.305803441	1.856491883
H	-3.792202214	0.687957178	0.792831825
H	-1.246324386	-2.669720841	-0.037767560
H	-5.754220162	-0.801850076	0.799162095
H	-3.212129150	-4.152598914	-0.076713977
H	-5.475755635	-3.228256327	0.351237199
H	0.098177274	2.296328015	1.558319212
H	-2.737721689	1.302726102	-1.510893232
H	-0.224655673	4.693352592	1.081539922
H	-2.998846234	3.696726248	-2.043444302
H	-1.759670812	5.404274671	-0.735903668
H	3.924483155	-1.093779410	-1.985016181
H	3.080086127	0.285014183	-2.721279620
H	2.904596190	-1.342914614	-3.403176568
H	2.678043869	-2.867373499	-0.742929836
H	1.584754281	-3.144731188	-2.101643241
H	0.932021839	-2.763617521	-0.499357300
H	0.516686392	-1.305915246	-3.335072356

H	0.438890116	0.332189492	-2.651804797
H	-0.413131494	-1.013382353	-1.867900241
H	5.298153833	0.880559032	0.862005499
H	4.050026663	1.903015601	0.118373351
H	4.671253017	0.488891809	-0.743120843
H	4.718967839	-1.348635081	1.865608984
H	4.293292880	-1.815699782	0.218153152
H	3.156883569	-2.111597621	1.538439498
H	2.561714953	1.661337782	2.145946029
H	3.952012975	0.807539676	2.833478495
H	2.340717414	0.080818738	2.909583054
H	1.283953707	-1.695052157	2.273620114
H	-0.549336839	-1.625446892	2.366512427

TS14_PB[c]

Total number of atoms = 57

C	-0.177888351	-0.355410553	-1.012939247
P	-1.617401068	-0.211804785	0.130551382
C	-2.875326934	0.988985447	-0.613276227
C	-3.728095760	0.458832595	-1.772360059
C	-3.796297817	1.446977138	0.534940362
C	-2.076567855	2.210813895	-1.095389680
C	-2.305212368	-1.969994846	0.282581826
C	-2.476876233	-2.718082560	-1.046393356
C	-3.649643100	-1.924694654	1.026904492
C	-1.306008264	-2.752336256	1.157638146
B	1.253028651	0.026924086	-0.443515892
C	1.560725767	1.559108025	-0.231784846
C	2.107921376	2.091514163	0.947160397
C	1.328207531	2.445374866	-1.294564780
C	2.386331243	3.450401874	1.064623557
C	1.629488545	3.800811622	-1.193217680
C	2.150557230	4.308940332	-0.006773946
C	2.378317122	-1.053392034	-0.344473878
C	3.689593974	-0.709125999	0.029370983
C	2.124560669	-2.406526141	-0.631842931
C	4.689962933	-1.669088733	0.137085451
C	3.118525687	-3.372901060	-0.530387402
C	4.403806930	-3.004327941	-0.139243503
C	-0.293876141	-0.664317518	-2.313235680
C	-0.592772555	0.357162421	2.258226504
O	-1.361598144	1.022027539	2.870101481
O	0.444093714	-0.221977442	2.127172306
H	-4.383332802	1.264630857	-2.128318233
H	-3.119756886	0.135634350	-2.622286140

H	-4.372085880	-0.371737478	-1.469646144
H	-3.223597135	1.851061204	1.374214751
H	-4.461962953	2.235466940	0.161076841
H	-4.427387491	0.639391906	0.913871994
H	-2.776844449	3.012960522	-1.359196644
H	-1.400592091	2.593628157	-0.323242462
H	-1.479384324	1.976036566	-1.980193579
H	-2.927087435	-3.698899276	-0.846410293
H	-3.130722513	-2.191992858	-1.747205270
H	-1.514606054	-2.889450092	-1.536257289
H	-4.452953556	-1.509936808	0.411026330
H	-3.938857063	-2.948513436	1.295115050
H	-3.585127840	-1.343890739	1.953628058
H	-0.286295314	-2.718974123	0.764174107
H	-1.276107563	-2.369615219	2.181809598
H	-1.618732900	-3.803333257	1.200781873
H	2.369978838	5.368834205	0.084498518
H	1.444663857	4.461756569	-2.035438584
H	2.791501942	3.839313557	1.994452746
H	2.296679902	1.433764838	1.790559736
H	0.902639493	2.067265548	-2.221441786
H	1.128659821	-2.703104967	-0.948623931
H	2.894107241	-4.412261030	-0.752266418
H	5.183349597	-3.756485476	-0.055782084
H	5.693945896	-1.377754500	0.432042652
H	3.926856975	0.330397725	0.235807109
H	-1.243853600	-0.847310566	-2.808496277
H	0.586210718	-0.737177053	-2.953026792

4PB[c]

Total number of atoms = 57

C	-0.933741050	-0.057560611	1.666445912
O	0.344763348	-0.190672943	1.594073787
C	-0.110126055	-0.269473394	-0.910167369
O	-1.625010718	0.064567605	2.656982900
B	1.079593979	-0.061852715	0.216864759
P	-1.674463653	-0.131872528	-0.063971313
C	-2.560300696	1.473486318	-0.408934702
C	-3.937597648	1.502248755	0.266747054
C	-1.677294707	2.595879790	0.169377688
C	-2.693697237	1.665315606	-1.927630941
C	-2.667372126	-1.714928373	-0.139367309
C	-3.327027505	-1.860419731	-1.518211544
C	-1.656386818	-2.857196510	0.083549872
C	-3.732406891	-1.775758740	0.969547944

C	1.694848942	1.435755379	0.149577572
C	1.906932299	2.114195997	-1.058231263
C	2.065037253	2.104435512	1.326285131
C	2.463142232	3.392088193	-1.099130014
C	2.614219985	3.384104568	1.298907244
C	2.816607152	4.034577695	0.083751272
C	2.164652622	-1.245934308	0.106221003
C	3.234693670	-1.152111189	-0.794661868
C	2.042150591	-2.441685412	0.827587583
C	4.126584583	-2.205181066	-0.986529203
C	2.933846851	-3.497450488	0.651584700
C	3.977039798	-3.386120521	-0.264308410
C	0.028876664	-0.533751883	-2.213079667
H	-4.350406435	2.512453353	0.163057708
H	-3.872638240	1.272298652	1.334752069
H	-4.641101380	0.811316428	-0.207649730
H	-2.141549463	3.556862338	-0.080617893
H	-0.666470015	2.590582484	-0.249300192
H	-1.600417534	2.533787161	1.259061359
H	-3.195261035	2.622088376	-2.112726155
H	-3.291409199	0.880403348	-2.401887169
H	-1.713791838	1.701430618	-2.412268140
H	-4.085820899	-1.091010545	-1.693103881
H	-3.828589208	-2.833942859	-1.565232053
H	-2.595507852	-1.829443853	-2.331813990
H	-2.197737964	-3.808909777	0.035901315
H	-1.184673117	-2.793402783	1.069550655
H	-0.865730635	-2.871222897	-0.670330440
H	-4.540799340	-1.058530750	0.815957940
H	-3.303934856	-1.603984896	1.960034121
H	-4.174811192	-2.778715047	0.955236845
H	1.619581076	1.641793275	-1.995974193
H	1.914770019	1.611668186	2.283496981
H	2.615343158	3.886761011	-2.055145532
H	2.885908950	3.875136580	2.229760284
H	3.247246246	5.031758611	0.059230318
H	3.386162601	-0.225614381	-1.345711706
H	1.242860451	-2.541189077	1.558855639
H	4.945724575	-2.099535402	-1.693413497
H	2.816191923	-4.409093387	1.232190486
H	4.675027166	-4.207059122	-0.404165988
H	-0.797255819	-0.629556305	-2.915307484
H	1.023962268	-0.678028701	-2.631629374

1PB[d]

Total number of atoms = 67

C	0.228501111	-1.198776298	-1.070768551
B	1.776407622	-1.046808750	-0.730843714
C	2.509100974	0.326109734	-0.924130439
C	2.042353948	1.300022347	-1.823066979
C	3.619492732	0.669296174	-0.129974536
C	2.652965118	2.543392628	-1.936825444
C	4.224632625	1.917910468	-0.220825262
C	3.745356270	2.856066505	-1.131652248
C	2.554098593	-2.295273074	-0.183933729
C	3.909843299	-2.509644667	-0.490599340
C	1.910284244	-3.267811901	0.603255885
C	4.589206209	-3.637269894	-0.038664029
C	2.589772484	-4.382124458	1.082158032
C	3.931464995	-4.571538597	0.757189860
P	-0.789631199	-0.785213926	0.448244210
C	-2.609331660	-0.843900644	0.083365552
C	-3.415519515	-0.289342168	1.107333671
C	-3.252152569	-1.444409027	-1.022651237
C	-4.804136178	-0.267481281	0.966431663
C	-4.643850576	-1.402797960	-1.112547249
C	-5.442786956	-0.802409442	-0.144478846
C	-0.414748045	1.028993292	0.524907358
C	-0.924332791	1.995373313	-0.366928940
C	0.536335701	1.422192832	1.492214739
C	-0.461168523	3.310073140	-0.282348532
C	0.979685923	2.742416569	1.527736005
C	0.501757651	3.701277752	0.640350404
C	1.121751495	0.452524731	2.494761415
C	1.054979369	5.101831346	0.648608576
C	-1.953500256	1.700727585	-1.433823407
C	-2.531392635	-2.157009829	-2.144953431
C	-6.940496457	-0.737219731	-0.300504513
C	-2.842056820	0.299064478	2.376621708
H	-0.055582763	-0.564146953	-1.916214191
H	0.022395671	-2.240619218	-1.329265715
H	1.174274789	1.088900959	-2.441426412
H	3.996666555	-0.049026890	0.592963080
H	2.267164933	3.275294866	-2.640453781
H	5.069666343	2.160091470	0.417461039
H	4.220332384	3.830160467	-1.212625251
H	4.437868889	-1.785931607	-1.106412008
H	0.863031790	-3.134366400	0.864203182
H	5.632987881	-3.784632374	-0.301118721
H	2.071948325	-5.107302660	1.703463595
H	4.461388156	-5.447495890	1.120856154
H	-5.400903072	0.176401903	1.760985685
H	-5.121541543	-1.860750139	-1.976632414

H	-0.850785967	4.047202366	-0.982127995
H	1.732199472	3.025947319	2.260452804
H	0.343531473	-0.022061994	3.101205745
H	1.683344386	-0.357716675	2.015727868
H	1.809846889	0.973915729	3.166968698
H	1.208827777	5.468202163	1.668960455
H	2.027553974	5.125820072	0.141070382
H	0.390915043	5.800740958	0.130850831
H	-2.004814518	2.529064177	-2.146827517
H	-1.725902832	0.791587460	-1.996761222
H	-2.950866946	1.560862871	-1.004457963
H	-1.864847567	-1.494690954	-2.703917386
H	-1.932999701	-2.996584161	-1.777915766
H	-3.256506362	-2.563050733	-2.855837774
H	-7.435868149	-0.591296771	0.664380655
H	-7.231047174	0.096966298	-0.950831568
H	-7.335601437	-1.654146288	-0.750099386
H	-2.067675629	-0.347286604	2.805544755
H	-2.384102223	1.278932124	2.204441424
H	-3.629127707	0.421684253	3.126395158

TS14_PB[d]

Total number of atoms = 70

C	0.572900652	-0.756759311	-0.944009074
B	2.084945775	-0.527290165	-0.474193162
C	3.173358479	-1.633960456	-0.687797197
C	2.857310950	-3.002911869	-0.709273158
C	3.832951394	-3.975244824	-0.893153434
C	5.160227160	-3.598160200	-1.088047074
C	5.503057147	-2.248845645	-1.086743817
C	4.521432552	-1.283841257	-0.879522178
C	2.527707467	0.912458414	-0.015889654
C	3.359946326	1.082906342	1.105113466
C	3.738727370	2.348583381	1.540018039
C	3.317429610	3.480022350	0.842545253
C	2.517619814	3.336508600	-0.286780887
C	2.121721629	2.066929844	-0.701397237
C	0.387423333	-0.915050768	2.341101697
O	1.423910244	-1.348106914	1.915359951
O	-0.359409995	-0.730402947	3.249160211
P	-0.652288108	-0.241039414	0.348729996
C	-2.205974593	-1.238696162	0.222181764
C	-3.473576926	-0.652022281	0.457753194
C	-2.141480659	-2.633806038	0.001474254
C	-4.622171200	-1.423520823	0.276671989

C	-3.321574696	-3.357739197	-0.169196971
C	-4.575769780	-2.766654997	-0.080101282
C	-1.055208344	1.471365033	-0.194250765
C	-1.585044757	1.732048852	-1.477253937
C	-0.770050052	2.543306213	0.674326261
C	-1.812633085	3.054563756	-1.856643974
C	-1.017209081	3.847573232	0.246685262
C	-1.533964079	4.127130630	-1.013408833
C	-0.182995847	2.348848631	2.049553444
C	-1.800005816	5.542403997	-1.458394238
C	-1.935609195	0.669237473	-2.497387488
C	-0.863411766	-3.445578404	0.007880939
C	-5.831874399	-3.563307735	-0.319097526
C	-3.687665949	0.755028918	0.974915477
H	0.389088202	-1.773873399	-1.285193743
H	0.420330369	-0.111456126	-1.817374617
H	-5.589717077	-0.955509138	0.445581887
H	-3.249493835	-4.428381370	-0.351705369
H	-2.228733813	3.249102641	-2.843776470
H	-0.787669603	4.669037179	0.921218717
H	-0.788722845	1.682949614	2.671629212
H	0.822286833	1.917772061	1.989259514
H	-0.097736446	3.309291778	2.564781327
H	-2.873163886	5.712684636	-1.602082309
H	-1.440918930	6.267660813	-0.722661886
H	-1.306738894	5.754267311	-2.413404431
H	-1.158160137	0.597916727	-3.268424497
H	-2.071864271	-0.323131991	-2.067291922
H	-2.866959482	0.936160315	-3.006605392
H	-0.485112345	-3.630894390	-1.004530227
H	-0.063697419	-2.984485439	0.591894878
H	-1.061103217	-4.423110550	0.457606565
H	-6.019875271	-3.679802627	-1.393154498
H	-5.752608288	-4.567600557	0.109818232
H	-6.706379450	-3.073874901	0.119796293
H	-2.941890955	1.033693738	1.723831924
H	-3.658537729	1.508957233	0.183294670
H	-4.667765916	0.814583995	1.457070004
H	2.180280917	4.211649135	-0.834329140
H	3.613670552	4.469602655	1.179265616
H	4.363217974	2.453375826	2.422583599
H	3.689680304	0.205695338	1.655233911
H	1.470165479	1.984363489	-1.568119682
H	4.804426643	-0.234650248	-0.868718315
H	6.536067378	-1.949433309	-1.239256438
H	5.925009287	-4.355075951	-1.238614896
H	3.561915015	-5.027167281	-0.884463697

H	1.830739617	-3.317090233	-0.550538060

4PB[d]

Total number of atoms = 70

C	-0.212734378	-0.285626530	1.751621162
O	-1.482325707	-0.337254834	1.566249930
C	-0.847269391	-0.536126041	-0.909536759
O	0.378206911	-0.247839261	2.807320699
B	-2.110193963	-0.219193269	0.152039964
C	-3.257815091	-1.342900908	0.041827249
C	-3.586772364	-1.955917442	-1.175191461
C	-3.999803188	-1.729179417	1.168470029
C	-4.601728531	-2.906944726	-1.271893123
C	-5.010284868	-2.683368777	1.086338843
C	-5.316639255	-3.276801491	-0.136654211
C	-2.628356356	1.303009836	-0.024421294
C	-2.188343389	2.352824518	0.793912818
C	-3.460154706	1.644096354	-1.102507280
C	-2.525378268	3.680420055	0.529435947
C	-3.804328109	2.965096044	-1.375812944
C	-3.327965974	3.993033580	-0.563193064
P	0.646083550	-0.225079137	0.034666978
C	1.472361939	1.401496476	0.016294088
C	2.535682937	1.586688407	0.936072795
C	1.068483374	2.466919111	-0.822154724
C	3.101631696	2.854942306	1.053780667
C	1.673662404	3.710953431	-0.649586792
C	2.673534006	3.935419831	0.290640279
C	1.828956195	-1.586023952	-0.232074258
C	2.881945743	-1.429303913	-1.159505062
C	1.641556363	-2.824320087	0.425955879
C	3.783689354	-2.479627763	-1.330847769
C	2.574565911	-3.836758473	0.211849382
C	3.664995562	-3.680152773	-0.639506462
C	0.473587422	-3.136467529	1.333610841
C	4.664105180	-4.792965093	-0.819689807
C	3.088867052	-0.197912428	-2.012347919
C	0.062848865	2.354144693	-1.940431516
C	3.304550871	5.295035022	0.437222307
C	3.173970123	0.476884219	1.741102335
H	-0.790064288	-1.607212193	-1.140860150
H	-0.913839651	-0.001437191	-1.854246146
H	-3.038580060	-1.688776282	-2.078673610
H	-3.775509521	-1.273767632	2.129947612
H	-4.828897142	-3.363052336	-2.232167913

H	-5.561506863	-2.965176622	1.979919037
H	-6.104444688	-4.022158635	-0.202937394
H	-1.564270570	2.137844076	1.658473659
H	-3.843905336	0.853988245	-1.745983580
H	-2.159944327	4.469647820	1.181432606
H	-4.448170590	3.194618689	-2.221122883
H	-3.590422605	5.026189325	-0.773682407
H	3.907327232	2.996842193	1.769836615
H	1.348563144	4.533546843	-1.281821177
H	4.597056920	-2.355646994	-2.041987022
H	2.434331931	-4.787111363	0.721790697
H	0.592405761	-2.677288533	2.319518520
H	-0.487215988	-2.805391368	0.925682002
H	0.397430842	-4.216937931	1.478601232
H	5.209353360	-4.977243966	0.112798703
H	4.165718365	-5.728298955	-1.095942665
H	5.395660939	-4.554189905	-1.596505419
H	2.152024252	0.178019746	-2.434788876
H	3.546626261	0.623339279	-1.451990461
H	3.747669953	-0.439088659	-2.850872511
H	0.340043701	1.569519376	-2.653265474
H	-0.945197891	2.151224612	-1.574322816
H	0.022317167	3.294240979	-2.495279390
H	3.788540299	5.407999812	1.411470759
H	4.067541506	5.452788348	-0.334539646
H	2.559593424	6.089470037	0.330192995
H	2.446061605	-0.173672683	2.226845630
H	3.817563101	-0.138576191	1.101188074
H	3.800279831	0.905254997	2.527840783

1PB[e]

Total number of atoms = 71

C	0.851659512	-1.144873730	-0.836383775
B	2.349888829	-1.202684174	-0.297355422
P	-0.267238218	-0.479487238	0.505170500
C	2.729183921	-2.405920487	0.722319482
C	3.417413276	-0.170321954	-0.922409609
C	-2.051575593	-0.869038166	0.158591813
C	-4.862967950	-1.274833712	-0.032410813
C	-2.943361766	-0.275753140	1.088046820
C	-2.593870182	-1.716302709	-0.836199468
C	-3.977135500	-1.891606905	-0.908805622
C	-4.318783728	-0.475388804	0.963788472
C	-0.172522871	1.346388756	0.190490038
C	0.084022379	4.151405403	-0.121362416

C	0.563834188	2.112670760	1.121066724
C	-0.772432841	2.003121924	-0.905755911
C	-0.627850518	3.385355781	-1.038527108
C	0.676448150	3.492628061	0.951150228
C	4.642973497	0.188589122	-0.063124043
C	2.814403215	1.168127339	-1.393178883
C	3.897890048	-0.919051441	-2.197607643
C	3.972351607	-3.204419438	0.269394655
C	1.601742916	-3.446400682	0.893360787
C	3.005011775	-1.811597226	2.123787626
C	-2.479899283	0.591642932	2.236961669
C	-1.783174579	-2.475225126	-1.863617013
C	1.300790373	1.489272637	2.283181623
C	-1.580044082	1.295395736	-1.967326074
C	-6.349352037	-1.501934773	-0.135764548
C	0.192145503	5.646784319	-0.275470897
H	-4.376746485	-2.536385245	-1.689273777
H	-4.981828089	0.007198208	1.679298547
H	-1.086817875	3.878089335	-1.893683607
H	1.253523558	4.066738003	1.673235898
H	5.339699519	0.805740828	-0.646785218
H	5.199047823	-0.682557144	0.290464702
H	4.350343839	0.776808108	0.815108076
H	1.960544094	1.042419084	-2.065698645
H	3.575864285	1.741791821	-1.939544964
H	2.480028773	1.785009511	-0.554868374
H	3.060440002	-1.181157392	-2.857438302
H	4.448767559	-1.836112033	-1.969250273
H	4.567940538	-0.264259242	-2.771059634
H	3.808738704	-3.687329064	-0.701957614
H	4.178714661	-4.001359762	0.996619899
H	4.876554754	-2.596314434	0.191923708
H	1.379878707	-3.967416529	-0.046952579
H	0.674127121	-2.997577865	1.264827790
H	1.906962192	-4.210885189	1.620104448
H	3.804182025	-1.064547578	2.117771238
H	3.309095385	-2.613284368	2.811167446
H	2.103288955	-1.348636213	2.538975709
H	-3.293448748	0.737101962	2.953554117
H	-2.148402093	1.579515085	1.899566875
H	-1.639500489	0.133969338	2.770751944
H	-2.452308614	-2.996626696	-2.553663223
H	-1.147722354	-3.236550478	-1.398448073
H	-1.141034890	-1.824573054	-2.462386054
H	2.135753027	0.869960352	1.934403438
H	0.658087883	0.842736762	2.887149659
H	1.718429620	2.264438735	2.932665908

H	-1.684595106	1.932842170	-2.850273742
H	-2.583943245	1.048093343	-1.607354769
H	-1.117300735	0.359029465	-2.285856290
H	-6.910895672	-0.661779665	0.284482326
H	-6.646600177	-2.404650579	0.411924603
H	-6.660868905	-1.633386484	-1.177038225
H	-0.667220324	6.148365267	0.185948599
H	0.214240243	5.937696781	-1.330576942
H	1.096335409	6.034093251	0.204174928
H	0.540002628	-2.176410141	-1.003084420
H	0.736375233	-0.596395529	-1.774882217

TS14_PB[e]

Total number of atoms = 74

C	1.057240273	-0.481360600	-0.911846347
P	-0.286544846	-0.108591650	0.305317798
C	-0.725426217	1.657443653	-0.042271256
C	-1.293798966	2.059359898	-1.275443705
C	-0.456216528	2.638447856	0.937401019
C	-1.556594905	3.409438997	-1.499693518
C	-0.737803979	3.978568024	0.660786167
C	-1.283975885	4.388506322	-0.547999874
C	-1.843781364	-1.077701039	-0.005426233
C	-2.867431222	-0.818594443	0.945188038
C	-2.092517367	-2.054073002	-1.002231567
C	-4.084243210	-1.492499357	0.867022129
C	-3.329205190	-2.707240533	-1.023314577
C	-4.340081663	-2.447818383	-0.108595204
C	3.553208148	0.600025233	-0.428977828
C	3.028562470	-2.229013991	-0.261807004
B	2.562209157	-0.675500992	-0.342113215
C	0.979499234	-0.724318808	2.380653799
C	-1.138961141	-2.478224152	-2.099380888
C	-5.652012746	-3.186989697	-0.152496257
C	-2.715531456	0.179068485	2.068664920
C	0.128484629	2.335804450	2.298024048
C	-1.581320933	5.838687024	-0.828836214
C	-1.648879924	1.098005238	-2.384009670
C	4.258850771	0.493640833	-1.803888223
C	4.638647247	0.701625651	0.661094756
C	2.796062834	1.941775821	-0.406013967
C	3.101119166	-2.745333869	-1.724879102
C	4.398721968	-2.495086240	0.381482060
C	2.008013944	-3.118972937	0.482208723
O	2.065448391	-0.459185106	1.963545364

O	0.208277451	-1.113784174	3.184371075
H	-1.991729008	3.705894536	-2.452029928
H	-0.518865297	4.724461035	1.421324119
H	-4.852296413	-1.264950056	1.603049597
H	-3.505555553	-3.450011929	-1.798177589
H	-0.768766925	-1.636072845	-2.688163422
H	-0.277213919	-3.029240504	-1.708169132
H	-1.652952486	-3.151044450	-2.790706510
H	-6.493282360	-2.513184829	0.040208824
H	-5.811197178	-3.662347089	-1.125037896
H	-5.680726578	-3.973259130	0.611044085
H	-3.577210405	0.126517727	2.739668531
H	-1.823443398	-0.033089350	2.664603361
H	-2.646575079	1.206644964	1.697011382
H	-0.491615518	1.637892966	2.866713552
H	1.131170628	1.905854154	2.229802237
H	0.209530567	3.255080775	2.884458968
H	-1.064152388	6.177834447	-1.733224033
H	-2.654071178	5.995686273	-0.988832604
H	-1.267212653	6.479829781	-0.000141198
H	-0.784966662	0.512095361	-2.710870507
H	-2.423876939	0.391375507	-2.073748713
H	-2.019871514	1.643780647	-3.255669442
H	4.953394266	-0.352289532	-1.843980419
H	3.544754821	0.387512550	-2.631794017
H	4.841098810	1.405957528	-1.992037561
H	5.348435226	-0.126641876	0.637607463
H	5.215319116	1.625915685	0.517599724
H	4.195528281	0.738318937	1.660982286
H	2.049921894	2.037366841	-1.201451626
H	2.283250882	2.090286616	0.547763548
H	3.503082862	2.773722712	-0.526282075
H	2.126441332	-2.739333065	-2.226377473
H	3.793780876	-2.163860724	-2.341900923
H	3.456490754	-3.784528211	-1.725607054
H	4.585234545	-3.576827551	0.435763451
H	5.217540723	-2.056214988	-0.198411970
H	4.448289766	-2.097654654	1.400349215
H	2.088776895	-2.995148234	1.566380822
H	0.965710903	-2.921891192	0.203559592
H	2.203510163	-4.178154591	0.266091274
H	1.051067772	0.299889946	-1.677450211
H	0.786802690	-1.405062685	-1.408935541

4PB[e]

Total number of atoms = 74

C	1.100852988	-0.439940753	-1.034175310
P	-0.267692315	-0.076319870	0.067840881
C	-0.677207461	1.703708069	-0.073902023
C	-1.299071384	2.104710208	-1.282370849
C	-0.364293939	2.670303153	0.908799504
C	-1.593657769	3.451078294	-1.478952764
C	-0.681427954	4.005304755	0.649133202
C	-1.294625165	4.420239955	-0.526390252
C	-1.812917470	-1.066773608	-0.007689230
C	-2.813573539	-0.768951766	0.952353671
C	-2.048616086	-2.094826425	-0.957332650
C	-3.986252515	-1.523376422	0.970197483
C	-3.243322504	-2.811045280	-0.882881177
C	-4.218986846	-2.558113845	0.074529641
C	3.595307481	0.516142549	-0.277055951
C	2.888121974	-2.286470141	-0.119121662
B	2.463226355	-0.673493998	-0.051096615
C	0.666770497	-0.507682992	1.683344063
C	-1.135380671	-2.487241572	-2.097982437
C	-5.475403415	-3.385355717	0.135817234
C	-2.712879650	0.348214875	1.962636233
C	0.286595998	2.383572607	2.241507574
C	-1.640274855	5.867214321	-0.760983921
C	-1.665982908	1.148355932	-2.393677861
C	4.447845140	0.266719882	-1.533105034
C	4.542703245	0.653441434	0.932593657
C	2.947928923	1.905455282	-0.456986492
C	3.098418829	-2.806110932	-1.556297598
C	4.167493743	-2.609121608	0.674089782
C	1.772105874	-3.149461644	0.511972022
O	1.921774264	-0.483668082	1.422478318
O	0.117651002	-0.759278104	2.732478963
H	-2.067242434	3.750988608	-2.410849797
H	-0.431042139	4.748848299	1.401455862
H	-4.740952264	-1.286786561	1.715887279
H	-3.418115938	-3.598444373	-1.612012120
H	-0.835136066	-1.632205287	-2.707973703
H	-0.231026470	-2.995542894	-1.750817840
H	-1.658406004	-3.184619725	-2.756675455
H	-5.840393937	-3.628968641	-0.866963607
H	-5.286409723	-4.331841583	0.655709825
H	-6.272592955	-2.864191600	0.673801884
H	-1.780903822	0.286216032	2.526549273
H	-2.778892279	1.330482351	1.483573035
H	-3.532281161	0.273960587	2.681970384
H	-0.353546797	1.782352556	2.891705730
H	1.238956982	1.857231350	2.144802859

H	0.490801870	3.323958998	2.758882070
H	-1.470311992	6.149979998	-1.804534047
H	-2.697570210	6.053308092	-0.537962508
H	-1.044119334	6.528073789	-0.125420622
H	-0.794811953	0.598581209	-2.764093553
H	-2.411440428	0.414515834	-2.072493838
H	-2.084427933	1.697999752	-3.240332760
H	5.088970291	-0.614300164	-1.425633461
H	3.826573250	0.120061527	-2.427549983
H	5.107303867	1.124591789	-1.731454565
H	5.120837405	-0.253627647	1.120393801
H	5.261170663	1.469533128	0.764900138
H	3.986243186	0.882441516	1.848677616
H	2.372694908	1.995996011	-1.386423869
H	2.279799970	2.161500404	0.370940351
H	3.722484785	2.684538829	-0.492785720
H	2.186892783	-2.752924727	-2.166193236
H	3.878550888	-2.258704096	-2.092213773
H	3.396957436	-3.864236804	-1.536273445
H	4.322237968	-3.697009050	0.731137910
H	5.059889512	-2.182352830	0.203787231
H	4.107763403	-2.228847232	1.699997221
H	1.713482720	-3.010805232	1.596411733
H	0.773321927	-2.933111364	0.105336987
H	1.957320994	-4.217361098	0.328949176
H	0.905835034	-1.333459565	-1.612868386
H	1.213761495	0.390085761	-1.733545529

1PB[f]

Total number of atoms = 72

C	-0.462662118	-1.172172257	-0.559151691
C	0.070506454	-1.692570089	-1.674229021
P	0.512112792	-0.322609043	0.772033677
B	-2.019917934	-1.416917758	-0.313143778
C	-3.090356378	-0.584407156	-1.195474037
C	-2.462164863	0.209869688	-2.354440344
C	-4.218210432	-1.433737749	-1.818294332
C	-3.717855238	0.456266815	-0.232566794
C	-2.439361420	-2.593359859	0.710855498
C	-2.538348497	-3.838466249	-0.214273512
C	-3.768681191	-2.419446579	1.468194173
C	-1.376894535	-2.928523585	1.772170534
C	-0.096711910	1.394383390	0.426175785
C	-1.235309715	3.961454736	0.079428822
C	-0.866741988	1.984326542	1.452165528
C	0.101180073	2.104976897	-0.780292246

C	-0.471747452	3.369882577	-0.923237977
C	-1.416565019	3.253313170	1.262566489
C	2.315908167	-0.402208905	0.347256397
C	5.060487308	-0.656090605	-0.346344820
C	3.185080146	0.714497638	0.419024530
C	2.898008175	-1.677255474	0.135013102
C	4.238336626	-1.771876116	-0.243866480
C	4.522069120	0.564543873	0.045803432
C	-1.869613361	5.313375080	-0.124159998
C	-1.149811862	1.283736670	2.763778931
C	0.913557277	1.578308069	-1.938407049
C	2.796549180	2.074185247	0.964271769
C	6.489996594	-0.770078056	-0.808260663
C	2.175526547	-2.972490197	0.428186983
H	-1.212885067	-2.103052550	2.471893031
H	-1.697981977	-3.803612990	2.354303626
H	-3.988586329	-3.331724031	2.039588369
H	-2.740531640	-4.726893894	0.398954042
H	-3.338880134	-3.760899918	-0.954943718
H	-4.626006024	-2.230846880	0.819106728
H	-3.707182970	-1.595088521	2.188950101
H	-0.415338529	-3.171666165	1.315455661
H	-1.595261064	-4.017469201	-0.745594692
H	-3.244892816	0.763571179	-2.890993801
H	-4.921923750	-0.774720552	-2.344797009
H	-4.796142817	-2.004596841	-1.088616304
H	-1.733938025	0.938019822	-1.994102335
H	-3.822787126	-2.140541698	-2.558198313
H	-1.961455390	-0.439613053	-3.080437421
H	-4.423730624	1.084134890	-0.793701395
H	-4.269730205	-0.003465617	0.591364637
H	-2.960968765	1.125850854	0.189852980
H	5.170165152	1.438313013	0.086301283
H	4.658483754	-2.758718475	-0.427791039
H	-0.315505115	3.909855846	-1.855006409
H	-2.007452429	3.696149778	2.061558798
H	1.135549118	-1.648246208	-1.898419418
H	6.893271749	-1.770150612	-0.620184337
H	7.133094501	-0.043157729	-0.301646155
H	6.568447137	-0.581776469	-1.886024405
H	3.689180162	2.565448143	1.363256469
H	1.932240565	1.312973705	-1.644926104
H	2.367840931	2.736624065	0.206505295
H	2.069341160	2.004357484	1.776645133
H	2.886802275	-3.803188855	0.436505158
H	1.387334054	-3.211361833	-0.289950946
H	1.709119523	-2.927131071	1.418868844

H	0.973102215	2.329398932	-2.731115248
H	-1.246844630	5.955752036	-0.754713396
H	-2.844070010	5.213105050	-0.617266349
H	-2.033386107	5.824748396	0.829375027
H	-1.732262090	1.933799404	3.423530594
H	-0.230553790	0.999294111	3.285065595
H	-1.723023257	0.361533410	2.613252009
H	0.462935514	0.676139984	-2.360370566
H	-0.544707578	-2.200047467	-2.417678350

TS14_PB[f]

Total number of atoms = 75

C	1.029105932	0.933994796	-1.974932819
C	1.185996260	0.319214228	-0.793647673
P	-0.290393862	0.080175207	0.301335539
C	-1.406231488	1.497898015	-0.093713792
C	-2.323642041	1.508617215	-1.167145039
C	-1.333441139	2.623568553	0.760283900
C	-3.115569249	2.642485906	-1.370347292
C	-2.142086165	3.729685730	0.511147669
C	-3.041861053	3.761814500	-0.551186397
C	-1.336801418	-1.429737689	0.053841570
C	-2.349958993	-1.567494708	1.042931681
C	-1.218598469	-2.431200553	-0.930190119
C	-3.160303777	-2.698971074	1.045476906
C	-2.048488692	-3.555094447	-0.869810172
C	-3.015843955	-3.720362240	0.109281557
C	3.694717555	1.320113065	-0.170323358
C	3.216183884	-1.503750189	-0.380423918
B	2.694828353	0.028843055	-0.268075395
C	1.083623847	-0.257671892	2.407616774
C	-0.293906053	-2.385643768	-2.123168907
C	-3.878412985	-4.954312076	0.165919339
C	-2.650994379	-0.504943802	2.075275817
C	-0.435468997	2.671330063	1.973931547
C	-3.915257542	4.967142782	-0.786580123
C	-2.541625828	0.356472874	-2.121049860
C	4.546543705	1.377633488	-1.463476824
C	4.685382266	1.282376839	1.015801184
C	2.951105927	2.663938429	-0.039255117
C	3.303458057	-1.809306414	-1.898556819
C	4.596688570	-1.816681749	0.222365625
C	2.239370144	-2.511578163	0.258244397
O	2.132323643	0.041669038	1.926464804
O	0.366608631	-0.625604792	3.266548813

H	0.063792819	1.215622399	-2.387645841
H	-3.815515102	2.644776401	-2.203246008
H	-2.071480798	4.590755321	1.172558154
H	-3.930753786	-2.784190595	1.808866885
H	-1.934405391	-4.317391405	-1.638718815
H	-0.872319047	-2.540287899	-3.041316969
H	0.236741443	-1.443118750	-2.216149751
H	0.452928208	-3.185402145	-2.070913091
H	-4.915375100	-4.705271515	0.414404760
H	-3.875715828	-5.487537020	-0.789476806
H	-3.515321409	-5.647399064	0.934168652
H	-3.340154011	-0.896606658	2.828537601
H	-1.753114494	-0.168343654	2.597696915
H	-3.121487618	0.371391190	1.615080182
H	-0.754619462	1.946139558	2.730989282
H	0.606871344	2.454951377	1.728953934
H	-0.466090821	3.663802760	2.432110208
H	-4.423753474	4.909620316	-1.753345904
H	-4.683368218	5.050359781	-0.008745643
H	-3.328371758	5.891632929	-0.765228053
H	-1.610485238	-0.110762298	-2.445793789
H	-3.149434884	-0.429950834	-1.661356573
H	-3.064872622	0.706665569	-3.015541456
H	5.212889728	0.514177895	-1.555604376
H	3.942882867	1.431853874	-2.376871628
H	5.178769321	2.275850352	-1.443403580
H	5.397676786	0.459324854	0.955848542
H	5.270372881	2.212540902	1.022159865
H	4.166679351	1.211407890	1.975382842
H	2.244154549	2.851892193	-0.851003666
H	2.395523217	2.707734869	0.903437237
H	3.673797977	3.490927831	-0.026652274
H	4.044229920	-1.179758481	-2.403045235
H	3.610452929	-2.853874765	-2.044724857
H	2.348564463	-1.671604213	-2.410871716
H	4.817095236	-2.885930377	0.094741925
H	5.405677836	-1.263965575	-0.265046331
H	4.628329264	-1.600126423	1.295080728
H	2.317415120	-2.497482015	1.350504525
H	1.194147877	-2.333852697	-0.000604445
H	2.481741560	-3.532996413	-0.066280060
H	1.884108689	1.201840867	-2.592558791

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Total number of atoms = 75

C	1.195946666	0.082800262	-2.272430905
C	1.185917058	-0.169057531	-0.960960735
P	-0.287731642	-0.025922394	0.070698676
C	-0.981923447	1.664096096	-0.055867020
C	-1.838691279	1.931009234	-1.148503673
C	-0.654031482	2.699090117	0.850906054
C	-2.316125902	3.226987345	-1.332954920
C	-1.162034358	3.976050602	0.609930754
C	-1.986730122	4.267162162	-0.470931031
C	-1.650865353	-1.248959539	0.014304344
C	-2.694215688	-1.078404442	0.959707306
C	-1.693550612	-2.337410661	-0.889313757
C	-3.716462978	-2.024478148	1.008277732
C	-2.741680695	-3.252081770	-0.781765607
C	-3.753291877	-3.127585070	0.163308747
C	3.611304306	0.850772579	-0.149323146
C	3.041752101	-1.986222207	-0.061203596
B	2.520273663	-0.404157783	0.010211570
C	0.666397565	-0.353603951	1.697998075
C	-0.724721787	-2.569986688	-2.024085668
C	-4.840419395	-4.162525100	0.282406426
C	-2.812523710	0.095941029	1.904319699
C	0.162047295	2.525972264	2.110112724
C	-2.533592148	5.654775950	-0.680525088
C	-2.343121465	0.882954479	-2.114757528
C	4.661076880	0.624801972	-1.254582510
C	4.370127873	1.080218652	1.175840925
C	2.927414546	2.194022104	-0.483892818
C	3.312337467	-2.455985807	-1.502413033
C	4.316972048	-2.239097946	0.765721013
C	1.976467115	-2.928062349	0.544239907
O	1.922949577	-0.267325621	1.464836656
O	0.110747677	-0.609569030	2.742591229
H	0.321850290	0.316889161	-2.874646661
H	-2.969338800	3.425681376	-2.179711919
H	-0.900095252	4.772641664	1.301875223
H	-4.508373628	-1.892611420	1.741589723
H	-2.765165168	-4.091742522	-1.472096250
H	-0.865334334	-1.834164376	-2.824159133
H	0.319186797	-2.515739177	-1.723445181
H	-0.896490413	-3.557344460	-2.459641864
H	-5.031729443	-4.654189880	-0.676077377
H	-4.549874255	-4.938346038	1.000495120
H	-5.776272449	-3.719813722	0.636488396
H	-1.877855081	0.293129455	2.430660194
H	-3.119163816	1.003170555	1.372526422
H	-3.569625304	-0.117549820	2.663101366

H	-0.372797119	1.923856338	2.851069873
H	1.129947198	2.051104768	1.941797369
H	0.358065362	3.502604825	2.559000249
H	-2.716855732	5.854336005	-1.740525887
H	-3.485785839	5.778873936	-0.151142998
H	-1.843701305	6.415166627	-0.302844768
H	-1.601528594	0.124887296	-2.367019072
H	-3.204947112	0.352630708	-1.693905504
H	-2.659604538	1.354935271	-3.048712112
H	5.305232686	-0.235747823	-1.052364335
H	4.203270649	0.471728650	-2.239940824
H	5.314632510	1.505443921	-1.339923626
H	4.910091452	0.191981113	1.512324312
H	5.106928643	1.888184447	1.055749666
H	3.687148096	1.370616887	1.981535599
H	2.505042885	2.208851093	-1.493917446
H	2.112098096	2.433001654	0.206736672
H	3.654730115	3.016094372	-0.419923357
H	2.413881251	-2.407762605	-2.128888411
H	4.085270724	-1.859420243	-1.996538306
H	3.655212180	-3.500785001	-1.507659606
H	4.553167392	-3.313829312	0.778443693
H	5.192406620	-1.722705174	0.360630834
H	4.184762318	-1.919950255	1.805620066
H	1.900067048	-2.805126488	1.629688500
H	0.971092602	-2.773767988	0.133605265
H	2.233955589	-3.979178678	0.351699434
H	2.138854221	0.069584887	-2.813890347

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Total number of atoms = 82

C	1.150918710	0.394804325	-1.103463963
C	0.850645878	-0.326989718	-0.006780833
B	1.833515547	-1.052908758	1.018317299
P	-0.825878855	-0.145639974	0.780200471
C	1.713784859	-2.650554363	1.304625223
C	2.888731353	-0.097750360	1.803024093
C	-2.121464137	-1.135731325	-0.106948882
C	-4.357670580	-2.560516753	-1.129179118
C	-3.374274201	-1.102890235	0.555525353
C	-2.000124475	-1.915989359	-1.281044747
C	-3.116849487	-2.609854211	-1.753591278
C	-4.462794184	-1.795063424	0.025819017
C	-1.306214157	1.623981966	0.468462721
C	-1.911456339	4.391185683	0.249078767

C	-1.103692642	2.503017746	1.561110542
C	-1.879271958	2.145660279	-0.716412872
C	-2.155976627	3.512015232	-0.799972381
C	-1.394060264	3.861218897	1.424730818
C	2.503224215	-0.122113577	3.309458257
C	2.878507473	1.377702752	1.353708708
C	4.350247508	-0.579213421	1.653715437
C	2.501899029	-3.348326345	0.166326400
C	0.268237805	-3.183556127	1.249852853
C	2.282661495	-3.175152854	2.638799812
C	-3.602755901	-0.327191864	1.834012227
C	-0.749881740	-2.038457380	-2.125467901
C	-0.609260266	2.040707652	2.913949902
C	-2.274884186	1.313862262	-1.914565921
C	2.431645834	0.498467811	-1.817596575
C	4.883437283	0.851256660	-3.144410211
C	2.682114839	1.653101978	-2.573753852
C	3.421225832	-0.488777963	-1.771410922
C	4.637486090	-0.313642335	-2.422854230
C	3.897599159	1.833540244	-3.221910897
C	-5.533757086	-3.337034872	-1.663270532
C	-2.242590995	5.856659886	0.129480441
H	0.377161844	1.024369375	-1.538457316
H	-3.011257509	-3.201950235	-2.660513363
H	-5.419038444	-1.741215114	0.542449389
H	-2.584774587	3.900605287	-1.721825767
H	-1.217481249	4.522343218	2.270690432
H	2.911766115	0.766449103	3.807497837
H	2.905559721	-0.996151609	3.823635889
H	1.417911779	-0.117478867	3.468842147
H	3.248137237	1.496221906	0.332468232
H	3.536533945	1.965567630	2.007855407
H	1.882619331	1.828617559	1.391072933
H	4.705177650	-0.441838380	0.626637989
H	4.492659325	-1.629564159	1.920042289
H	5.001702173	0.015944054	2.308539430
H	2.084213241	-3.128190158	-0.822673090
H	2.448509186	-4.436832041	0.302911680
H	3.564012307	-3.073168831	0.164296638
H	-0.220971473	-2.995498448	0.294631745
H	-0.355757880	-2.743866075	2.035284699
H	0.270694262	-4.272081228	1.398566598
H	3.333885168	-2.925508001	2.799180332
H	2.207506830	-4.270982815	2.655942363
H	1.709234127	-2.801169541	3.492622176
H	-4.613809536	-0.505043655	2.211540847
H	-3.485950773	0.752455530	1.687021028

H	-2.891610986	-0.625097713	2.612503049
H	-0.884341388	-2.825643569	-2.872946897
H	0.142030192	-2.275651297	-1.545693303
H	-0.524295134	-1.112259123	-2.664115370
H	0.437010521	1.726686501	2.888290337
H	-1.188099189	1.189987509	3.285765818
H	-0.687628866	2.853979611	3.641773984
H	-2.452803278	1.960254513	-2.779120598
H	-3.195160576	0.753568903	-1.718268739
H	-1.517052831	0.583921461	-2.196085926
H	1.918135024	2.424867061	-2.628123804
H	3.233779379	-1.410351698	-1.235083063
H	5.391752014	-1.093487347	-2.371898687
H	4.077650072	2.742804556	-3.787833038
H	5.833169560	0.989141474	-3.652368832
H	-6.475400146	-2.806568040	-1.488981568
H	-5.612602077	-4.314468258	-1.171876003
H	-5.437458672	-3.516196514	-2.738684913
H	-3.295682182	6.039910282	0.375265099
H	-2.076858125	6.220807641	-0.889538319
H	-1.634499666	6.460641505	0.809893910

TS14_PB[a]

Total number of atoms = 85

C	1.090643275	0.652975282	-1.031652051
C	0.860097493	-0.195603223	-0.004903999
P	-0.896109978	-0.116493011	0.603477790
C	-1.338603139	1.679883563	0.498500210
C	-1.954420141	2.301781501	-0.614364855
C	-1.021565811	2.466989518	1.630982528
C	-2.223266272	3.672470780	-0.560078079
C	-1.303410423	3.831555494	1.626638239
C	-1.910626616	4.456958971	0.543121047
C	-2.110349282	-1.014893794	-0.456206132
C	-3.432305640	-0.997572185	0.055124745
C	-1.846200878	-1.739476444	-1.642933096
C	-4.426164335	-1.742384055	-0.578860296
C	-2.879485773	-2.474311412	-2.227685889
C	-4.169403332	-2.507324125	-1.709999830
C	3.178500756	-0.227162252	1.519907852
C	1.914338608	-2.700485377	0.783510034
B	1.947630429	-1.065496069	0.825699527
C	-0.741372368	-1.250257684	2.725463865
C	2.287465041	0.884702027	-1.855224510
C	2.483232479	2.173999914	-2.373939193

C	3.208694014	-0.111485104	-2.184232430
C	3.597504036	2.468953601	-3.147602296
C	4.321355221	0.178476741	-2.968524190
C	4.524751550	1.470128987	-3.443807053
C	-0.543301152	-1.720286068	-2.411998323
C	-5.247189769	-3.345957416	-2.345943222
C	-3.870216313	-0.118559103	1.205000366
C	-0.406585946	1.894550589	2.884342099
C	-2.238149253	5.927201402	0.577199469
C	-2.368891168	1.600318282	-1.889377784
C	4.554001788	-0.719548944	1.002436771
C	3.190754516	-0.383279220	3.062415457
C	3.151790976	1.295734775	1.266994828
C	2.686346397	-3.149794370	-0.486339024
C	2.575833364	-3.408687888	1.984012041
C	0.508874669	-3.332386274	0.671428096
O	0.440055698	-1.191566081	2.905079488
O	-1.824599925	-1.606592019	3.054762991
H	0.275783900	1.299994464	-1.349647560
H	-2.691440525	4.141785584	-1.422747870
H	-1.042992711	4.421184187	2.503035770
H	-5.433574566	-1.718482119	-0.168890556
H	-2.665336520	-3.032777163	-3.136327746
H	1.760064679	2.952314007	-2.141781412
H	3.045070622	-1.122792582	-1.838713044
H	3.742350555	3.476244751	-3.526456145
H	5.026908693	-0.610252134	-3.212604621
H	5.393970642	1.696876981	-4.053855015
H	-0.375939126	-0.747624430	-2.889588239
H	0.332025074	-1.913495237	-1.795872176
H	-0.571007881	-2.472999128	-3.204373760
H	-6.229955894	-2.874771648	-2.244560412
H	-5.053362363	-3.508252652	-3.410683012
H	-5.304417807	-4.330379007	-1.866221125
H	-4.826555762	-0.468605396	1.603071113
H	-3.160985828	-0.109200032	2.033164769
H	-4.004406509	0.916147884	0.866199354
H	-1.131434698	1.282470736	3.434084558
H	0.464802629	1.267656458	2.684287772
H	-0.085390558	2.698887479	3.551878543
H	-2.328414488	6.341818884	-0.431429901
H	-3.191187436	6.099527099	1.091577595
H	-1.469646171	6.493682788	1.112578460
H	-1.611276267	0.910764138	-2.263838674
H	-3.286937516	1.019937448	-1.751879723
H	-2.555995042	2.340763278	-2.672271512
H	4.747202310	-1.770641339	1.230940088

H	4.661626912	-0.577290445	-0.077380503
H	5.347975053	-0.133385471	1.484835551
H	3.186945945	-1.419736551	3.399065222
H	4.100809271	0.091173508	3.454360912
H	2.332681438	0.112033242	3.522950040
H	3.374275889	1.549653738	0.228779957
H	2.188492236	1.749112974	1.519661287
H	3.916994354	1.780103712	1.888114315
H	2.155830855	-2.887534312	-1.408276821
H	3.700176757	-2.741785568	-0.541003995
H	2.779247172	-4.243850656	-0.478798429
H	2.505776568	-4.496197705	1.842597526
H	3.635361602	-3.168843503	2.102103091
H	2.060738854	-3.165730487	2.917615865
H	-0.017909168	-3.329142208	1.628405335
H	-0.136818238	-2.855842039	-0.066524037
H	0.603665008	-4.385740123	0.374582373

4PB[a]

Total number of atoms = 85

C	-1.196179372	0.558548763	1.137241532
C	-0.872430667	-0.232754385	0.091272565
P	0.856216255	-0.043839508	-0.412592895
C	1.350910129	1.723967383	-0.419597048
C	1.906610131	2.298226924	0.751422243
C	1.104583173	2.540135411	-1.550796162
C	2.177094970	3.666014683	0.765075926
C	1.398962967	3.901530405	-1.470597160
C	1.931715627	4.487762036	-0.329282815
C	2.161717261	-1.032632675	0.408319219
C	3.453236744	-0.999452430	-0.165096727
C	1.929529216	-1.808059916	1.575245579
C	4.464913332	-1.774511719	0.409744515
C	2.977740300	-2.564640439	2.089071726
C	4.249619781	-2.576422814	1.519239126
C	-3.018712840	-0.231582549	-1.713510840
C	-1.812193000	-2.741876316	-0.905406919
B	-1.695304670	-1.083926098	-1.125047955
C	0.613768891	-0.798346151	-2.141342152
C	-2.461546340	0.761721589	1.864501924
C	-2.745455738	2.058411745	2.319304647
C	-3.350996038	-0.266171607	2.180994724
C	-3.911763518	2.328275081	3.022366352
C	-4.512077491	-0.001050314	2.901303434
C	-4.801610347	1.295606920	3.314611187

C	0.638861438	-1.844372222	2.361749003
C	5.343435085	-3.432154385	2.101097824
C	3.873792571	-0.180442272	-1.366083951
C	0.594401759	2.040106428	-2.881204673
C	2.260668857	5.956700268	-0.285954246
C	2.268783548	1.540334047	2.010777491
C	-4.373942466	-0.676538644	-1.128395545
C	-3.116612146	-0.386255950	-3.250098293
C	-2.931612391	1.289822031	-1.461760931
C	-2.587548083	-3.160817529	0.353514015
C	-2.482322967	-3.436825616	-2.109278254
C	-0.416093481	-3.398140665	-0.809410237
O	-0.637332667	-1.002308070	-2.310768906
O	1.524428606	-1.026759540	-2.906462243
H	-0.426168524	1.217209782	1.542288430
H	2.595521886	4.102585284	1.668992375
H	1.202396196	4.522928980	-2.340670989
H	5.453569413	-1.743347273	-0.042613037
H	2.796193583	-3.162193310	2.979217667
H	-2.048724832	2.862854709	2.094253893
H	-3.128578108	-1.276089597	1.867582481
H	-4.124904324	3.342060016	3.347905480
H	-5.192935241	-0.813351055	3.137626056
H	-5.712136990	1.500937381	3.869575337
H	0.436768292	-0.889914479	2.860157684
H	-0.232179471	-2.064906763	1.747250922
H	0.705360148	-2.610473528	3.138189719
H	5.437184135	-3.275111056	3.180928652
H	5.126762933	-4.494663038	1.942528676
H	6.310602522	-3.215622560	1.638966629
H	3.911831999	-0.811678702	-2.257024864
H	3.211032436	0.651692440	-1.596846822
H	4.871214998	0.234661501	-1.188012568
H	1.353139843	1.441921170	-3.395819314
H	-0.305567537	1.428891954	-2.800517557
H	0.345759554	2.887894242	-3.524126538
H	2.102535613	6.371279385	0.714426268
H	3.312105730	6.123757637	-0.548374213
H	1.648465964	6.524530367	-0.992478777
H	1.502249872	0.833546127	2.331570134
H	3.196449604	0.974005128	1.881629405
H	2.417974599	2.246630331	2.831741429
H	-4.612063956	-1.718422645	-1.361442217
H	-4.414718533	-0.555875699	-0.042420946
H	-5.182240791	-0.060507356	-1.549449968
H	-3.178096841	-1.427521941	-3.573319959
H	-4.018142436	0.126114546	-3.616226371

H	-2.253567920	0.059357798	-3.755880119
H	-3.112464277	1.548478653	-0.415809359
H	-1.959423017	1.712170932	-1.737348433
H	-3.692904912	1.813017797	-2.057992182
H	-2.069252994	-2.860672060	1.272243449
H	-3.598447204	-2.743354979	0.380075780
H	-2.687787674	-4.255194814	0.395778013
H	-2.437271356	-4.528800321	-1.981987881
H	-3.536828310	-3.171247147	-2.223291275
H	-1.967310723	-3.194384432	-3.044827476
H	0.124685304	-3.346319415	-1.760135223
H	0.225723279	-2.958071823	-0.040634615
H	-0.514793366	-4.463728933	-0.557917852

TS13_^{t}Bu$_3$P/BPh$_3$

Total number of atoms = 76

P	1.903338595	0.007319955	0.477979804
C	2.352882923	-1.742999440	1.082482831
C	1.754407755	-1.971723847	2.484064753
C	1.640459924	-2.761741160	0.166229266
C	3.855417217	-2.060624985	1.134305335
C	2.925444499	0.454624324	-1.069251210
C	2.959219465	-0.734436281	-2.046852614
C	4.378926917	0.868140624	-0.784047487
C	2.189150225	1.595812403	-1.804191796
C	2.247112183	1.275581931	1.864387103
C	2.205966830	2.704630971	1.289947499
C	1.074851395	1.201895182	2.869156646
C	3.574404306	1.090760064	2.615577959
B	-1.825206558	-0.034765430	-0.296636386
C	-3.011822135	-0.019212847	0.789922892
C	-4.151303319	0.772294958	0.586675267
C	-5.205533072	0.785833142	1.498042946
C	-5.141992769	0.010919494	2.652903803
C	-4.018013730	-0.778589085	2.885328168
C	-2.975107888	-0.790201604	1.962567826
C	-1.573393761	1.366917013	-1.038514128
C	-1.769372013	1.558786910	-2.413032811
C	-1.545270068	2.793480334	-3.022923893
C	-1.116327251	3.880347010	-2.267430516
C	-0.940359986	3.727325580	-0.893175225
C	-1.175045556	2.491629857	-0.298661868
C	-1.590565031	-1.390324645	-1.124491859
C	-2.219316442	-2.595415548	-0.772576867
C	-1.934763062	-3.792740366	-1.425117842

C	-1.010899232	-3.821026750	-2.467269903
C	-0.385767753	-2.639174147	-2.854011066
C	-0.675141913	-1.449932105	-2.188331715
H	0.037132538	-0.034566500	0.437134052
H	1.864776017	-3.034346660	2.731832351
H	0.684272079	-1.741138859	2.516263173
H	2.263364024	-1.406190938	3.267419595
H	1.812798003	-3.767490220	0.570005043
H	2.005556789	-2.757990962	-0.859478562
H	0.559445903	-2.595008341	0.133957211
H	3.993005285	-3.063776172	1.558432589
H	4.412108309	-1.358844990	1.760777734
H	4.313595745	-2.067095137	0.142370688
H	3.397863324	-0.386279859	-2.990000432
H	1.961196204	-1.118330270	-2.267709578
H	3.580183983	-1.558750867	-1.689635681
H	4.889278572	1.043299597	-1.739923869
H	4.934197989	0.091016624	-0.251137384
H	4.449908730	1.793978876	-0.209514487
H	2.698157517	1.781538660	-2.758419040
H	2.183992289	2.535014396	-1.252007355
H	1.147714024	1.338578950	-2.021176787
H	2.219269546	3.411488510	2.128744041
H	1.293726103	2.889910280	0.716544240
H	3.067836727	2.938946292	0.662222036
H	1.203247420	1.995687559	3.615688167
H	1.020908494	0.258100324	3.410456493
H	0.109134627	1.362825438	2.380558764
H	3.686090859	1.900892183	3.347916799
H	4.438921316	1.127087531	1.947363989
H	3.611932317	0.149796802	3.169559353
H	-0.813050647	-0.083691789	0.677056709
H	0.330096814	-2.642513846	-3.672699231
H	-0.789480648	-4.753442953	-2.979239670
H	-2.440568526	-4.706186732	-1.123358092
H	-2.949317166	-2.595613931	0.032455973
H	-0.176899548	-0.538642871	-2.507909627
H	-2.103747423	-1.415543728	2.158639821
H	-3.953423459	-1.382552220	3.786852393
H	-5.958236152	0.025226813	3.369839962
H	-6.076336287	1.408039639	1.308304416
H	-4.210071050	1.396788891	-0.302046700
H	-2.105778214	0.724986360	-3.024541751
H	-1.057080895	2.394137901	0.779438102
H	-1.707328957	2.905533432	-4.091730525
H	-0.935235886	4.841348079	-2.740633083
H	-0.626694759	4.572780602	-0.285455928

3_^{t}Bu$_3$P/BPh$_3$

Total number of atoms = 76

P	-2.097253072	-0.043774168	-0.461297913
C	-2.398823027	-1.822777662	-1.000428926
C	-1.819863230	-2.034676331	-2.412575300
C	-1.619324536	-2.779818529	-0.075478967
C	-3.894135807	-2.179340956	-0.998498065
C	-2.936805543	0.421261614	1.158615161
C	-2.893642073	-0.758431325	2.147570338
C	-4.408316412	0.815558787	0.943693859
C	-2.147100905	1.581127106	1.805260189
C	-2.401090477	1.208512255	-1.843289965
C	-2.354285311	2.641543113	-1.279783009
C	-1.251702814	1.095265387	-2.871653795
C	-3.754794316	0.993359920	-2.538692626
B	1.750534370	0.017681774	-0.005304541
C	3.194343405	0.003799492	-0.752272514
C	4.347975507	0.540746206	-0.159560334
C	5.592032227	0.493016510	-0.784051800
C	5.725183108	-0.100367946	-2.037998837
C	4.599531526	-0.637338689	-2.656027651
C	3.360718946	-0.577204036	-2.018742467
C	1.481503059	1.448215921	0.729637937
C	1.728442310	1.708056216	2.088446662
C	1.483854711	2.952997026	2.669905990
C	0.992484434	4.004003689	1.900398292
C	0.781210702	3.797637941	0.538520086
C	1.025157864	2.545099674	-0.021652849
C	1.523816295	-1.302972418	0.935022087
C	2.053279839	-2.549198113	0.549448310
C	1.777612437	-3.727180950	1.238860841
C	0.962596739	-3.708048048	2.370535437
C	0.441658570	-2.491478385	2.798159778
C	0.717779715	-1.321919140	2.086273205
H	-0.702627504	0.025978514	-0.243145755
H	-1.868525305	-3.107346971	-2.629883217
H	-0.768605404	-1.735940589	-2.472254676
H	-2.389356014	-1.523217902	-3.191128364
H	-1.752932040	-3.794090762	-0.469204302
H	-1.969821133	-2.784273744	0.954201838
H	-0.547936330	-2.562662974	-0.068019645

H	-4.004410044	-3.196608241	-1.391355053
H	-4.492419158	-1.516830116	-1.630739170
H	-4.322125878	-2.174843221	0.007154340
H	-3.280891166	-0.395912885	3.106483714
H	-1.878851411	-1.123876130	2.315794394
H	-3.528211256	-1.592220868	1.838982819
H	-4.857643461	1.007639179	1.924610642
H	-4.988078812	0.018159700	0.467914217
H	-4.523081849	1.726805486	0.353160658
H	-2.563758571	1.749782341	2.804887999
H	-2.223997949	2.520247469	1.259926351
H	-1.083267881	1.351437269	1.919043224
H	-2.417026748	3.332006616	-2.128347269
H	-1.419290058	2.847056277	-0.754036711
H	-3.193715288	2.869397083	-0.620394621
H	-1.281682437	1.984855248	-3.510620285
H	-1.348750060	0.228008858	-3.523632033
H	-0.267772131	1.054845752	-2.395572648
H	-3.880083591	1.778143074	-3.293572253
H	-4.598960290	1.063329629	-1.846274915
H	-3.811948221	0.034140725	-3.058409264
H	0.907729577	-0.080231362	-0.924000500
H	-0.178334488	-2.448746919	3.692237144
H	0.753645274	-4.623886977	2.917012577
H	2.209155703	-4.665338708	0.897509497
H	2.702218839	-2.591442265	-0.322600403
H	0.296441796	-0.388646295	2.453953343
H	2.488263317	-1.001946192	-2.516019598
H	4.685971573	-1.098623126	-3.637512220
H	6.694283575	-0.139118723	-2.528743442
H	6.462042872	0.923539481	-0.293310252
H	4.265664205	1.020072923	0.814648714
H	2.127385337	0.913237125	2.714817363
H	0.881913095	2.413128169	-1.093537799
H	1.684256994	3.103846137	3.728092585
H	0.801136655	4.975084580	2.349072134
H	0.434338462	4.616576989	-0.089044152

TS13_PB[b]

Total number of atoms = 55

C	-0.211363506	-0.508035182	-0.891567771
P	-1.647622472	-0.374178294	0.241829993
C	-2.863595551	0.940750053	-0.328221793

C	-3.728343002	0.491279169	-1.513145071
C	-3.753967059	1.335788108	0.863417010
C	-2.045470203	2.179283238	-0.738274687
C	-2.382548236	-2.099678121	0.366005849
C	-2.680544559	-2.755093930	-0.990394232
C	-3.654834374	-2.093504488	1.225291833
C	-1.300604346	-2.923107225	1.097016926
B	1.081943515	-0.073353814	0.035515669
C	1.260903254	1.521907067	0.122935863
C	1.083821479	2.259543795	1.300311965
C	1.570127268	2.247257305	-1.038608480
C	1.188542634	3.651146730	1.321501223
C	1.680018894	3.634117533	-1.031543861
C	1.482019562	4.344478923	0.152049238
C	2.428100692	-0.938945183	-0.058477390
C	3.615315319	-0.458535672	0.520518302
C	2.490234888	-2.204670584	-0.660571162
C	4.793173303	-1.199037499	0.507279289
C	3.665117886	-2.953898680	-0.686604379
C	4.822922380	-2.453003180	-0.099490656
H	-0.322224677	0.154216639	-1.755410948
H	-0.147040014	-1.526788545	-1.283921332
H	0.635248217	-0.370296460	1.330431037
H	-0.343605947	-0.224826660	1.328224909
H	-4.319123036	1.343218610	-1.873093674
H	-3.117616413	0.132009335	-2.348623064
H	-4.432104093	-0.298400129	-1.232093969
H	-3.152009637	1.684493779	1.709318361
H	-4.414914752	2.157140811	0.560019452
H	-4.387861234	0.515034820	1.208683676
H	-2.743150262	2.994817530	-0.965300357
H	-1.373258448	2.517858023	0.055934839
H	-1.440522084	2.003259071	-1.631790523
H	-3.018888013	-3.785599768	-0.823157287
H	-3.467933783	-2.233640935	-1.539927719
H	-1.793760728	-2.801991315	-1.629357229
H	-4.496315568	-1.619860751	0.710019461
H	-3.946146392	-3.128351509	1.443468732
H	-3.500519682	-1.582533796	2.182368134
H	-0.344923219	-2.931758253	0.561699155
H	-1.116048470	-2.536694930	2.105143286
H	-1.638971513	-3.962374710	1.190699416
H	1.563915360	5.427812993	0.161400022
H	1.920089285	4.164050542	-1.949754921
H	1.039707882	4.190910080	2.253186029
H	0.853401980	1.734729716	2.226497204
H	1.728170218	1.711448542	-1.973797099

H	1.604188751	-2.623928753	-1.132914706
H	3.676617585	-3.928115596	-1.168595105
H	5.742473438	-3.031697129	-0.117831556
H	5.692083193	-0.795174577	0.965799699
H	3.611501345	0.522223684	0.991079770

3PB[b]

Total number of atoms = 55

C	-0.015519019	-0.749427818	0.625324127
P	-1.627812609	-0.425938531	-0.065784159
C	-2.407361293	-1.962216008	-0.773659351
C	-3.052263953	-2.806122076	0.335266975
C	-3.450104201	-1.580323017	-1.838132161
C	-1.295069763	-2.779018186	-1.460414858
C	-2.689681006	0.596377669	1.070450124
C	-2.786422738	-0.046814794	2.462353208
C	-4.092691114	0.818456777	0.489373218
C	-1.971170318	1.957124558	1.184612812
B	1.150063094	-0.274947055	-0.503852562
C	2.602103610	-0.833221207	-0.062572215
C	3.602275884	-1.021606198	-1.031044699
C	2.965189402	-1.110578965	1.263505667
C	4.883674630	-1.452754280	-0.701744144
C	4.244948323	-1.544319629	1.611070846
C	5.212332536	-1.717442070	0.627200425
C	1.086761629	1.349283127	-0.589610209
C	0.508467226	2.022145324	-1.677123762
C	1.525025840	2.155655057	0.474649584
C	0.333890959	3.407930593	-1.692365171
C	1.363482549	3.538464795	0.475219000
C	0.752373815	4.172232169	-0.606953610
H	0.060309702	-1.814304194	0.870833431
H	0.086702630	-0.183114571	1.557327238
H	0.832012440	-0.738625553	-1.600364643
H	-1.479824298	0.417241013	-1.175186349
H	-3.385931361	-3.758287424	-0.092659493
H	-2.344284315	-3.035065510	1.139482507
H	-3.928735569	-2.316328926	0.770158618
H	-3.004523636	-0.981341638	-2.639695957
H	-3.841222245	-2.498653131	-2.291128957
H	-4.299340273	-1.030632227	-1.426756216
H	-1.757075046	-3.657370672	-1.926294965
H	-0.780725430	-2.204394968	-2.234816428
H	-0.536905445	-3.129826913	-0.755933790
H	-3.339080745	0.629859756	3.124322393

H	-3.317601794	-1.002520582	2.447669859
H	-1.799066918	-0.209372649	2.905207178
H	-4.687494730	-0.100036837	0.479478890
H	-4.622986646	1.543930890	1.117014461
H	-4.056700823	1.227467079	-0.526550055
H	-0.972953511	1.868221642	1.620988533
H	-1.855603750	2.452488836	0.214882587
H	-2.566888277	2.609082962	1.834198630
H	6.210947856	-2.056868093	0.889717699
H	4.484696265	-1.747019698	2.652461792
H	5.629510341	-1.586159156	-1.481995315
H	3.361983425	-0.820649650	-2.073881605
H	2.231351556	-0.985071966	2.059828796
H	2.012399498	1.680103732	1.325703105
H	1.717048145	4.127148495	1.318489820
H	0.621617179	5.251045491	-0.610414835
H	-0.121920188	3.889529692	-2.554582610
H	0.195701676	1.440383106	-2.543914010

TS13_PB[c]

Total number of atoms = 56

C	0.188185537	0.495294411	0.710633000
P	1.669791046	0.308216189	-0.342970391
C	2.537807922	1.974858904	-0.462531654
C	3.409835011	2.323913139	0.749349272
C	3.381519237	1.997047084	-1.749821283
C	1.426245254	3.032505320	-0.601282949
C	2.776854736	-1.080234940	0.286709817
C	3.028004257	-0.997905148	1.799214839
C	4.112178178	-1.079687660	-0.472107756
C	2.038149256	-2.395448027	-0.019737400
B	-1.103078426	0.086396358	-0.188234569
C	-2.421087700	0.987545916	-0.079726594
C	-2.359916278	2.362189035	0.200611186
C	-3.696428422	0.438291414	-0.285776169
C	-3.505037637	3.150535032	0.269930258
C	-4.849708748	1.216415984	-0.215914301
C	-4.757365737	2.577620220	0.062037549
C	-1.321184812	-1.507258791	-0.228095612
C	-1.296871293	-2.260901848	-1.407569449
C	-1.536731892	-2.203735195	0.970933674
C	-1.462944710	-3.645496411	-1.396630889
C	-1.710411990	-3.584449229	0.994783226
C	-1.666796830	-4.313126630	-0.193102226
C	0.171724904	0.886332369	1.989681236

H	-0.626832408	0.340461824	-1.479343043
H	0.347620668	0.189469555	-1.439748554
H	3.801599609	3.342506578	0.631738435
H	2.837595529	2.295881088	1.682104900
H	4.267954197	1.652494208	0.848093234
H	2.767162367	1.783393479	-2.631233364
H	3.816929814	2.996051422	-1.877366630
H	4.205527298	1.280163519	-1.727845324
H	1.882574266	3.996936964	-0.855764687
H	0.710147644	2.780757691	-1.391933200
H	0.872269781	3.152497115	0.332513191
H	3.665536513	-1.839097248	2.100190819
H	3.535731395	-0.074933442	2.093872711
H	2.090123322	-1.072284685	2.356145061
H	4.738040875	-0.219761072	-0.214968915
H	4.671648408	-1.983642718	-0.201958189
H	3.965459775	-1.094317557	-1.557897300
H	1.081988759	-2.463131082	0.505451629
H	1.840733871	-2.513748895	-1.089866459
H	2.664533552	-3.235146053	0.306991390
H	-5.655198762	3.187331911	0.118148849
H	-5.822317304	0.758456218	-0.376077258
H	-3.420936552	4.212251185	0.487718879
H	-1.392002485	2.826521400	0.371198434
H	-3.786822744	-0.623915982	-0.499864506
H	-1.553561684	-1.651323827	1.909020522
H	-1.874146868	-4.094530946	1.940492530
H	-1.794852050	-5.391936274	-0.178908896
H	-1.431934055	-4.202017748	-2.329837413
H	-1.139388483	-1.754933921	-2.358901322
H	1.064350967	1.105417595	2.573458248
H	-0.777118200	1.013075298	2.510578315

3PB[c]

Total number of atoms = 56

C	-0.053166101	-0.641667520	0.517096113
B	-1.184476607	-0.084058354	-0.553819699
P	1.605196611	-0.414080587	-0.124568701
C	2.746898322	0.615495791	0.931461716
C	4.120881738	0.753587715	0.258781190
C	2.084890857	2.003393191	1.024469484
C	2.901948691	0.045813151	2.349075764
C	2.306003032	-2.019344835	-0.776848817
C	3.009372025	-2.804042908	0.339201799
C	1.126010407	-2.851359592	-1.314459010

C	3.274944402	-1.733490622	-1.936075558
C	-1.035019268	1.536042168	-0.576294185
C	-1.292698966	2.317208165	0.563331893
C	-0.565564274	2.224070039	-1.705441214
C	-1.092652660	3.695046576	0.582196593
C	-0.345812254	3.603030835	-1.700449947
C	-0.606109022	4.344892850	-0.551392692
C	-2.648296417	-0.673284169	-0.186977051
C	-3.754782479	0.115886614	0.156286008
C	-2.865967576	-2.062157678	-0.220599441
C	-4.998339157	-0.441174533	0.459890966
C	-4.097978846	-2.633492352	0.080700507
C	-5.175572716	-1.820174328	0.428716467
C	-0.232774872	-1.257917500	1.693947145
H	4.713154215	1.482238626	0.824090263
H	4.039917487	1.123317081	-0.769542947
H	4.679257931	-0.187273137	0.253116574
H	2.740015158	2.659788253	1.609403166
H	1.114147057	1.956804453	1.522317973
H	1.925726497	2.463875428	0.043648925
H	3.566381655	0.707354690	2.917038221
H	3.341680522	-0.955264960	2.362846654
H	1.942080987	0.017255822	2.870859294
H	3.914949047	-2.303073180	0.693933629
H	3.306085971	-3.783567342	-0.052881649
H	2.344806513	-2.979360624	1.192358280
H	1.528826088	-3.766026527	-1.765195632
H	0.553579018	-2.312083181	-2.074537869
H	0.433965681	-3.132087081	-0.516821177
H	4.152969719	-1.160967151	-1.628503736
H	2.776881422	-1.195747844	-2.750042935
H	3.629684978	-2.688671178	-2.340365067
H	-1.649483418	1.824120427	1.467096506
H	-0.375963022	1.660289006	-2.618420947
H	-1.308450570	4.263479307	1.483818753
H	0.020753340	4.098231724	-2.596634867
H	-0.441239012	5.419003625	-0.541045900
H	-3.649102985	1.197926439	0.176656039
H	-2.039937065	-2.715390991	-0.501144861
H	-5.831405813	0.208343448	0.718778632
H	-4.223266496	-3.713110758	0.038094267
H	-6.142154423	-2.258194949	0.663338694
H	0.564268791	-1.615893839	2.344136495
H	-1.248096324	-1.447398676	2.037460553
H	1.459165339	0.379213134	-1.268168833
H	-0.832053541	-0.513795771	-1.657763874

TS13_PB[d]

Total number of atoms = 69

C	0.811768827	-0.835432130	0.852378182
B	2.133000217	-0.527876781	-0.075721209
C	3.336213579	-1.581085677	-0.038931275
C	3.396168613	-2.654217744	0.859983969
C	4.401607062	-1.450896377	-0.946016899
C	4.460380502	-3.556703272	0.856068223
C	5.459427720	-2.352790624	-0.970930441
C	5.492661729	-3.412406743	-0.065116332
C	2.553197537	1.022764492	-0.108727480
C	1.993797482	1.972869844	-0.973946855
C	3.458204853	1.497732103	0.855255730
C	2.281569803	3.332072256	-0.860011258
C	3.755612805	2.852406331	0.977511196
C	3.158606167	3.778278943	0.123549821
P	-0.616090496	-0.323637923	-0.175304150
C	-1.224893680	1.394535767	-0.075925857
C	-2.023664962	1.784126267	-1.177529534
C	-0.898212684	2.343944785	0.914998220
C	-2.488832379	3.095281460	-1.255346811
C	-1.381603596	3.645534866	0.782148075
C	-2.177528551	4.044421107	-0.286966620
C	-2.003514076	-1.493183191	0.068670676
C	-3.040889743	-1.313759771	1.008100008
C	-1.994977949	-2.639403846	-0.755209145
C	-4.055640389	-2.266382095	1.080091998
C	-3.029908008	-3.567972091	-0.639839807
C	-4.074436846	-3.394893937	0.262547754
C	-0.898350894	-2.904413847	-1.762565241
C	-5.201470231	-4.391139935	0.357490744
C	-3.089900545	-0.145476681	1.960649607
C	-0.040185835	2.045212451	2.117163695
C	-2.703569971	5.453506018	-0.380550255
C	-2.394868842	0.831527079	-2.290777308
H	0.652738729	-1.915065787	0.980125245
H	0.866341496	-0.396872643	1.849043283
H	2.602668093	-2.789149248	1.592432952
H	4.395309882	-0.619890437	-1.649182803
H	4.480736274	-4.372518879	1.574026562
H	6.261665608	-2.229521943	-1.693829493
H	6.318875939	-4.117985668	-0.076236355
H	1.304062888	1.651744248	-1.752817769
H	3.934580906	0.787045095	1.528297805
H	1.815676488	4.040831244	-1.539298183
H	4.456951906	3.186556100	1.737652286

H	3.383222314	4.836913941	0.219597321
H	-3.103307488	3.384070415	-2.105417315
H	-1.118968500	4.375229790	1.544772429
H	-4.851777867	-2.128855454	1.809153418
H	-3.016400744	-4.451165213	-1.274761490
H	-0.871287195	-2.131385057	-2.538735357
H	0.095473054	-2.932831096	-1.300101781
H	-1.056687574	-3.868457181	-2.253787963
H	-4.952666224	-5.328374020	-0.148672219
H	-5.439589509	-4.619950630	1.401552865
H	-6.111965563	-3.993006809	-0.105842030
H	-2.133668932	-0.013934471	2.476025041
H	-3.313168640	0.794245659	1.446420534
H	-3.857671829	-0.305723092	2.722819684
H	-0.386128712	1.161761996	2.661657882
H	1.001421609	1.878165793	1.826625610
H	-0.058360010	2.887716074	2.813540386
H	-2.893891379	5.738588114	-1.419800661
H	-3.648268621	5.554489659	0.167333820
H	-1.996736817	6.171699168	0.046590525
H	-1.504538610	0.379799061	-2.744066553
H	-3.028671120	0.011057094	-1.935389475
H	-2.941171121	1.358524425	-3.077798844
H	0.662635789	-0.566547538	-1.318117797
H	1.608316602	-0.727584799	-1.384943947

3PB[d]

Total number of atoms = 69

C	0.755451222	-1.278423739	0.558385872
B	2.023198519	-1.117788076	-0.544933028
C	3.360918837	-1.824182463	0.029409891
C	3.653072437	-1.991442644	1.390677087
C	4.342296597	-2.269989034	-0.872663293
C	4.846777102	-2.564178801	1.833400515
C	5.538459405	-2.839707173	-0.448807882
C	5.797254052	-2.991456293	0.912969790
C	2.229954455	0.466032254	-0.867304217
C	1.724913562	1.060118620	-2.035099016
C	2.818415075	1.338826266	0.063260172
C	1.730382421	2.441190018	-2.233845562
C	2.831870136	2.718903515	-0.117168916
C	2.267241473	3.280110270	-1.262094151
P	-0.661142753	-0.407715343	-0.109968202
C	-0.864067167	1.365808615	0.220553013
C	-1.518803581	2.104386590	-0.791891589

C	-0.379881555	2.020232921	1.370749012
C	-1.664566540	3.479748750	-0.635294562
C	-0.550007068	3.399909270	1.470952301
C	-1.174629845	4.149894052	0.480767248
C	-2.230253789	-1.329476492	0.020699155
C	-3.213168147	-1.071627056	0.996546857
C	-2.422718962	-2.363301974	-0.926067799
C	-4.377946357	-1.839201998	0.991992098
C	-3.604246884	-3.099776724	-0.882918971
C	-4.595516390	-2.852859079	0.063562193
C	-1.411657452	-2.701736119	-1.999547530
C	-5.850747021	-3.685355176	0.097520144
C	-3.073159713	-0.005231203	2.055379100
C	0.333412989	1.337670999	2.511337520
C	-1.286338311	5.646731718	0.598260242
C	-2.048117834	1.481745359	-2.062432061
H	0.452941518	-2.327229867	0.666490674
H	0.995338582	-0.903372509	1.552337824
H	2.931857511	-1.670788952	2.142204023
H	4.155429249	-2.159025253	-1.939513616
H	5.030568386	-2.679727298	2.899192992
H	6.271409662	-3.171345315	-1.180588569
H	6.727577699	-3.440570437	1.250608089
H	1.313657047	0.414061994	-2.811570160
H	3.280318634	0.915558799	0.955179461
H	1.315637270	2.862180188	-3.147180003
H	3.283956017	3.361766097	0.634685168
H	2.267636779	4.357611260	-1.404372839
H	-2.165944126	4.044571403	-1.417706670
H	-0.170525400	3.904989100	2.355950832
H	-5.136844278	-1.638212663	1.744652610
H	-3.752886855	-3.892566130	-1.612585806
H	-1.394825845	-1.938640866	-2.788450136
H	-0.387774159	-2.793852187	-1.622140329
H	-1.672634219	-3.650943510	-2.474081935
H	-6.208009495	-3.905427010	-0.913384209
H	-5.665192534	-4.644068597	0.596001477
H	-6.653539222	-3.178244037	0.640688405
H	-2.125819174	-0.090479461	2.594967044
H	-3.120390533	1.001552405	1.629536790
H	-3.874576097	-0.097260337	2.793122282
H	-0.132964663	0.396678342	2.813528194
H	1.371835497	1.126824588	2.236790977
H	0.347323812	1.990404187	3.388180639
H	-2.168011006	6.026605344	0.073345536
H	-1.345414234	5.963482730	1.643940591
H	-0.405061241	6.127015727	0.156466739

H	-1.220933515	1.204807465	-2.728786758
H	-2.653886162	0.587536830	-1.880004133
H	-2.675037848	2.196938409	-2.600594164
H	-0.450812308	-0.411927610	-1.485529223
H	1.649185148	-1.684411725	-1.574913642

TS13_PB[e]

Total number of atoms = 73

C	1.140269028	-0.649140050	-0.936235109
B	2.486891045	-0.892268766	0.018804500
P	-0.191871681	-0.131389305	0.207327296
C	2.727565179	-2.507406285	0.281127051
C	3.728919223	0.169601434	-0.227326263
C	-1.817720836	-0.989468448	0.091449784
C	-4.362320898	-2.234102335	0.204045137
C	-2.686553184	-0.769263917	1.190506177
C	-2.228257982	-1.867686162	-0.936799900
C	-3.490600556	-2.463345320	-0.851956036
C	-3.935015953	-1.382973715	1.219182855
C	-0.486325747	1.670669771	0.003262744
C	-0.897731894	4.452525203	-0.257537790
C	-0.037655184	2.553866179	1.012118721
C	-1.125843234	2.193372539	-1.141287673
C	-1.323065751	3.569401023	-1.245336566
C	-0.257866379	3.923015287	0.858583793
C	4.522813281	0.451266550	1.063442180
C	3.216815833	1.536675275	-0.725820491
C	4.712870116	-0.351620249	-1.291981740
C	3.012496058	-3.267333736	-1.030999820
C	1.457914640	-3.132740096	0.899833907
C	3.878796844	-2.808481269	1.254199577
C	-2.307785967	0.099476402	2.365819560
C	-1.401432118	-2.242106021	-2.145797050
C	0.701943924	2.105568978	2.252365905
C	-1.587904038	1.323938898	-2.283134981
C	-5.724707431	-2.874994389	0.257934801
C	-1.089141031	5.939397874	-0.408298337
H	-3.798821250	-3.134703353	-1.650315269
H	-4.590475053	-1.196962512	2.067352529
H	-1.817243746	3.962566749	-2.131147748
H	0.088980671	4.598877125	1.637029751
H	5.337514917	1.164631797	0.869485003
H	4.971557800	-0.450049976	1.487596664
H	3.880506070	0.891866608	1.837336178
H	2.808719118	1.482607446	-1.741832256

H	4.035666974	2.270008095	-0.750863141
H	2.430876019	1.948700012	-0.082079169
H	4.199412705	-0.600871667	-2.229916153
H	5.244679714	-1.247482659	-0.954631519
H	5.471360450	0.410660901	-1.524999091
H	2.205027906	-3.151637033	-1.765646200
H	3.114890522	-4.345070479	-0.835986522
H	3.938095789	-2.932848453	-1.508387743
H	0.572844421	-3.028286562	0.258221897
H	1.218433778	-2.679072288	1.870775672
H	1.596844997	-4.210292325	1.069475993
H	4.849634356	-2.507524810	0.846661684
H	3.937713903	-3.886527363	1.466001136
H	3.740661930	-2.291411797	2.212083005
H	-3.088188478	0.067441658	3.130636697
H	-2.168105274	1.146987327	2.078011995
H	-1.376248023	-0.248276308	2.826295595
H	-2.037153678	-2.720129851	-2.896068953
H	-0.616111970	-2.960254900	-1.883960493
H	-0.923043536	-1.382702115	-2.616942982
H	1.678348394	1.675764454	2.006141816
H	0.150567436	1.351273478	2.819930993
H	0.877756833	2.957126136	2.915010912
H	-2.000561517	1.935563193	-3.089894486
H	-2.359016672	0.613399843	-1.970491706
H	-0.754391546	0.748637762	-2.699489514
H	2.047837926	-0.506967569	1.287034279
H	1.044535231	-0.396054119	1.286162831
H	-5.842734963	-3.632216259	-0.522523855
H	-6.513599793	-2.126020483	0.121813016
H	-5.895331559	-3.356320723	1.226851275
H	-0.213581071	6.394417173	-0.886674916
H	-1.221750887	6.424672604	0.563609849
H	-1.961110187	6.169992784	-1.027934461
H	0.866419830	-1.580688567	-1.424545050
H	1.269345903	0.100679823	-1.721282032

3PB[e]

Total number of atoms = 73

C	0.842080995	-1.268114381	-0.584259150
B	2.376303429	-0.961481509	0.083628847
P	-0.392047784	-0.351437080	0.313715824
C	2.806067412	-2.234115448	1.078663162
C	3.360713389	-0.476103819	-1.174419931
C	-2.166332965	-0.775898923	0.090108990

C	-4.928738438	-1.343694160	-0.123831949
C	-3.076724154	-0.302899108	1.066701407
C	-2.650496957	-1.553641383	-0.987810166
C	-4.020465163	-1.811371834	-1.066611558
C	-4.433014241	-0.591671777	0.935822441
C	-0.170248079	1.449164809	0.187920002
C	0.251608657	4.219586769	-0.063451040
C	0.374516995	2.176595623	1.270865810
C	-0.508298305	2.110098315	-1.011922147
C	-0.289194603	3.480643704	-1.112149250
C	0.569592682	3.549372996	1.112606104
C	4.819698067	-0.281140960	-0.730786230
C	2.873011875	0.898262844	-1.674454932
C	3.377702611	-1.421814597	-2.391181913
C	3.184777859	-3.514228801	0.316104877
C	1.651224098	-2.595120431	2.036295210
C	3.981589678	-1.860108125	2.001515359
C	-2.653016602	0.499535556	2.273618225
C	-1.794486775	-2.147072319	-2.084240070
C	0.776220774	1.567791465	2.594179184
C	-1.077509609	1.396799363	-2.213820616
C	-6.395815259	-1.667713106	-0.228677137
C	0.463586507	5.704815826	-0.198313396
H	-4.388203680	-2.403143123	-1.901485295
H	-5.122816987	-0.217870182	1.688913481
H	-0.538241003	3.983837161	-2.043478153
H	0.997059968	4.109971304	1.940181940
H	5.408158195	0.218399177	-1.516780263
H	5.311735319	-1.238296294	-0.524966670
H	4.883886533	0.332643303	0.176172736
H	1.851713981	0.858357802	-2.075936256
H	3.514187552	1.278195647	-2.485454811
H	2.872418784	1.639800749	-0.866340591
H	2.380452547	-1.558234512	-2.832728927
H	3.755496068	-2.416786772	-2.134850257
H	4.022023574	-1.023835160	-3.190538173
H	2.409619720	-3.810007443	-0.405152420
H	3.336460276	-4.363927611	1.000512366
H	4.117213070	-3.380926770	-0.243705672
H	0.749336715	-2.950409700	1.517704872
H	1.370936907	-1.734774495	2.661914644
H	1.947161742	-3.401680833	2.724070621
H	4.914728075	-1.709464414	1.454341393
H	4.167966029	-2.650584356	2.746158162
H	3.769640933	-0.931439295	2.547525770
H	-3.526269441	0.778701350	2.868298051
H	-2.134241259	1.422194123	1.996550885

H	-1.990106927	-0.079570438	2.927639764
H	-2.433684483	-2.595247471	-2.849121343
H	-1.135769992	-2.933184824	-1.705720974
H	-1.164952050	-1.405309503	-2.578972796
H	1.546756632	0.803227375	2.455119036
H	-0.070361123	1.111431792	3.118140245
H	1.182001545	2.339913456	3.252600930
H	-1.272999971	2.108543238	-3.019653029
H	-2.018988233	0.887641775	-1.985522281
H	-0.372934977	0.655720239	-2.606985934
H	2.283738238	0.020382782	0.822207605
H	-0.194035781	-0.624122710	1.663696578
H	-7.012401980	-0.868702033	0.193877919
H	-6.626397257	-2.588588440	0.320166662
H	-6.696863525	-1.820228489	-1.269315962
H	-0.482918187	6.243735504	-0.071919921
H	0.857516279	5.958759031	-1.187382365
H	1.164054608	6.078296570	0.554008938
H	0.574643412	-2.328507178	-0.537745820
H	0.784176966	-0.963695279	-1.630753971

TS13_PB[f]

Total number of atoms = 74

C	-1.326204977	0.087779650	2.172743653
C	-1.305802833	-0.141545232	0.856659710
B	-2.621740659	-0.381130579	-0.102438709
P	0.180143441	-0.006891880	-0.210164636
C	-3.004535389	-1.980232299	-0.279180114
C	-3.783654323	0.797521889	0.017568487
C	1.494651986	-1.288297467	-0.131339137
C	3.612488810	-3.155909687	-0.316989936
C	2.386716648	-1.262130659	-1.233456362
C	1.652521238	-2.282080766	0.858412128
C	2.707165713	-3.191274623	0.735795186
C	3.429404400	-2.182187616	-1.295125131
C	0.973552476	1.634674580	0.003637790
C	2.095673516	4.213614213	0.234272708
C	0.618872814	2.649832904	-0.914379231
C	1.912081657	1.911638011	1.019280147
C	2.451391598	3.194495417	1.112419406
C	1.183319006	3.917291730	-0.774058673
C	-4.433737054	1.079388341	-1.352040774
C	-3.211787503	2.143063041	0.511441207
C	-4.901103318	0.412390625	1.008131568
C	-3.369299603	-2.607422796	1.080663282

C	-1.799740248	-2.765856840	-0.836620735
C	-4.164501681	-2.238331793	-1.255767200
C	2.250245408	-0.277473945	-2.371464587
C	0.767567852	-2.438168745	2.070906148
C	-0.317961465	2.422949858	-2.079361016
C	2.398098944	0.877116593	2.003748967
C	4.752576161	-4.136709253	-0.409235295
C	2.665067672	5.600813178	0.382038422
H	-0.447621704	0.307986860	2.774684576
H	2.820624759	-3.955065331	1.501813989
H	4.111088672	-2.145933805	-2.142382202
H	3.174104872	3.402129824	1.898666470
H	0.903821917	4.695128679	-1.481140081
H	-4.899736993	0.192862172	-1.788415241
H	-3.693010298	1.449703829	-2.073136624
H	-5.213296136	1.849800763	-1.258757738
H	-2.882482333	2.094778471	1.553609267
H	-3.977030050	2.929705411	0.442387371
H	-2.347714949	2.474080929	-0.075501107
H	-4.503385278	0.190396590	2.006422179
H	-5.469612684	-0.461967212	0.676883800
H	-5.614839967	1.241964798	1.120346212
H	-4.282289126	-2.175831121	1.503007362
H	-2.569813631	-2.470207401	1.818471966
H	-3.537078172	-3.688974366	0.972820603
H	-0.925845666	-2.726675855	-0.178791243
H	-1.491341962	-2.389490764	-1.821173965
H	-2.051386164	-3.829067658	-0.960456250
H	-5.108519815	-1.804770324	-0.911932915
H	-4.329815793	-3.319036245	-1.377258587
H	-3.948640159	-1.826704346	-2.249668442
H	2.984979605	-0.494608365	-3.151350822
H	2.406495697	0.756674960	-2.045550183
H	1.254419767	-0.334412812	-2.825575147
H	0.996014907	-3.378945505	2.578888429
H	-0.293926168	-2.439585907	1.823638823
H	0.924173573	-1.632358298	2.795614336
H	-1.305225442	2.070888955	-1.768152340
H	0.084785417	1.681571854	-2.778377781
H	-0.464996237	3.355288796	-2.631134567
H	2.921155324	1.357090832	2.835531861
H	3.087452350	0.168464782	1.532228569
H	1.577223595	0.293594129	2.424612363
H	-2.094563853	-0.109906123	-1.369456581
H	-1.107917205	-0.089815762	-1.303122673
H	5.715947435	-3.630636586	-0.277004765
H	4.773601263	-4.626412310	-1.388720482

H	4.675010153	-4.913844624	0.356552414
H	2.004036162	6.227022295	0.993206316
H	2.776909077	6.091641885	-0.589736566
H	3.644217549	5.580668997	0.869970422
H	-2.267825674	0.072146122	2.719898394

3PB[f]

Total number of atoms = 74

C	1.289573916	-0.008524717	-2.029887787
C	1.306619295	-0.230366712	-0.709106758
B	2.633673701	-0.498888702	0.269421878
P	-0.241598206	-0.022882690	0.198223609
C	2.881561698	-2.150567517	0.371467243
C	3.902106001	0.526232186	-0.126639304
C	-1.639678139	-1.204592567	0.139874858
C	-3.914102327	-2.869823700	0.221243131
C	-2.577501330	-1.081024271	1.196440547
C	-1.826437027	-2.188772933	-0.852332710
C	-2.963929108	-2.995706759	-0.784703910
C	-3.697071996	-1.908479883	1.204965536
C	-0.876556305	1.678699762	0.038590831
C	-1.689304162	4.354976170	-0.230660125
C	-0.375704850	2.656498645	0.926131745
C	-1.789595618	2.034783399	-0.974746701
C	-2.174565398	3.369167277	-1.086607480
C	-0.795459570	3.976456613	0.766137079
C	4.742824572	0.787652230	1.140993281
C	3.408793893	1.916889712	-0.579694993
C	4.861984818	0.015872494	-1.217396433
C	3.097175702	-2.844151519	-0.984711136
C	1.652770676	-2.806305881	1.033886634
C	4.079732119	-2.496752375	1.270745100
C	-2.421903913	-0.107526087	2.343409729
C	-0.879222299	-2.441818055	-1.998153042
C	0.561011944	2.340330077	2.068601847
C	-2.402309431	1.042206751	-1.934451832
C	-5.124513026	-3.764802038	0.271505347
C	-2.141355895	5.785567284	-0.368053152
H	0.410085553	0.239388409	-2.621692017
H	-3.106071866	-3.752103594	-1.552739962
H	-4.419032305	-1.803278786	2.011632593
H	-2.873944957	3.647369454	-1.871760412
H	-0.405986655	4.731967707	1.444238097
H	5.587131465	1.460399739	0.921161624
H	5.158012168	-0.129619731	1.566917302

H	4.133904413	1.261670381	1.921382387
H	2.935327499	1.899745038	-1.566703392
H	4.248427434	2.626784055	-0.634775186
H	2.674552868	2.336605830	0.119947511
H	4.345089884	-0.211492554	-2.158711324
H	5.385107403	-0.894888939	-0.906801438
H	5.632162894	0.769348654	-1.445949355
H	2.288658023	-2.622377307	-1.692583964
H	3.142476831	-3.938384630	-0.869274179
H	4.031551702	-2.529329887	-1.459216706
H	0.741699939	-2.709653612	0.427807398
H	1.449701664	-2.360326782	2.016738331
H	1.804794566	-3.886302987	1.185103687
H	5.028508221	-2.163058984	0.837801895
H	4.158436128	-3.585477981	1.419679707
H	3.980413095	-2.030966901	2.259131947
H	-3.293205597	-0.158795206	3.000746339
H	-2.323584123	0.929058199	2.006782496
H	-1.542413459	-0.346162469	2.954278761
H	-1.163623858	-3.360488193	-2.517320278
H	0.154023740	-2.550406234	-1.666529548
H	-0.898200729	-1.633344001	-2.736007140
H	1.417929893	1.729561980	1.768764428
H	0.035989656	1.799565741	2.867849176
H	0.949728710	3.264284184	2.503873684
H	-2.863935002	1.565118724	-2.776147099
H	-3.175865550	0.440148784	-1.445501004
H	-1.668677208	0.347201118	-2.350030717
H	2.277984137	-0.153756626	1.405474009
H	0.144125006	-0.120039688	1.530835236
H	-6.025022099	-3.200104243	0.533887252
H	-4.995317864	-4.546133513	1.029657282
H	-5.297266561	-4.258030451	-0.689150086
H	-3.080058615	5.948520515	0.174869344
H	-2.318586914	6.046101124	-1.415981649
H	-1.399226466	6.480031609	0.036279629
H	2.220136079	-0.057369676	-2.589513494

TS13_PB[a]

Total number of atoms = 84

C	1.167182404	0.409966670	-1.110199926
C	0.870094096	-0.244990108	0.030867322
B	1.746574814	-0.931300952	1.274395707
P	-0.868691021	-0.076802180	0.599461723
C	1.746652381	-2.592499513	1.357325871

C	3.046500946	-0.040790294	1.829556880
C	-2.147170963	-1.155012407	-0.151060190
C	-4.310473490	-2.731713408	-1.055100249
C	-3.359773587	-1.192984794	0.574020755
C	-2.012125987	-1.936873436	-1.321673391
C	-3.097938109	-2.704691191	-1.739930335
C	-4.418507811	-1.968494566	0.100779013
C	-1.427402019	1.662858737	0.415232516
C	-2.126233996	4.396536371	0.294732252
C	-1.189211937	2.511682104	1.520121079
C	-2.053264821	2.184427294	-0.739020266
C	-2.384392058	3.539503930	-0.771113036
C	-1.537261931	3.858998486	1.434499690
C	3.034080839	0.025169861	3.374555950
C	3.019679620	1.425579284	1.351121477
C	4.419389706	-0.608653464	1.411190538
C	2.530931896	-3.243491889	0.203371096
C	0.315493872	-3.163207890	1.289654277
C	2.328449329	-3.125243415	2.680547337
C	-3.568519943	-0.420985489	1.856919501
C	-0.769417606	-1.989935373	-2.179385073
C	-0.602130447	2.012711543	2.819466052
C	-2.426671300	1.356593400	-1.946157132
C	2.437251655	0.524924121	-1.846817840
C	4.822064266	0.862251482	-3.287825174
C	2.693613146	1.714032826	-2.544865439
C	3.380040902	-0.502976486	-1.916163115
C	4.563410126	-0.335960442	-2.628564090
C	3.879667642	1.888396266	-3.246485533
C	-5.450953956	-3.586844490	-1.543426669
C	-2.458689425	5.863412925	0.205302160
H	0.377534065	0.986122001	-1.596281058
H	-2.992645756	-3.301473167	-2.643522267
H	-5.350268030	-1.981242112	0.661889469
H	-2.860498119	3.938430732	-1.664433970
H	-1.344249367	4.505235122	2.287778150
H	3.899082130	0.600343813	3.735698784
H	3.079891808	-0.959429869	3.845250340
H	2.131686000	0.525482608	3.748173375
H	3.231094198	1.514844316	0.283314122
H	3.784279731	2.010130715	1.883166256
H	2.053064448	1.910274269	1.530477808
H	4.539075716	-0.632684545	0.324439625
H	4.590335065	-1.619940260	1.792387709
H	5.224528627	0.026440972	1.809671228
H	2.068911130	-3.027403911	-0.767668030
H	2.540018760	-4.337879604	0.314487995

H	3.574157086	-2.911672896	0.168253845
H	-0.188299796	-2.935993241	0.347399811
H	-0.314933144	-2.787122892	2.106323870
H	0.334409095	-4.259038639	1.378690546
H	3.385427394	-2.880190245	2.814522915
H	2.244570530	-4.221466474	2.715318573
H	1.779435277	-2.730224013	3.544076130
H	-4.533992351	-0.675618400	2.302169907
H	-3.552727671	0.662548538	1.692466482
H	-2.789467125	-0.651578572	2.592563887
H	-0.888526072	-2.747306424	-2.958938477
H	0.126765536	-2.233812859	-1.606411951
H	-0.567575888	-1.035622128	-2.676221596
H	0.385244242	1.561844346	2.686271820
H	-1.245907320	1.255465939	3.282087413
H	-0.491103356	2.836336919	3.529860944
H	-2.692583187	2.008784266	-2.782673952
H	-3.284462391	0.709418655	-1.735311800
H	-1.613413439	0.708757284	-2.278902666
H	1.958996918	2.515423147	-2.513196857
H	3.180193466	-1.438867437	-1.412387320
H	5.285643654	-1.146258232	-2.666390995
H	4.068652068	2.824318489	-3.764027492
H	5.749199119	0.994144388	-3.837643273
H	0.853100440	-0.701621772	2.323907635
H	-0.065125603	-0.519444341	1.995550455
H	-5.243715347	-4.649079215	-1.368765513
H	-5.610055678	-3.457741733	-2.619211172
H	-6.384824147	-3.340734020	-1.029693636
H	-1.660008892	6.409349331	-0.311225033
H	-2.574619998	6.309019224	1.197811174
H	-3.384983304	6.029089407	-0.353865406

3PB[a]

Total number of atoms = 84

C	1.097069002	-0.463476760	1.028276796
C	0.893393426	0.183991620	-0.143770703
B	1.820671358	0.788037678	-1.429841451
P	-0.859101428	0.063381686	-0.580550593
C	1.881247286	2.462740751	-1.479549242
C	3.211677498	-0.113268604	-1.742989957
C	-2.085527282	1.235701888	0.097212487
C	-4.152601009	2.920624649	1.005479560
C	-3.301610023	1.320908397	-0.622224621
C	-1.895797844	2.015389994	1.258004608
C	-2.940084245	2.837607446	1.681504014

C	-4.310450910	2.155168135	-0.145898251
C	-1.507607831	-1.636402142	-0.423344754
C	-2.327481014	-4.324947486	-0.288063040
C	-1.233632255	-2.513638852	-1.496793210
C	-2.198565432	-2.102461746	0.716170837
C	-2.589292896	-3.440265335	0.755006788
C	-1.651428313	-3.840204680	-1.402854471
C	3.361579991	-0.233852503	-3.277449971
C	3.117536830	-1.567943873	-1.238657055
C	4.542633023	0.451300442	-1.210234689
C	2.596333003	3.142733588	-0.300582657
C	0.455432407	3.046319814	-1.521635589
C	2.555428590	2.953020812	-2.773914507
C	-3.568148540	0.562528349	-1.904067335
C	-0.636091567	2.027328359	2.090803257
C	-0.532402133	-2.075782832	-2.760887587
C	-2.562432946	-1.240683433	1.903725376
C	2.305376693	-0.569113845	1.861307309
C	4.531030040	-0.845557154	3.544454910
C	2.493826037	-1.735494964	2.616659988
C	3.232685798	0.467013713	1.989187868
C	4.337129739	0.329440408	2.823999162
C	3.602913051	-1.880357761	3.439615431
C	-5.248073410	3.838133645	1.481762282
C	-2.780941914	-5.759720639	-0.214384911
H	0.271592922	-1.016002001	1.485784974
H	-2.795726437	3.434994679	2.578382896
H	-5.246475878	2.212441019	-0.696689138
H	-3.111732012	-3.804608615	1.636725157
H	-1.432161146	-4.515326172	-2.226508439
H	4.262762548	-0.812665199	-3.535295872
H	3.445496911	0.736590566	-3.773087034
H	2.498370207	-0.749414625	-3.717404739
H	3.224571255	-1.644805478	-0.153850051
H	3.919687600	-2.178307124	-1.681471903
H	2.164395288	-2.040376282	-1.508631455
H	4.554893255	0.524846646	-0.119168907
H	4.760606761	1.445094941	-1.615598569
H	5.381315956	-0.202684760	-1.496902115
H	2.074035024	2.961767225	0.647932055
H	2.631516373	4.235368303	-0.434999221
H	3.628960942	2.796397687	-0.187366375
H	-0.097738775	2.870600881	-0.592530086
H	-0.126199278	2.622623617	-2.351965944
H	0.475028340	4.138076016	-1.663279751
H	3.618109305	2.696326273	-2.819369509
H	2.484898884	4.049307950	-2.856080582

H	2.069424908	2.522878235	-3.657997561
H	-4.601012211	0.718829883	-2.224497820
H	-3.416765251	-0.516439690	-1.795290727
H	-2.919821740	0.911925734	-2.717134386
H	-0.707029791	2.803760957	2.856635355
H	0.253566169	2.224232078	1.490003197
H	-0.463840187	1.075211097	2.603012069
H	0.378944156	-1.500521342	-2.572559494
H	-1.188608474	-1.448843239	-3.379725147
H	-0.254633146	-2.946548935	-3.359992983
H	-2.891516163	-1.870564113	2.734389642
H	-3.375014302	-0.547344033	1.664053921
H	-1.722412449	-0.642000844	2.264472179
H	1.768522187	-2.542268619	2.536548872
H	3.081701726	1.381969459	1.432450542
H	5.050517407	1.144105921	2.906788131
H	3.743388964	-2.799106433	4.001454368
H	5.396254358	-0.952486220	4.192041714
H	1.080589176	0.513930269	-2.385541299
H	-0.930046813	0.329176485	-1.943697083
H	-6.237025169	3.409097333	1.293205451
H	-5.199410976	4.799534534	0.957040296
H	-5.160235272	4.040965999	2.553057813
H	-3.842707015	-5.845096363	-0.474415240
H	-2.657549638	-6.164067854	0.795254832
H	-2.217060946	-6.392165896	-0.905924639

1PAl[b]

Total number of atoms = 53

C	-0.728060106	-0.421035659	-1.661681573
AL	0.869559141	0.170415249	-0.651490167
C	2.239791189	-1.180310269	-0.262318696
C	3.216849219	-0.959664728	0.724077636
C	2.308928942	-2.397330394	-0.961220207
C	4.194038024	-1.909953048	1.015069062
C	3.282335867	-3.353687506	-0.683339447
C	4.225473440	-3.111986038	0.312577216
C	1.230951053	2.057018454	-0.235618707
C	1.325442750	3.036384113	-1.238797817
C	1.386394410	2.492626133	1.092400867
C	1.560353009	4.376746046	-0.938707985
C	1.618408446	3.830606743	1.405286870
C	1.705748930	4.776778468	0.387318254
P	-1.472736480	-0.424180604	0.044328518
C	-2.145213008	-2.168795913	0.340011888

C	-2.989798926	-2.207059427	1.621529389
C	-2.954851178	-2.740667718	-0.831416010
C	-0.899960148	-3.048474421	0.554980856
C	-2.831554672	0.889107452	0.059177837
C	-3.184599971	1.214978639	1.521209649
C	-4.089801797	0.474113306	-0.712702077
C	-2.260788514	2.172871153	-0.570539512
H	-0.635378479	-1.440082925	-2.050268293
H	-1.263639671	0.193179725	-2.387999215
H	-3.950725418	-1.698738356	1.496196738
H	-3.205056715	-3.251798761	1.879043184
H	-2.464643513	-1.755706747	2.470839323
H	-3.900443057	-2.215734437	-0.983352050
H	-2.394938096	-2.706322660	-1.770994793
H	-3.189313075	-3.793317365	-0.626410940
H	-0.259847581	-3.081935876	-0.331434779
H	-0.287805671	-2.693129145	1.390028512
H	-1.214961875	-4.077225688	0.771852344
H	-3.917100628	2.031883472	1.542731193
H	-3.624598994	0.366045996	2.050129818
H	-2.298118845	1.541604003	2.075233022
H	-4.621206457	-0.345930570	-0.220334473
H	-4.781856429	1.324443791	-0.767727139
H	-3.854928945	0.168000329	-1.738278409
H	-1.357882904	2.517265149	-0.059210092
H	-2.025124453	2.050630012	-1.631727598
H	-3.015829513	2.965032564	-0.491117160
H	1.202815860	2.755847758	-2.284473312
H	1.626549009	5.110510335	-1.737679597
H	1.885330500	5.821569418	0.625236045
H	1.729780419	4.135409356	2.442578229
H	1.310917895	1.774603499	1.908366417
H	3.223544699	-0.019862887	1.274533907
H	4.933725979	-1.711320095	1.786130033
H	4.985681619	-3.855263914	0.536606079
H	3.307075448	-4.286166094	-1.241137985
H	1.584235460	-2.609771321	-1.746699604

TS13_PAl[b]

Total number of atoms = 55

C	0.662053673	0.014383571	0.988135551
AL	-1.059097229	0.070255653	-0.104297496
P	2.009386973	-0.027085617	-0.227779411
C	3.270806455	1.286803262	0.225686020
C	4.533743024	1.168444004	-0.638047399

C	2.574703375	2.625030896	-0.093237327
C	3.652904201	1.254461022	1.712472621
C	2.679544160	-1.774626455	-0.301709200
C	3.500812428	-2.169055919	0.931157159
C	1.446722726	-2.694234257	-0.417516942
C	3.518622701	-1.947520212	-1.579547016
C	-1.944575924	1.836770933	-0.100905428
C	-3.181997219	2.039623416	0.533502228
C	-1.346571999	2.965147411	-0.688939801
C	-3.786066269	3.295303715	0.588934043
C	-1.937489678	4.225879202	-0.640911517
C	-3.161873930	4.393052116	0.002245970
C	-2.203390997	-1.535390169	-0.009470636
C	-3.226808213	-1.748141379	-0.950152660
C	-2.052518370	-2.515148848	0.986669276
C	-4.045326131	-2.875052683	-0.909085890
C	-2.866966626	-3.645318332	1.043805279
C	-3.865233969	-3.828465777	0.090529895
H	0.710047677	0.955866624	1.547551360
H	0.730369582	-0.799253674	1.718187728
H	4.298186185	1.100819242	-1.706125969
H	5.155843924	2.059492446	-0.489423845
H	5.137431591	0.298749858	-0.359504608
H	1.633469104	2.749261965	0.453363559
H	3.234153423	3.453728593	0.192526804
H	2.359519104	2.718498223	-1.163470434
H	4.149709676	0.320937587	1.989810128
H	4.346932531	2.077796070	1.924569456
H	2.780253026	1.379862710	2.360085525
H	3.731762544	-3.241011414	0.887257243
H	4.452535067	-1.629737454	0.975967253
H	2.954330282	-1.983766117	1.862386222
H	0.800112655	-2.417260787	-1.257714122
H	1.787213449	-3.723013692	-0.586892690
H	0.834070631	-2.694193653	0.487332633
H	4.445129901	-1.368399889	-1.558458656
H	3.793664182	-3.003863943	-1.687846608
H	2.953025766	-1.657279100	-2.471823857
H	-3.693986047	1.194540728	0.992738899
H	-0.395419188	2.858920696	-1.211509773
H	-4.745218881	3.417203076	1.085814894
H	-1.449234697	5.077264722	-1.108842037
H	-3.629645543	5.373144087	0.041679364
H	-3.394376815	-1.013482542	-1.737175710
H	-1.280881125	-2.395819387	1.747556284
H	-4.825016111	-3.009543922	-1.654494026
H	-2.724332389	-4.382498210	1.830082659

H	-4.502014778	-4.708329328	0.127981569
H	0.830597711	0.154439498	-1.431583305
H	-0.177333526	0.098214671	-1.669152673

3PAl[b]

Total number of atoms = 55

C	0.053824138	-0.936802345	0.570660159
AL	-1.296579278	-0.184488720	-0.851208256
P	1.702299580	-0.643690633	0.014517084
C	2.730555151	0.290691632	1.254744311
C	4.160051647	0.512414244	0.742063298
C	2.039989813	1.660289144	1.416319745
C	2.748706875	-0.433445657	2.608583906
C	2.481315192	-2.169725656	-0.720836432
C	3.119006386	-3.046008763	0.366663224
C	1.373692035	-2.967794799	-1.435633235
C	3.529937912	-1.753592738	-1.766654784
C	-0.811345337	1.759557971	-0.797778725
C	-1.194607415	2.587778264	0.272395244
C	0.064380898	2.332723682	-1.737594241
C	-0.717450562	3.889687132	0.417177059
C	0.554263265	3.634457482	-1.608986249
C	0.170196912	4.414465904	-0.520775682
C	-3.094919350	-0.680167613	-0.165277946
C	-4.096123541	-1.200721700	-1.003776790
C	-3.437360360	-0.532313919	1.191029416
C	-5.358987968	-1.549149406	-0.525808769
C	-4.695030088	-0.873988495	1.685253984
C	-5.662053615	-1.384975247	0.823209247
H	-0.137229459	-0.373364298	1.489179279
H	-0.112589256	-1.999131914	0.765023283
H	4.171078992	0.989888318	-0.244180920
H	4.684483305	1.180165486	1.435248279
H	4.732180579	-0.418821499	0.689313120
H	1.025227366	1.571895942	1.812915935
H	2.623436772	2.260847173	2.123994619
H	1.975419202	2.212830144	0.473187058
H	3.279161191	-1.388526316	2.566880430
H	3.262321070	0.200986939	3.340109364
H	1.736746193	-0.618509237	2.982441916
H	3.445375793	-3.988865300	-0.086768430
H	3.998525141	-2.575421114	0.816159853
H	2.407913944	-3.291007999	1.163240930
H	0.817171930	-2.358297504	-2.153443176
H	1.843836044	-3.799402440	-1.973317898

H	0.652629919	-3.392834819	-0.732002591
H	4.353983614	-1.176741563	-1.339997573
H	3.958037136	-2.657714710	-2.214604311
H	3.077773491	-1.167403309	-2.573812225
H	-1.891687932	2.206437009	1.019380331
H	0.369136670	1.747069462	-2.606236863
H	-1.038661821	4.498691663	1.259000826
H	1.228813437	4.041216839	-2.359144664
H	0.548155880	5.427593596	-0.411202028
H	-3.885494325	-1.342710775	-2.063194531
H	-2.700990402	-0.139747439	1.894264733
H	-6.107474861	-1.948289281	-1.206212986
H	-4.921259627	-0.742349530	2.740796980
H	-6.644921839	-1.654021788	1.201446636
H	1.692409193	0.254046636	-1.067198738
H	-0.870722436	-0.825070204	-2.283175993

TS14_PAl[b]

Total number of atoms = 56

C	-0.305896260	0.674462133	2.353368247
O	0.562727446	0.119356469	1.769722810
C	-0.679955535	-0.040379836	-1.152647378
O	-0.978735002	1.234823025	3.113127595
AL	1.133402792	0.038958871	-0.343198782
P	-2.030840718	0.000840809	0.104526089
C	-3.419385699	0.980766597	-0.737955737
C	-4.730354182	0.828606545	0.045826666
C	-2.968005581	2.451607756	-0.634675526
C	-3.657832733	0.649949331	-2.217820845
C	-2.516808554	-1.819323295	0.313348209
C	-3.238619391	-2.443586242	-0.886464668
C	-1.218816516	-2.607606966	0.567220942
C	-3.393778358	-1.950422457	1.571127635
C	1.961731419	1.820416030	-0.313415485
C	3.351742267	1.996763757	-0.415342149
C	1.183491925	2.984470336	-0.176144973
C	3.935781836	3.262172980	-0.383174775
C	1.755102824	4.254722418	-0.135153544
C	3.137173419	4.394081747	-0.241034613
C	2.291791105	-1.542140107	-0.300210167
C	3.336968974	-1.670732113	0.631527304
C	2.129398765	-2.593381307	-1.218718492
C	4.167358555	-2.789592174	0.655130503
C	2.957913408	-3.713926696	-1.211438080
C	3.978680448	-3.813948912	-0.269595779

H	-0.752665206	0.891117886	-1.730724100
H	-0.813362745	-0.860529772	-1.870759882
H	-4.584693715	1.000457475	1.118681453
H	-5.461393295	1.564020280	-0.314025003
H	-5.174326536	-0.162767174	-0.088435355
H	-2.037359264	2.635460959	-1.183934550
H	-3.735512943	3.105450173	-1.068340380
H	-2.814393340	2.753054910	0.407421643
H	-4.062027640	-0.354429100	-2.361974538
H	-4.383071283	1.360249357	-2.636545799
H	-2.738384155	0.732731802	-2.805781149
H	-3.352089889	-3.523925107	-0.727126500
H	-4.241614359	-2.027149444	-1.018938140
H	-2.682375919	-2.303337901	-1.819745086
H	-0.637059262	-2.197513317	1.400104164
H	-1.470855319	-3.643832562	0.826011948
H	-0.568340284	-2.639751458	-0.310816136
H	-4.356264287	-1.442859522	1.467855981
H	-3.599181776	-3.010932716	1.765954218
H	-2.890235295	-1.538201930	2.452664268
H	3.996725082	1.125836413	-0.524288132
H	0.098401007	2.904276372	-0.096090610
H	5.013973586	3.366938093	-0.470652445
H	1.125655297	5.133754795	-0.024356369
H	3.590006662	5.381296906	-0.213162291
H	3.509279700	-0.880213056	1.361229853
H	1.334999676	-2.543131056	-1.963433358
H	4.962264558	-2.861990383	1.392632454
H	2.808048371	-4.508020672	-1.938148509
H	4.626194824	-4.686450827	-0.256931885

4PAl[b]

Total number of atoms = 56

C	-1.153538776	0.155478359	1.613230513
O	0.128732912	0.125895211	1.665811243
C	-0.362744807	0.106028480	-1.199986102
O	-1.948593320	0.258639694	2.527991360
AL	1.209606593	0.058987709	0.135614700
P	-1.804141620	0.005446296	-0.166212527
C	-2.925084421	1.474546953	-0.426222108
C	-4.248508948	1.344947389	0.341166485
C	-2.142778005	2.694411055	0.104785762
C	-3.205322383	1.664717921	-1.926032864
C	-2.565892647	-1.696080014	-0.273244337
C	-3.220124512	-1.887496665	-1.650206835

C	-1.408925835	-2.702203916	-0.097176451
C	-3.597905846	-1.943521026	0.839641690
C	2.177103722	1.771915095	0.049537243
C	3.227737316	1.967667960	-0.863731642
C	1.783034718	2.889593599	0.806154645
C	3.846336810	3.206606379	-1.023490893
C	2.394867503	4.133700384	0.658299527
C	3.427471105	4.295072402	-0.262125614
C	2.124885542	-1.684586073	0.055550284
C	2.568157403	-2.361266632	1.205308707
C	2.328622602	-2.335030338	-1.174041475
C	3.176513966	-3.613357687	1.134695402
C	2.939131102	-3.585486993	-1.260513886
C	3.363717543	-4.228673331	-0.100887216
H	-0.332309205	1.065974636	-1.722309572
H	-0.339766110	-0.698496569	-1.939116686
H	-4.087986677	1.093933856	1.393181941
H	-4.769927002	2.308280112	0.294586192
H	-4.906045101	0.596515652	-0.112009102
H	-1.147958266	2.791291960	-0.344899422
H	-2.704603919	3.602666671	-0.141835313
H	-2.029022038	2.655965139	1.192201813
H	-3.728094273	0.810388706	-2.364929590
H	-3.846672117	2.545066695	-2.049010767
H	-2.290303949	1.838497886	-2.499451881
H	-3.510068972	-2.938830630	-1.759145107
H	-4.127222622	-1.283875145	-1.754967127
H	-2.540094035	-1.644082569	-2.473609216
H	-0.895508933	-2.581595561	0.862619508
H	-1.830804711	-3.713360016	-0.120970951
H	-0.655751916	-2.637601454	-0.886431574
H	-4.477952142	-1.304703817	0.746751293
H	-3.934585869	-2.983960691	0.761560910
H	-3.172765065	-1.794400641	1.834875124
H	3.582490639	1.130600668	-1.465452120
H	0.985647499	2.786528271	1.541592663
H	4.656420895	3.322928469	-1.739037402
H	2.069315448	4.976353869	1.263245148
H	3.907524059	5.262646098	-0.381639274
H	2.432599411	-1.903529749	2.184020717
H	1.999867184	-1.858575782	-2.098881995
H	3.506347186	-4.109715701	2.043707742
H	3.083536022	-4.057745360	-2.229001566
H	3.839297470	-5.203878669	-0.160133410

1PAl[c]

Total number of atoms = 54

C	0.616309274	-0.521258803	1.554493734
P	1.351251310	-0.621469861	-0.140645015
C	2.925551600	0.431638379	-0.177518919
C	4.149727367	-0.255019198	0.439494458
C	3.210955547	0.818600322	-1.638949108
C	2.634022714	1.723115355	0.607055413
C	1.664324193	-2.440970880	-0.552194427
C	2.399946412	-3.220781533	0.545363403
C	2.430708736	-2.546288306	-1.879178484
C	0.271808607	-3.067616812	-0.742517248
AL	-0.891437101	0.294853336	0.598961794
C	-0.882790174	2.221303475	0.202669460
C	-0.796740390	2.677627132	-1.124809402
C	-0.916020601	3.200679347	1.209138403
C	-0.742606615	4.035392209	-1.433858333
C	-0.864392976	4.561439455	0.912459472
C	-0.775507115	4.981331112	-0.412348135
C	-2.493644190	-0.762778477	0.207037597
C	-3.430577395	-0.310607700	-0.738087211
C	-2.776203478	-1.975639122	0.857859445
C	-4.579795716	-1.040777936	-1.036977472
C	-3.923647812	-2.711169635	0.571469815
C	-4.825697680	-2.245150170	-0.382523854
C	1.148510610	-0.891687772	2.722440555
H	4.991641571	0.449668920	0.445844223
H	3.962815388	-0.556376947	1.475349895
H	4.465102184	-1.135517849	-0.128252741
H	2.353443136	1.336926209	-2.081147422
H	4.070753457	1.500071504	-1.671758822
H	3.449862690	-0.045161553	-2.265517933
H	3.505692229	2.385446687	0.529131416
H	1.768947978	2.259614540	0.206958293
H	2.451167713	1.522690328	1.666128273
H	2.524204607	-4.263299758	0.224071268
H	3.394099521	-2.818858382	0.755529197
H	1.825693903	-3.226922463	1.475926412
H	3.469023237	-2.214115711	-1.786163313
H	2.451641777	-3.596015694	-2.198633453
H	1.949692325	-1.965631475	-2.674545602
H	-0.321164238	-3.021843361	0.175085488
H	-0.297376204	-2.570907080	-1.534702329
H	0.386597514	-4.125337445	-1.012298519
H	-0.729776761	6.041323291	-0.646577637
H	-0.889684758	5.294966388	1.713884873
H	-0.670499332	4.355550263	-2.470054776
H	-0.754344290	1.956531557	-1.940584623

H	-0.974353470	2.902336234	2.255319322
H	-2.082930542	-2.355907424	1.607463367
H	-4.115459542	-3.646879573	1.090026752
H	-5.722021011	-2.815838115	-0.610340020
H	-5.285398555	-0.669504660	-1.775490670
H	-3.265812315	0.637494955	-1.248432399
H	2.139777016	-1.336214757	2.826696436
H	0.603131856	-0.757616673	3.657141977

TS13_PAl[c]

Total number of atoms = 56

C	0.312182297	-0.704861817	0.804195266
P	1.779032864	-0.567856796	-0.257192627
C	3.049210951	0.617321399	0.462986164
C	3.936910570	-0.026130926	1.535809864
C	3.912356847	1.155024965	-0.691135907
C	2.273981511	1.793371291	1.083386046
C	2.416245778	-2.301627998	-0.605741435
C	2.652160193	-3.143497534	0.654961965
C	3.697777468	-2.241522031	-1.449253139
C	1.302268936	-2.967117924	-1.439746818
AL	-1.205680819	0.072135884	-0.273983824
C	-1.090704913	2.048167534	-0.290498031
C	-0.500010884	2.760828722	-1.347822196
C	-1.467913772	2.796561070	0.838153983
C	-0.285953151	4.137781519	-1.283701856
C	-1.260411659	4.172280202	0.916806979
C	-0.662434082	4.846406757	-0.145738457
C	-2.937598113	-0.845233387	-0.118342186
C	-4.135216598	-0.263353609	-0.570165611
C	-3.032484984	-2.121633199	0.464000376
C	-5.359570909	-0.917873234	-0.454060027
C	-4.251601395	-2.785246478	0.589161674
C	-5.418965577	-2.182464704	0.127352696
C	0.311193866	-1.129245186	2.075586401
H	-0.323589336	-0.218295091	-1.804271527
H	0.657988461	-0.184971377	-1.482459155
H	4.602104676	0.738786534	1.956490180
H	3.344648179	-0.437813389	2.359504848
H	4.568964643	-0.821403399	1.129412877
H	3.294002918	1.645652817	-1.450180453
H	4.616793470	1.898972424	-0.298644702
H	4.497731598	0.370763648	-1.179306860
H	2.996687774	2.541953981	1.430999200
H	1.606900921	2.277074158	0.362935785

H	1.669681983	1.476758966	1.937620628
H	3.000462319	-4.141001285	0.357616717
H	3.408320957	-2.712430272	1.316617332
H	1.726371715	-3.271683031	1.222628247
H	4.552487156	-1.868312147	-0.876462615
H	3.949145841	-3.253260755	-1.790821515
H	3.573288918	-1.611804106	-2.337399850
H	0.349099220	-2.992138719	-0.900873031
H	1.142497159	-2.451185944	-2.392404544
H	1.588358575	-4.002918749	-1.660488522
H	-0.494665852	5.918448339	-0.087401122
H	-1.562843014	4.719076812	1.806342419
H	0.175689763	4.656780159	-2.120059844
H	-0.189129466	2.227836228	-2.246213688
H	-1.932970385	2.296394019	1.687805570
H	-2.131232750	-2.608707559	0.835896768
H	-4.293451591	-3.770128834	1.047460103
H	-6.372687896	-2.694602178	0.222938840
H	-6.268111937	-0.442583008	-0.814785903
H	-4.113541688	0.727687480	-1.021466706
H	1.197910739	-1.453115708	2.623851869
H	-0.617089757	-1.167357112	2.647623299

3PAl[c]

Total number of atoms = 56

C	0.071008942	-0.940528539	0.377207282
P	1.753852559	-0.575048460	-0.080719110
C	2.726934220	0.479836894	1.116196274
C	3.472962049	-0.367847994	2.155770169
C	3.707516024	1.351669069	0.312024891
C	1.728034764	1.408524957	1.829515292
C	2.616069570	-2.089078378	-0.743685009
C	2.660397002	-3.204246588	0.310786708
C	4.031137377	-1.748685701	-1.232266296
C	1.766068620	-2.558560952	-1.940746387
AL	-1.290026145	-0.139228173	-0.962205021
C	-0.875607787	1.813811419	-0.752555063
C	0.038347534	2.465521550	-1.600620982
C	-1.332502633	2.559553567	0.349636535
C	0.491764709	3.764130131	-1.358235235
C	-0.902377180	3.862296592	0.599919435
C	0.022968351	4.465846636	-0.250021171
C	-3.092319530	-0.700628988	-0.339308945
C	-4.132904480	0.221591502	-0.131370319
C	-3.388234054	-2.046006624	-0.053950775

C	-5.388625954	-0.168052709	0.334342201
C	-4.637424796	-2.451838466	0.413023679
C	-5.643385044	-1.508807968	0.609834656
C	-0.187244073	-1.571929476	1.533095356
H	-0.747704077	-0.653670244	-2.405572982
H	1.670429435	0.253567341	-1.207895271
H	3.944972418	0.305879492	2.880265674
H	2.796659794	-1.024836495	2.712775550
H	4.264549425	-0.977769730	1.710609961
H	3.167976034	2.014532081	-0.373202295
H	4.269114021	1.983189007	1.010093163
H	4.432564620	0.766874847	-0.260400413
H	2.296054669	2.085699524	2.478481946
H	1.154214683	2.016667062	1.125022147
H	1.020553119	0.850387042	2.447996239
H	3.103013287	-4.097515626	-0.144651684
H	3.268700717	-2.940243141	1.180480252
H	1.655524006	-3.468226137	0.653293497
H	4.703541308	-1.474208227	-0.414222782
H	4.454526487	-2.633665409	-1.721231665
H	4.025333607	-0.937788577	-1.968998041
H	0.744988494	-2.813627076	-1.645275101
H	1.699554268	-1.796725670	-2.723439176
H	2.235646394	-3.451554252	-2.370112519
H	0.367225264	5.478328441	-0.056277300
H	-1.282413961	4.405473234	1.461839799
H	1.199140869	4.232313021	-2.039208700
H	0.402899229	1.945954758	-2.488161737
H	-2.039218030	2.105940079	1.044286290
H	-2.620514937	-2.806947259	-0.200806394
H	-4.828362944	-3.502190442	0.620380360
H	-6.619889915	-1.817776225	0.973920603
H	-6.169163723	0.574758709	0.481010248
H	-3.961161524	1.277085450	-0.339230193
H	0.559030219	-1.893816187	2.263901303
H	-1.220733370	-1.789815777	1.802227380

1PAl[d]

Total number of atoms = 67

AL	-1.352812880	1.445960150	-0.692553398
C	0.045105593	0.442339634	-1.649679611
C	-1.114671583	3.340490726	-0.244839751
C	-0.554379473	4.236813248	-1.171999915
C	-0.384812694	5.588217601	-0.879842759
C	-0.770844166	6.081619855	0.363874490

C	-1.324940021	5.219355080	1.306670164
C	-1.495782683	3.871027838	1.000287794
C	-3.041762139	0.522551879	-0.330387100
C	-4.060429325	1.103689086	0.445346701
C	-5.232992072	0.415121574	0.749904373
C	-5.418134187	-0.882098561	0.277454812
C	-4.433535586	-1.480107069	-0.505316034
C	-3.266319299	-0.782200802	-0.805240084
P	0.583654793	-0.115427836	0.060335922
C	2.429822560	-0.058321531	0.226568643
C	3.161081525	-1.078720890	0.878972623
C	3.124524776	1.082953528	-0.232676066
C	4.555889637	-1.008253887	0.894607115
C	4.518398611	1.103824169	-0.189442427
C	5.259921625	0.052724400	0.336918185
C	0.051415862	-1.874574607	0.009172752
C	0.498508355	-2.763820863	-0.994616530
C	-0.900247925	-2.309066522	0.952869386
C	-0.073227600	-4.031961020	-1.075799293
C	-1.441640441	-3.590468279	0.830270177
C	-1.059124402	-4.457925661	-0.186375454
C	-1.357635831	-1.456216632	2.113819408
C	-1.692232464	-5.817846975	-0.332404158
C	1.644411220	-2.447284078	-1.928058770
C	2.441996002	2.345002096	-0.711618042
C	6.765786660	0.106792123	0.377913501
C	2.539301778	-2.238953084	1.627942364
H	5.107997734	-1.810574459	1.380400586
H	5.035547238	1.986002953	-0.563022563
H	0.271597684	-4.715379897	-1.849439070
H	-2.187776270	-3.914250957	1.552406543
H	-0.516531852	-1.000698187	2.646019728
H	-2.010080173	-0.643568070	1.779643069
H	-1.922109265	-2.063979386	2.826855723
H	-2.140741748	-6.154102551	0.607249478
H	-2.485647712	-5.796446052	-1.089228541
H	-0.959563840	-6.567151659	-0.649034141
H	1.669100602	-3.158442403	-2.758863072
H	1.597166324	-1.438897130	-2.342652302
H	2.601012119	-2.521080695	-1.397151446
H	1.459451909	2.492695667	-0.256578577
H	3.048085312	3.214633893	-0.439780418
H	2.315630143	2.372216923	-1.799484042
H	7.112610059	0.755697877	1.191182486
H	7.197791575	-0.885611979	0.538683083
H	7.174203616	0.507721966	-0.555638014
H	1.664478585	-1.933102256	2.207690052

H	2.221573646	-3.052809984	0.969788106
H	3.270189800	-2.647285832	2.332303219
H	0.805979858	1.015613406	-2.177912834
H	-0.264124879	-0.406517067	-2.262546916
H	-2.505747913	-1.280218093	-1.403699334
H	-4.571546884	-2.491563271	-0.877965064
H	-3.938825715	2.117869189	0.822622612
H	-6.001765775	0.889173922	1.354326718
H	-6.329964949	-1.423215244	0.515522342
H	-0.228325966	3.872204426	-2.145734914
H	0.048781258	6.256119728	-1.619427874
H	-0.637386870	7.134201910	0.597743422
H	-1.623320791	5.598680806	2.280368455
H	-1.926705337	3.217784004	1.757729955

pre-1PAl[d]

Total number of atoms = 67

C	-0.290246171	-1.079876105	-1.585328295
AL	1.513655928	-0.444430227	-1.053461235
C	2.040847487	1.411299247	-1.396563859
C	1.282538450	2.213348674	-2.266352715
C	3.087583919	2.045251087	-0.704608367
C	1.541063084	3.571937638	-2.433153518
C	3.358212499	3.402720237	-0.863267184
C	2.580452978	4.171094004	-1.726245326
C	2.821051546	-1.820473377	-0.570563319
C	4.175076008	-1.552049407	-0.306739793
C	2.417832499	-3.167262143	-0.506688860
C	5.075191787	-2.564378692	0.019065864
C	3.308104628	-4.188407766	-0.181692159
C	4.640733385	-3.886059190	0.085369257
P	-1.109988054	-1.385869498	0.049737916
C	-2.896374203	-0.893026860	-0.041579203
C	-3.535748673	-0.390008576	1.113224855
C	-3.677390655	-1.120263931	-1.197113179
C	-4.872182371	0.008820601	1.044064125
C	-5.009078138	-0.705445663	-1.217394533
C	-5.620483111	-0.103924791	-0.121560671
C	-0.276647037	0.045206452	0.923066921
C	-0.510677661	1.414158089	0.623724409
C	0.685988391	-0.279852555	1.913640877
C	0.240332578	2.392622057	1.268242844
C	1.441110497	0.741620933	2.500381852
C	1.238799954	2.080159507	2.187482677
C	0.893062791	-1.688524928	2.424142909

C	2.086742791	3.166420693	2.792805591
C	-1.561222209	1.897306829	-0.347785183
C	-3.173550729	-1.859627061	-2.418651829
C	-7.046520032	0.378834183	-0.192490396
C	-2.853893414	-0.275867793	2.458840097
H	-0.779112626	-0.297620636	-2.176016190
H	-0.277045203	-1.997346016	-2.181729491
H	0.451101149	1.775782823	-2.817430303
H	3.694628193	1.477612020	-0.002253161
H	0.931324654	4.164390935	-3.110213073
H	4.176200361	3.862447397	-0.314054484
H	2.785779713	5.230732333	-1.850860382
H	4.546637496	-0.531234139	-0.366351467
H	1.378025714	-3.426989617	-0.703027234
H	6.116498863	-2.324676069	0.217089040
H	2.962646288	-5.217657978	-0.134720550
H	5.340070737	-4.677461391	0.340559015
H	-5.342386785	0.409522862	1.940338942
H	-5.592917540	-0.877446926	-2.119976573
H	0.068805022	3.435829789	1.012258672
H	2.194180259	0.475510497	3.238468427
H	-0.041425327	-2.102403176	2.817713434
H	1.245880972	-2.374143376	1.650750744
H	1.633453292	-1.689848389	3.229056967
H	2.664436215	2.799146994	3.646085406
H	2.790337785	3.551765532	2.045194846
H	1.473410895	4.008761922	3.129583100
H	-1.275277157	2.871887601	-0.753314919
H	-1.721334510	1.215968771	-1.182387977
H	-2.529651912	2.004172563	0.154964642
H	-2.560361451	-1.232623152	-3.072097031
H	-2.574489699	-2.734496160	-2.146573057
H	-4.022571505	-2.216490446	-3.009217886
H	-7.495564976	0.450314879	0.803038496
H	-7.100555354	1.373932075	-0.650819991
H	-7.665836725	-0.291653786	-0.797448916
H	-2.174100781	-1.113376459	2.646506783
H	-2.268717358	0.645086279	2.552885122
H	-3.604040060	-0.276270438	3.255283005

TS13_PAl[d]

Total number of atoms = 69

C	-0.295161366	-1.337367219	-0.869527062
AL	-1.984011538	-0.950134488	0.203250682
C	-3.434622879	-2.266964063	0.028194838

C	-3.244578501	-3.521013131	-0.577495586
C	-4.725329171	-1.986121198	0.511108661
C	-4.277458111	-4.449042906	-0.692448377
C	-5.766135640	-2.906452707	0.405298366
C	-5.542461254	-4.142193108	-0.196887215
C	-2.488699735	0.957237430	0.367200356
C	-1.942912239	1.814504070	1.337560671
C	-3.355630835	1.545798694	-0.570627694
C	-2.221141510	3.179506457	1.362656027
C	-3.639068609	2.910851830	-0.562822772
C	-3.067167186	3.732857300	0.404745820
P	0.951794231	-0.451317227	0.089678016
C	0.996535818	1.357425970	-0.152874605
C	1.546427626	2.079347416	0.931750027
C	0.397857876	2.061554517	-1.220803010
C	1.468645741	3.470076616	0.939995436
C	0.333017186	3.452266551	-1.154744898
C	0.841525381	4.175077379	-0.081395411
C	2.625146506	-1.181078454	-0.038635689
C	3.518016084	-0.899284140	-1.092531547
C	3.010234885	-2.074309815	0.984876292
C	4.786310681	-1.478475590	-1.077936645
C	4.284708280	-2.638336941	0.948654073
C	5.193349164	-2.341623333	-0.063742648
C	2.089436996	-2.453724480	2.123172823
C	6.581938663	-2.926890354	-0.052376218
C	3.135981617	-0.030872486	-2.263837177
C	-0.204684382	1.408087540	-2.438627769
C	0.671722229	5.669460241	-0.012725390
C	2.185827433	1.395761875	2.117523790
H	-0.073844152	-2.398202319	-0.669368545
H	-0.293987791	-1.199877033	-1.950095701
H	-2.265219297	-3.783940555	-0.976704069
H	-4.923812292	-1.022778340	0.979134446
H	-4.098385863	-5.410032804	-1.167906048
H	-6.751927302	-2.661288401	0.792219927
H	-6.350844633	-4.863621055	-0.281190785
H	-1.265095601	1.412987639	2.090030108
H	-3.824597340	0.925878046	-1.335268255
H	-1.769828905	3.812113377	2.122709783
H	-4.311124341	3.331321020	-1.306761156
H	-3.285004496	4.797792722	0.416752182
H	1.888568450	4.013419267	1.783642837
H	-0.153084065	3.986992173	-1.967514906
H	5.473509596	-1.256061840	-1.891603454
H	4.576529811	-3.329580858	1.736356438
H	1.852060190	-1.591749842	2.756409099

H	1.136806406	-2.863696941	1.768289894
H	2.558361516	-3.213218509	2.754892017
H	6.986101883	-3.021561416	-1.064872053
H	7.265844055	-2.286503622	0.517644269
H	6.593660622	-3.916488519	0.414669264
H	2.264172839	-0.447574203	-2.780398216
H	2.883903105	0.989122556	-1.958670146
H	3.953040663	0.023337297	-2.988388500
H	0.453620594	0.651734986	-2.871406156
H	-1.160902486	0.933892226	-2.199062303
H	-0.398248705	2.159565717	-3.208745137
H	-0.349928564	5.916189864	0.301538280
H	1.362233855	6.121732847	0.705447780
H	0.835595899	6.137750083	-0.988681424
H	1.457859399	0.771592275	2.650785481
H	3.019431716	0.747702505	1.825738360
H	2.569261176	2.135922983	2.825038519
H	-0.104549668	-0.809970704	1.397460935
H	-1.004724218	-1.127777519	1.724263315

3PAl[d]

Total number of atoms = 69

C	0.064732850	-1.798831657	-0.915421276
AL	1.775558939	-1.127787896	-1.963019172
C	3.379864051	-1.660476282	-0.896661893
C	3.504950910	-2.936204255	-0.316113824
C	4.443968617	-0.770893348	-0.665466415
C	4.606157235	-3.301941404	0.456234126
C	5.553399025	-1.119851019	0.104702215
C	5.635349439	-2.388135795	0.672742805
C	1.559694083	0.871279659	-2.088080784
C	0.906016832	1.452025281	-3.192286246
C	1.944026734	1.759490686	-1.066095140
C	0.647133702	2.821527705	-3.275256378
C	1.697134415	3.131150379	-1.133292448
C	1.043966196	3.667611808	-2.240490676
P	-0.902801108	-0.449175481	-0.305855965
C	-0.261200750	0.523483815	1.087477711
C	-0.707257279	1.864932616	1.150423585
C	0.680406674	0.044592666	2.022492073
C	-0.206178382	2.694238728	2.149653465
C	1.152994904	0.925222486	2.996106838
C	0.732308503	2.248631678	3.075574311
C	-2.691047934	-0.769496548	-0.133196739
C	-3.237534732	-1.332486440	1.037224470

C	-3.527158881	-0.464948718	-1.230987825
C	-4.613168248	-1.538044050	1.107132493
C	-4.897695328	-0.693243910	-1.109520823
C	-5.461621529	-1.220015811	0.048834357
C	-3.015230601	0.095715992	-2.541141255
C	-6.942168286	-1.482137235	0.142886523
C	-2.384137979	-1.747237449	2.209325511
C	1.237655974	-1.355817277	2.032926401
C	1.298411167	3.181333007	4.113978079
C	-1.661039115	2.471773696	0.149254730
H	-0.564003393	-2.269148865	-1.683342724
H	0.271983200	-2.546612279	-0.148932686
H	2.713963796	-3.673189492	-0.463675788
H	4.409822916	0.226508855	-1.101426362
H	4.664594510	-4.298052589	0.888738886
H	6.354905696	-0.401418781	0.260157212
H	6.496980143	-2.665655682	1.274588100
H	0.596874502	0.813868373	-4.020268659
H	2.444100740	1.370566361	-0.179721143
H	0.149760230	3.231360337	-4.151366450
H	2.010163471	3.779766232	-0.318574891
H	0.852003302	4.735711994	-2.301658902
H	-0.550003332	3.724830346	2.194447753
H	1.881497100	0.558382665	3.715008482
H	-5.033787068	-1.967019908	2.013880527
H	-5.544068258	-0.453246263	-1.950599641
H	-2.636782579	1.119359377	-2.433424975
H	-2.207613465	-0.507483314	-2.970372648
H	-3.822705241	0.123761408	-3.276961900
H	-7.506358282	-0.849441689	-0.548412007
H	-7.164194657	-2.526697242	-0.106133123
H	-7.315204045	-1.300277039	1.155513019
H	-1.629948415	-2.480573973	1.902543665
H	-1.862320614	-0.898094460	2.660904731
H	-2.995814420	-2.217238914	2.983670051
H	0.455450940	-2.119224147	2.018630012
H	1.898108252	-1.528849144	1.178309419
H	1.830591426	-1.516492078	2.936560608
H	0.579984586	3.960537059	4.385386115
H	1.581804506	2.642794072	5.023247445
H	2.197810667	3.677951863	3.731125070
H	-1.166363640	2.601347506	-0.822252564
H	-2.566497671	1.873651813	0.005627024
H	-1.975254030	3.463474371	0.484261143
H	-0.880631286	0.492191556	-1.330199316
H	1.594507098	-1.817967438	-3.415934554

1PAl[e]

Total number of atoms = 71

C	0.413207479	-1.247890083	-1.000394032
AL	2.300686481	-1.088965265	-0.406258721
P	-0.607176018	-0.696448913	0.434932101
C	2.976527257	-2.591743954	0.732777115
C	3.481018071	0.360325657	-1.096408928
C	-2.437665334	-0.825884279	0.132575899
C	-5.271018160	-0.870232799	-0.082248449
C	-3.249305755	-0.136949049	1.064604268
C	-3.072532104	-1.598361406	-0.866105525
C	-4.464616733	-1.594741455	-0.954888445
C	-4.638696757	-0.159920438	0.929648369
C	-0.289863080	1.131524431	0.293677843
C	0.387102750	3.882808413	0.147014418
C	0.571728842	1.716404465	1.245967980
C	-0.825043337	1.950296095	-0.729323500
C	-0.476845528	3.299690317	-0.777682668
C	0.897196198	3.072651931	1.152869743
C	4.244329117	1.050330380	0.046496371
C	2.683892508	1.418782138	-1.874372949
C	4.502954993	-0.279937059	-2.059165552
C	4.421602507	-2.965624819	0.359128336
C	2.076570565	-3.822424153	0.519194121
C	2.946010731	-2.233653598	2.229875608
C	-2.684821098	0.650771217	2.225198064
C	-2.336552304	-2.458647879	-1.868531851
C	1.190991125	0.938810418	2.385959454
C	-1.791322720	1.456738427	-1.781249920
C	-6.773266947	-0.902693437	-0.202126287
C	0.753197680	5.341060298	0.043810051
H	-4.936597817	-2.182543905	-1.740134201
H	-5.241311386	0.393988730	1.647175318
H	-0.890545152	3.917538919	-1.572681235
H	1.569539845	3.502732568	1.892465484
H	4.972314598	1.774562954	-0.354434752
H	4.805893707	0.337292476	0.664801710
H	3.567431394	1.610221935	0.704016827
H	2.123679150	0.979581389	-2.710258874
H	3.365349842	2.173498117	-2.300315660
H	1.966552185	1.946257178	-1.238232280
H	4.017880118	-0.785402561	-2.906643481
H	5.151372452	-1.009516689	-1.560539438
H	5.158746676	0.495428637	-2.487381105
H	4.519736905	-3.263943135	-0.693257193
H	4.768616066	-3.815714173	0.968571459

H	5.118738604	-2.136774117	0.534633355
H	2.076253921	-4.162113924	-0.525851027
H	1.036176298	-3.621376385	0.804786870
H	2.426554797	-4.668229374	1.132469308
H	3.588205788	-1.374129447	2.464617218
H	3.312228018	-3.081403693	2.831643235
H	1.930795139	-2.004524513	2.576058719
H	-3.458978886	0.818312539	2.979855918
H	-2.304417422	1.628625224	1.911052186
H	-1.856146003	0.121544008	2.708411057
H	-3.052286009	-3.000362834	-2.493444929
H	-1.705546319	-3.205085577	-1.375896713
H	-1.696407236	-1.872337655	-2.533241653
H	2.038478632	0.323761867	2.056668562
H	0.480878883	0.259676166	2.863119445
H	1.585330597	1.623079767	3.143199650
H	-1.837355726	2.167358653	-2.611825941
H	-2.801298464	1.349603575	-1.371645083
H	-1.511713340	0.483429020	-2.189114622
H	-7.229884308	-0.023897987	0.263627839
H	-7.187285824	-1.790703741	0.290863705
H	-7.088362375	-0.934404332	-1.250339500
H	-0.139597210	5.975815941	0.073892391
H	1.268347383	5.547527859	-0.901178953
H	1.413722280	5.647131459	0.860279181
H	0.254483520	-2.319137285	-1.163094559
H	0.210462744	-0.711024199	-1.933113485

TS13_PAl[e]

Total number of atoms = 73

C	-0.899968498	-0.613149743	-1.096692493
AL	-2.634825497	-0.491762667	0.001373127
P	0.421797869	-0.165914044	0.060031445
C	-3.508726360	1.308029594	0.177248660
C	-3.766331227	-2.149902839	-0.118920582
C	1.044373186	1.554262711	0.048323687
C	2.079502523	4.170436195	0.340075169
C	1.767892826	1.917174308	1.209004707
C	0.826744112	2.521619725	-0.958794279
C	1.348620983	3.803062217	-0.786524771
C	2.278850135	3.209495838	1.324085697
C	1.844219570	-1.314762360	-0.088435346
C	3.990295687	-3.140039976	-0.170354059
C	1.895247336	-2.390848584	0.822347154
C	2.852968370	-1.177270571	-1.064507402

C	3.908933146	-2.086426307	-1.078634015
C	2.968886666	-3.280024750	0.764250558
C	-4.423776260	-2.442695521	1.240027407
C	-2.916014899	-3.368219447	-0.510776083
C	-4.869800477	-1.968674232	-1.175550052
C	-4.012798293	1.797599103	-1.191315955
C	-2.526244478	2.343989188	0.745620712
C	-4.711265276	1.220498130	1.131601749
C	2.012495787	0.958990064	2.351783018
C	0.051266355	2.262564273	-2.227082876
C	0.823962488	-2.623996387	1.863421154
C	2.813627547	-0.102841997	-2.120451425
C	2.607847725	5.572751081	0.495276398
C	5.132533126	-4.121507347	-0.229038313
H	1.177237259	4.542484954	-1.565893476
H	2.839289478	3.472136321	2.218524496
H	4.687454195	-1.974405896	-1.830590886
H	3.005605290	-4.104479923	1.472918766
H	-5.044171072	-3.353842290	1.189230230
H	-5.076188614	-1.625589764	1.570144091
H	-3.674819860	-2.603321844	2.027172712
H	-2.467541169	-3.256467753	-1.506679486
H	-3.526644045	-4.286588446	-0.533226966
H	-2.098855203	-3.546103143	0.202811286
H	-4.455703064	-1.768523213	-2.173793212
H	-5.544446726	-1.139826033	-0.926210491
H	-5.490516498	-2.876965721	-1.260057185
H	-3.199882148	1.901084703	-1.922959737
H	-4.495838155	2.785722171	-1.105440032
H	-4.754151854	1.112363334	-1.623287194
H	-2.137702531	2.043288300	1.727942878
H	-3.016948701	3.323767706	0.875538391
H	-1.661525407	2.507397167	0.092182200
H	-5.486018600	0.540004512	0.756828850
H	-5.183363181	2.209388600	1.260395366
H	-4.418473425	0.868521800	2.129930953
H	2.534857627	1.465639618	3.167745752
H	2.621793561	0.100427432	2.048170149
H	1.069635159	0.568959326	2.752029730
H	0.475476842	1.440024102	-2.808753187
H	0.059385129	3.152533792	-2.861952240
H	-0.994220118	2.019528740	-2.017389404
H	-0.174781677	-2.705698665	1.418970038
H	0.783834245	-1.810861511	2.596457445
H	1.016390693	-3.553903884	2.405624270
H	3.613713368	-0.248680508	-2.851388803
H	2.922228961	0.898617483	-1.693070294

H	1.861867554	-0.131839636	-2.661446413
H	-1.694593964	-0.648762673	1.540890196
H	-0.723492144	-0.439394200	1.267334485
H	3.016837003	5.951038339	-0.447290578
H	3.395349421	5.621260948	1.252954296
H	1.807969564	6.256667902	0.802916537
H	4.947114512	-4.888008600	-0.991093301
H	5.269105301	-4.632865004	0.728465122
H	6.072314277	-3.623099984	-0.486957042
H	-0.750992012	-1.691965108	-1.251284637
H	-0.860876685	-0.148712307	-2.080666485

3PAl[e]

Total number of atoms = 73

C	-1.075936493	-0.034164973	-0.786819343
AL	-2.794048654	-0.008265671	0.430364672
P	0.397116429	-0.013693065	0.176911572
C	-3.088884589	1.969124731	0.769274363
C	-4.171103715	-1.040387060	-0.620890989
C	1.632636497	1.328246166	-0.007846848
C	3.631827308	3.322962934	-0.114620961
C	2.603396410	1.428521720	1.019139084
C	1.656179804	2.250931217	-1.079119461
C	2.660377068	3.219415838	-1.103855136
C	3.582640862	2.416411918	0.938336413
C	1.218563131	-1.637208708	0.093210196
C	2.458168170	-4.155228781	-0.089246751
C	1.071671438	-2.567583653	1.144259049
C	1.963073783	-1.976333408	-1.058504953
C	2.571099875	-3.226059295	-1.122208106
C	1.700939701	-3.808469888	1.024032850
C	-5.575489201	-0.827731324	-0.036187205
C	-3.825664759	-2.535572620	-0.538564727
C	-4.193290445	-0.631062872	-2.101564690
C	-3.554634032	2.706689882	-0.493434222
C	-1.787347076	2.624091724	1.257152173
C	-4.150505188	2.153068884	1.864724904
C	2.632147364	0.523904503	2.229643955
C	0.655632496	2.303028756	-2.211186388
C	0.267822429	-2.300129501	2.394261448
C	2.111807673	-1.047156519	-2.238322066
C	4.680121273	4.402789148	-0.168157844
C	3.145476931	-5.492312896	-0.183553815
H	2.678014204	3.924620281	-1.931339017
H	4.327553852	2.478530006	1.728006189

H	3.141412926	-3.486320593	-2.011177967
H	1.584938705	-4.529177576	1.829812864
H	-6.326759460	-1.445832349	-0.558807996
H	-5.898302676	0.217757228	-0.129711271
H	-5.622054872	-1.091840961	1.029215170
H	-2.827845358	-2.748167368	-0.950399500
H	-4.545145662	-3.148076079	-1.110169324
H	-3.834418077	-2.898148714	0.497475483
H	-3.223878123	-0.803149285	-2.590431267
H	-4.441033040	0.429959837	-2.233680872
H	-4.942463099	-1.212654615	-2.666873906
H	-2.837260989	2.606876209	-1.322599196
H	-3.682709010	3.788171880	-0.309813382
H	-4.517762943	2.323621504	-0.854050863
H	-0.993679379	2.594909538	0.494312290
H	-1.397720497	2.138571006	2.163734425
H	-1.936699426	3.690404911	1.502221460
H	-5.118675372	1.727685116	1.570994182
H	-4.319565672	3.221491995	2.087800696
H	-3.850746352	1.665404894	2.801709227
H	3.492911419	0.764874082	2.858049432
H	2.707909714	-0.533866540	1.959302153
H	1.735432378	0.650933680	2.848078944
H	1.009321369	2.990749471	-2.983455475
H	-0.312829519	2.679981769	-1.863503722
H	0.489057729	1.333845155	-2.683717726
H	-0.750418569	-1.961201480	2.174316828
H	0.739902192	-1.536530810	3.024440324
H	0.193764958	-3.211502250	2.993031150
H	2.623801428	-1.553188191	-3.060794932
H	2.688342585	-0.151509619	-1.985465712
H	1.135848405	-0.721380114	-2.613569499
H	-2.363675985	-0.734979470	1.830542392
H	0.063616826	0.121320963	1.527443888
H	5.591843416	4.102093271	0.356422049
H	4.310892778	5.319191688	0.307216256
H	4.943109060	4.650380954	-1.201008546
H	4.225110308	-5.383062822	-0.027489268
H	3.001385018	-5.942602781	-1.171029642
H	2.768274311	-6.191335974	0.568156347
H	-1.211810927	0.866635851	-1.379730130
H	-1.055462841	-0.909349716	-1.441582417

1PAl[f]

Total number of atoms = 72

C	-0.058059671	-1.117736745	-0.799515680
C	0.482364447	-1.554761518	-1.945753941
P	0.830733646	-0.404993470	0.636403326
AL	-1.992362274	-1.260567857	-0.412852403
C	-3.338244095	-0.223093762	-1.456954755
C	-2.719257439	0.440940478	-2.695443204
C	-4.516533511	-1.106561077	-1.901167090
C	-3.878231016	0.885734140	-0.530645498
C	-2.573869418	-2.601349480	0.945359417
C	-3.067398743	-3.814182025	0.124632124
C	-3.727358918	-2.098484959	1.827293299
C	-1.423460984	-3.079611900	1.843711020
C	0.041128072	1.270156507	0.509492023
C	-1.435198907	3.683111915	0.419585309
C	-0.690888718	1.707745573	1.637061507
C	0.042569266	2.066426776	-0.659791812
C	-0.694786546	3.250868357	-0.677756064
C	-1.410269389	2.902532633	1.571261940
C	2.638995888	-0.322662052	0.253708280
C	5.407062269	-0.477278494	-0.348424566
C	3.450677257	0.835400141	0.308034563
C	3.266603197	-1.575729686	0.045302742
C	4.624410465	-1.623008555	-0.276191792
C	4.804869178	0.731542244	-0.012577694
C	-2.262621155	4.940168598	0.349655169
C	-0.722705744	0.936080500	2.939356695
C	0.828423265	1.722230296	-1.902954672
C	2.967075754	2.194075074	0.768395326
C	6.861315650	-0.541177396	-0.738613551
C	2.552098378	-2.896423475	0.232224580
H	-1.035981058	-2.281934993	2.487141737
H	-1.763380137	-3.898646808	2.498481995
H	-4.067900970	-2.892071746	2.512058603
H	-3.401086753	-4.620481649	0.797634620
H	-3.915759609	-3.567216448	-0.525677882
H	-4.597410542	-1.785970560	1.236597546
H	-3.427084007	-1.244027276	2.448406140
H	-0.576499034	-3.456434163	1.256834513
H	-2.272268591	-4.238634505	-0.505183626
H	-3.487693919	0.993833332	-3.260224333
H	-5.266334906	-0.502349194	-2.437212580
H	-5.028285210	-1.574003828	-1.051161585
H	-1.942998702	1.160560754	-2.415910820
H	-4.202032766	-1.908253644	-2.582680157
H	-2.270867849	-0.287912556	-3.383113028
H	-4.636026477	1.489012954	-1.057745330
H	-4.360061111	0.479334397	0.368193875

H	-3.087293010	1.573281179	-0.206863509
H	5.415162329	1.632293987	0.021678383
H	5.085757055	-2.593668444	-0.447725832
H	-0.685256005	3.857237480	-1.581740206
H	-1.968181023	3.230150940	2.445835737
H	1.552400209	-1.502479741	-2.160128746
H	7.283894441	-1.532477489	-0.547066109
H	7.455831880	0.194193590	-0.186790422
H	6.988970023	-0.330336446	-1.807426814
H	3.824606220	2.803077456	1.069861896
H	1.750453867	1.181939928	-1.681403571
H	2.434232711	2.743185844	-0.013031381
H	2.293883027	2.124665531	1.626650436
H	3.282668063	-3.696610421	0.382455855
H	1.928170649	-3.168364879	-0.624295592
H	1.895056456	-2.872856223	1.109486405
H	1.087761403	2.635954882	-2.446937150
H	-1.797333784	5.689313957	-0.298646494
H	-3.256371168	4.722832688	-0.060472708
H	-2.403303352	5.383707519	1.340034933
H	-1.264610298	1.502929753	3.702301365
H	0.283798591	0.730896960	3.316895390
H	-1.217332143	-0.034745689	2.828942538
H	0.243437089	1.084801674	-2.573389106
H	-0.127279426	-1.971156638	-2.749335706

TS13_PAI[f]

Total number of atoms = 74

C	0.666770090	-1.230304139	2.107374969
C	0.890311595	-0.552960940	0.973231736
AL	2.624815156	-0.427110836	-0.107497974
P	-0.471398777	-0.132646069	-0.144226916
C	3.499765737	1.379458450	-0.205025165
C	3.762452957	-2.084644404	-0.013802179
C	-1.079169982	1.586628425	-0.099831168
C	-2.092421527	4.210572905	-0.304011544
C	-1.819840237	1.979662910	-1.238704904
C	-0.834237449	2.518130776	0.931098658
C	-1.346613370	3.809211164	0.800467828
C	-2.320711470	3.277553986	-1.311259912
C	-1.877020236	-1.292974466	0.009596901
C	-3.958086996	-3.189318298	0.101292086
C	-1.834448825	-2.434768571	-0.820084282
C	-2.956169024	-1.111116466	0.897925171
C	-3.975498120	-2.063860416	0.920211778

C	-2.872969504	-3.360812695	-0.755208415
C	4.485489131	-2.299020192	-1.354510760
C	2.934423268	-3.343583168	0.282135440
C	4.814926838	-1.922758062	1.097552818
C	3.967052931	1.829135650	1.190293389
C	2.526370560	2.428111736	-0.766494019
C	4.727880920	1.331847681	-1.129245075
C	-2.099472250	1.038663684	-2.387885124
C	-0.045248517	2.202335321	2.177664740
C	-0.697100886	-2.683865123	-1.782139980
C	-3.061611108	0.062590283	1.839516562
C	-2.609598201	5.620586565	-0.424099564
C	-5.088527831	-4.185498012	0.126172961
H	-0.327583767	-1.456755716	2.500375242
H	-1.155574076	4.526588885	1.595448171
H	-2.896631992	3.569687784	-2.186760536
H	-4.804871570	-1.924933393	1.610493244
H	-2.832874059	-4.241069371	-1.393189381
H	5.135249090	-1.456420159	-1.618298668
H	3.774063609	-2.437010334	-2.179622250
H	5.121092695	-3.200252296	-1.317426295
H	2.398134346	-3.278061826	1.236052139
H	3.582400113	-4.235245688	0.329460936
H	2.186656315	-3.533186265	-0.499464203
H	4.353937877	-1.778508074	2.085156335
H	5.477110646	-1.066741080	0.915758928
H	5.455460057	-2.818291401	1.168605155
H	4.702973538	1.135683524	1.618443335
H	3.137471594	1.905271768	1.905485868
H	4.445934520	2.821955947	1.145793773
H	2.170486216	2.158304604	-1.769827793
H	3.014614825	3.414253449	-0.848457144
H	1.641282667	2.564694130	-0.134698473
H	5.499504887	0.648359477	-0.753656127
H	5.192739319	2.328728581	-1.214965738
H	4.466429212	1.008158741	-2.145632921
H	-2.616326951	1.564469170	-3.195210446
H	-2.727985986	0.194249236	-2.082384458
H	-1.172515841	0.623566100	-2.800482230
H	0.003717877	3.081992223	2.825234727
H	0.976925990	1.895848412	1.944382023
H	-0.488339007	1.385189744	2.753416142
H	0.276897324	-2.674376546	-1.280054577
H	-0.662723378	-1.921289729	-2.568918100
H	-0.809074268	-3.658540513	-2.264748213
H	-3.852332999	-0.108336390	2.575275939
H	-3.287725133	0.992979632	1.308927427

H	-2.129166033	0.220833220	2.388031050
H	1.673645852	-0.515782256	-1.632252822
H	0.673668383	-0.343132554	-1.339243745
H	-2.720816400	6.091226534	0.557344758
H	-3.580725167	5.647051341	-0.928297020
H	-1.918302572	6.237331722	-1.010774833
H	-4.728412960	-5.201217242	-0.064351244
H	-5.830085675	-3.948718890	-0.646244997
H	-5.604161175	-4.180864686	1.091120306
H	1.494025673	-1.609585261	2.707636432

3PAl[f]

Total number of atoms = 74

C	0.146081321	-1.643245390	1.758150392
C	0.509763250	-0.983393321	0.651840139
AL	2.390439504	-0.892306724	-0.268205268
P	-0.738130439	-0.161721282	-0.336160430
C	3.636406351	0.254964608	0.844004474
C	2.980961088	-2.805374804	-0.598331062
C	-0.415097054	1.615560670	-0.369784189
C	0.184780418	4.353259170	-0.432495720
C	-0.288382655	2.272621198	-1.611592101
C	-0.255207052	2.322675172	0.837632575
C	0.033880441	3.683440513	0.777946002
C	0.010885414	3.632678802	-1.612203507
C	-2.496783088	-0.614654400	-0.089082511
C	-5.102734852	-1.615126734	0.345207289
C	-2.795381186	-1.977992362	-0.339743797
C	-3.534992717	0.265002283	0.304973700
C	-4.807588021	-0.266441778	0.519072281
C	-4.086148401	-2.448253038	-0.106585440
C	4.052138978	-2.797512541	-1.701883980
C	1.811468245	-3.671740785	-1.084269422
C	3.569170402	-3.467373808	0.656192757
C	3.566837075	-0.115960940	2.333008384
C	3.283958874	1.741500372	0.694806162
C	5.085685775	0.068729866	0.365268592
C	-0.457115797	1.573899956	-2.938974375
C	-0.373191064	1.684384509	2.200847857
C	-1.791788734	-2.949216231	-0.914432842
C	-3.403818708	1.763998247	0.461913473
C	0.548523335	5.814095692	-0.470221616
C	-6.483017225	-2.146545238	0.628519631
H	-0.880276118	-1.723940723	2.128530968
H	0.157012018	4.231669785	1.708885881

H	0.114406000	4.144392405	-2.565953634
H	-5.603691425	0.409040664	0.823382695
H	-4.300267221	-3.497164642	-0.296035107
H	4.396875844	-3.821918434	-1.929383607
H	4.937473991	-2.215741629	-1.416032672
H	3.664973453	-2.366938949	-2.634834578
H	1.071468075	-3.827672700	-0.288795807
H	2.157059387	-4.671988103	-1.400155002
H	1.293530938	-3.222649903	-1.944474571
H	2.842433451	-3.499710576	1.480476583
H	4.456681497	-2.937994398	1.023456005
H	3.873903761	-4.509855594	0.455247423
H	2.555874834	0.020855450	2.742120388
H	4.247826283	0.509081010	2.937432253
H	3.847150578	-1.162720167	2.508805297
H	2.287583497	1.967358322	1.089663562
H	3.293962013	2.061774432	-0.355156676
H	3.999149591	2.378843458	1.245435612
H	5.438344250	-0.960687442	0.504601464
H	5.774696454	0.724058247	0.927079813
H	5.201040910	0.314155237	-0.699329276
H	-0.411289559	2.298735072	-3.755393906
H	-1.420294256	1.055363552	-3.017404148
H	0.346486237	0.843161262	-3.093652463
H	-0.596778864	2.445706326	2.953536300
H	0.565725446	1.195872613	2.480319614
H	-1.157475970	0.923446034	2.256571000
H	-0.870197709	-3.002975127	-0.333022397
H	-1.513872382	-2.674418219	-1.940113962
H	-2.216583105	-3.954936884	-0.955841376
H	-4.397257767	2.205502255	0.575662072
H	-2.929509076	2.230890479	-0.403985109
H	-2.823258034	2.046411058	1.343031795
H	1.970715072	-0.178510753	-1.690783154
H	-0.478887586	-0.587333880	-1.637437492
H	0.071481537	6.322359670	-1.313930626
H	1.632378322	5.932690979	-0.584079156
H	0.254332332	6.324613753	0.451380764
H	-7.254422616	-1.442484140	0.301223100
H	-6.620307965	-2.307080934	1.704354983
H	-6.654801891	-3.102694966	0.126047495
H	0.897082150	-2.154635243	2.358925786

1PAl[a]

Total number of atoms = 82

C	-0.238882947	-0.567895288	-0.045189507
C	-0.276253133	-1.716618887	-0.746898934
P	1.181748530	0.056138434	0.899221829
AL	-2.061581986	0.135703255	0.379993514
C	-2.811575473	1.888876547	-0.236518677
C	-2.424497320	2.307153765	-1.661556787
C	-4.347229664	1.866878453	-0.147570052
C	-2.273177251	2.961893047	0.733256523
C	-2.959876787	-0.843593568	1.879815624
C	-4.322095894	-1.418482116	1.457126811
C	-3.171740234	0.139026894	3.047866201
C	-2.082703028	-1.999371589	2.383226557
C	1.322379196	1.756996135	0.198373853
C	1.315439336	4.445820054	-0.671805706
C	1.454262207	2.810941572	1.128278703
C	1.224830909	2.060090088	-1.176848552
C	1.218534968	3.395399201	-1.580654800
C	1.452115468	4.131458647	0.676785923
C	2.666329182	-0.959600650	0.439437369
C	4.731102370	-2.806025851	-0.197306309
C	3.845386720	-0.523083967	-0.210377817
C	2.610973648	-2.304123903	0.893135378
C	3.622307298	-3.198659997	0.543705803
C	4.834974386	-1.459137240	-0.524080655
C	-1.557143101	-2.214211561	-1.291208263
C	-4.119801936	-3.075840741	-2.079599304
C	-2.484770395	-1.318919681	-1.850243668
C	-1.925927976	-3.561491181	-1.178267524
C	-3.191659282	-3.984058458	-1.565038337
C	-3.759995158	-1.742839078	-2.231309651
C	1.256136719	5.877752034	-1.137295159
C	1.599080955	2.569212275	2.614302870
C	1.159066945	1.008102828	-2.260108987
C	4.172677048	0.918601349	-0.538595594
C	5.792619732	-3.795837110	-0.602231075
C	1.525080076	-2.812863807	1.814881563
H	-1.102816843	-1.649540707	2.730285641
H	-2.569746675	-2.511126463	3.229792253
H	-3.635972399	-0.375692826	3.905104778
H	-4.813189195	-1.910405658	2.313311575
H	-5.009144052	-0.646272027	1.090662214
H	-3.831777732	0.972577065	2.778901836
H	-2.224953145	0.566396585	3.407349478
H	-1.910532745	-2.750033871	1.602388327
H	-4.216414903	-2.171353770	0.666527425
H	-2.812406455	3.315425876	-1.880459373
H	-4.765243732	2.841310447	-0.449130352

H	-4.704462589	1.664780804	0.868609183
H	-1.339591858	2.344713711	-1.800333678
H	-4.785973215	1.106592262	-0.808109388
H	-2.847913348	1.639295618	-2.423994676
H	-2.726950487	3.941996607	0.511388031
H	-2.504171548	2.736705262	1.783142940
H	-1.187309461	3.083649695	0.644562537
H	5.731378131	-1.110395706	-1.033251346
H	3.549462173	-4.228867777	0.887014018
H	1.139200837	3.619902961	-2.642850149
H	1.550718760	4.936090739	1.402281452
H	0.598681552	-2.354474127	-0.896980225
H	-2.167009909	-0.305796264	-2.089515076
H	-4.455649173	-1.029543255	-2.663829778
H	-5.108807941	-3.413740322	-2.372471050
H	-3.464186739	-5.029512033	-1.453879226
H	-1.218045569	-4.271394589	-0.758402046
H	5.909953725	-4.584448664	0.148183334
H	6.763063039	-3.308346859	-0.738515421
H	5.532351962	-4.281457397	-1.550671245
H	5.246963303	1.014131837	-0.722025482
H	1.722088678	0.107347332	-2.005951608
H	3.656881114	1.280417249	-1.431551915
H	3.915563925	1.597989241	0.276704200
H	1.784165744	-3.806193733	2.192508150
H	0.548661043	-2.885068247	1.327723577
H	1.399751483	-2.145871384	2.675041340
H	1.560268764	1.411042845	-3.195673201
H	1.762308850	6.006565887	-2.099380284
H	0.215017424	6.196042845	-1.269587562
H	1.719408867	6.554637787	-0.413113373
H	1.782909340	3.513189238	3.135877025
H	2.427677769	1.890157166	2.840547580
H	0.696555595	2.115987959	3.037813452
H	0.127770110	0.693080564	-2.449213955

TS13_PAl[a]

Total number of atoms = 84

C	-0.868384590	0.993636394	1.194885471
C	-0.630785038	0.104182517	0.211696535
AL	-1.898155999	-0.838901806	-1.102812192
P	1.022322952	0.012952672	-0.502451270
C	-2.082741943	-2.839379369	-0.948476360
C	-3.453214021	0.255762241	-1.779564364
C	2.098133845	-1.300984708	0.165708264

C	3.883854670	-3.340974976	0.942173597
C	3.226493819	-1.604501860	-0.630609071
C	1.858025449	-2.033109591	1.348223227
C	2.759305089	-3.037241301	1.703453710
C	4.101616716	-2.608157834	-0.220972383
C	1.867401603	1.632111786	-0.426555418
C	3.023510449	4.200016544	-0.469774490
C	1.603026726	2.512547165	-1.500155426
C	2.702953236	2.043589476	0.629900291
C	3.268566835	3.320096678	0.578771278
C	2.182856644	3.777466968	-1.498639456
C	-3.480342232	0.106157867	-3.313172837
C	-3.327968641	1.750912033	-1.451221545
C	-4.798539644	-0.244203638	-1.224765487
C	-2.868972656	-3.265008940	0.301782211
C	-0.703212726	-3.516289125	-0.913592530
C	-2.823206101	-3.362364993	-2.191933447
C	3.530433328	-0.866983636	-1.914483168
C	0.687966751	-1.799992269	2.274523324
C	0.714443561	2.119469182	-2.656369399
C	3.023257820	1.176109911	1.823032508
C	-2.160341401	1.187748466	1.871940703
C	-4.629359276	1.615939666	3.130080436
C	-2.468279260	2.431526992	2.437823394
C	-3.095751507	0.152643033	1.980854691
C	-4.322163206	0.365214458	2.600244219
C	-3.696164637	2.648200430	3.051453714
C	4.818846881	-4.451644520	1.344834320
C	3.627584103	5.580502677	-0.493852515
H	-0.074793329	1.653087638	1.563176174
H	2.574363511	-3.600559515	2.615273100
H	4.971972490	-2.829139376	-0.835226899
H	3.915813469	3.636238332	1.394013575
H	1.973780451	4.453494814	-2.325057320
H	-4.326800024	0.668216849	-3.743117227
H	-3.593719119	-0.938555683	-3.629059422
H	-2.562878714	0.491098005	-3.777488030
H	-3.361008792	1.941203553	-0.373026758
H	-4.156317366	2.317564407	-1.909704446
H	-2.394505917	2.184482223	-1.834058149
H	-4.874144612	-0.095989504	-0.141215175
H	-4.964542316	-1.309397971	-1.428030908
H	-5.637204680	0.305604471	-1.685143212
H	-2.338804741	-3.003462573	1.228417015
H	-3.020376091	-4.357673067	0.323353906
H	-3.863779510	-2.800847309	0.344582709
H	-0.092375894	-3.245400688	-1.785432937

H	-0.804853219	-4.615109317	-0.916394147
H	-0.128346585	-3.253687584	-0.018558356
H	-3.839665713	-2.959172437	-2.274251333
H	-2.912323725	-4.461710573	-2.159987519
H	-2.292434013	-3.107353734	-3.119007392
H	4.400528446	-1.305911409	-2.409876646
H	3.745826438	0.192931189	-1.736437555
H	2.687953307	-0.914340136	-2.614529728
H	0.711020685	-2.525671178	3.091904205
H	-0.270780539	-1.898709735	1.759839567
H	0.700186972	-0.798537608	2.715606578
H	-0.278473486	1.794461025	-2.323973825
H	1.147308125	1.293252077	-3.232409885
H	0.571760334	2.963317459	-3.336709878
H	3.504454997	1.770054175	2.605045940
H	3.696930531	0.354524709	1.558947600
H	2.122491365	0.729350340	2.253178055
H	-1.742029723	3.238315172	2.373746081
H	-2.853233551	-0.832134314	1.592673442
H	-5.037135907	-0.449188078	2.671113640
H	-3.925563872	3.622642584	3.472293011
H	-5.587640110	1.782828519	3.612613421
H	-0.649884004	-0.725632940	-2.382777598
H	0.262324725	-0.462300946	-1.880202648
H	5.858386749	-4.205920090	1.105504602
H	4.569652891	-5.378103799	0.813796548
H	4.754401033	-4.657954117	2.417310763
H	2.857051336	6.345826183	-0.344336682
H	4.106223821	5.783952818	-1.457706615
H	4.379263732	5.703464150	0.291193866

3PAl[a]

Total number of atoms = 84

C	0.780422524	1.147277633	-0.997150515
C	0.645419798	0.192097302	-0.049831395
AL	1.988217818	-0.778274743	1.273081178
P	-1.033842744	-0.004283568	0.507166936
C	2.380082049	-2.712127160	0.794076868
C	3.565086844	0.406563520	1.767394865
C	-1.948872889	-1.440947405	-0.125103719
C	-3.509283118	-3.627841166	-0.955853992
C	-3.036460939	-1.876499277	0.667570491
C	-1.634090596	-2.106261078	-1.328696538
C	-2.427462526	-3.187609199	-1.712036574
C	-3.797990537	-2.956713267	0.229592693

C	-2.050638595	1.506242793	0.438609311
C	-3.534631257	3.892341844	0.501158838
C	-1.874408504	2.417684123	1.502751362
C	-2.943281871	1.802598360	-0.613032425
C	-3.669541182	2.989866523	-0.552568057
C	-2.625794462	3.592417100	1.510955289
C	3.817452329	0.142081018	3.265040812
C	3.248985153	1.900616868	1.608030132
C	4.869853050	0.103744531	1.014871378
C	3.097733264	-2.937619338	-0.543671782
C	1.081160259	-3.533279549	0.797654972
C	3.275986029	-3.271522553	1.914444274
C	-3.411568754	-1.229765162	1.982177813
C	-0.488215631	-1.731335278	-2.238362670
C	-0.904692302	2.173025361	2.635787022
C	-3.147419630	0.908614494	-1.812724103
C	2.006983900	1.463197482	-1.742585708
C	4.306767843	2.099767367	-3.207812780
C	2.170657315	2.740331691	-2.295068955
C	3.000149649	0.503152533	-1.958652959
C	4.141658592	0.819321219	-2.686262078
C	3.317122905	3.061673546	-3.011050590
C	-4.328838144	-4.815569074	-1.387525812
C	-4.354111108	5.156157392	0.534170780
H	-0.069758402	1.770051524	-1.300486144
H	-2.187008058	-3.703516028	-2.638332263
H	-4.636980790	-3.288140822	0.837109748
H	-4.358228724	3.222924985	-1.361727655
H	-2.488448000	4.295031333	2.329422432
H	4.659709878	0.753998616	3.633055586
H	4.068858172	-0.907668103	3.464685515
H	2.938259489	0.385635945	3.874886983
H	3.107503459	2.184080831	0.558968030
H	4.068851489	2.523465653	2.007163625
H	2.338815186	2.185624832	2.154990410
H	4.794748933	0.336825262	-0.052536980
H	5.161437023	-0.950381487	1.104978018
H	5.704382113	0.704294052	1.417906567
H	2.477670310	-2.642269462	-1.401957104
H	3.346157497	-4.003478878	-0.690928507
H	4.039398926	-2.375588972	-0.606103815
H	0.395673605	-3.239624838	-0.006259766
H	0.538209739	-3.422324689	1.745569013
H	1.287909115	-4.609660990	0.660102756
H	4.257194367	-2.782071421	1.944244892
H	3.457134857	-4.351511108	1.771838015
H	2.815803983	-3.146468572	2.903935465

H	-4.339062722	-1.663017326	2.364554933
H	-3.567248701	-0.149529312	1.888674984
H	-2.638376079	-1.393515661	2.742965479
H	-0.440843596	-2.427107977	-3.079914224
H	0.470251497	-1.765252016	-1.716001655
H	-0.587013818	-0.721067545	-2.647345814
H	0.079371369	1.842335097	2.286768903
H	-1.275459226	1.407725403	3.329369426
H	-0.756690121	3.090742529	3.210332208
H	-3.732186727	1.430831329	-2.574579172
H	-3.676931567	-0.013244133	-1.553268393
H	-2.197324846	0.621984422	-2.273119328
H	1.397147541	3.489816030	-2.143184350
H	2.872214024	-0.496180372	-1.557119605
H	4.905191369	0.062683154	-2.840547194
H	3.439048260	4.060106521	-3.420370412
H	5.201681368	2.347066654	-3.771120755
H	0.961584328	-0.805167624	2.562563938
H	-0.939088241	-0.287062806	1.868521034
H	-5.392651880	-4.660932637	-1.181533203
H	-4.015422863	-5.715392963	-0.845383287
H	-4.211262862	-5.014486131	-2.456585682
H	-5.404397916	4.932157461	0.754179335
H	-4.325695367	5.669585868	-0.432501077
H	-3.992634528	5.849420427	1.298782284

TS14_PAl[a]

Total number of atoms = 85

C	-0.2514800000	-1.4902900000	-0.9879600000
C	-0.2839400000	-0.4791700000	-0.1031600000
P	1.2301000000	0.1499900000	0.7123000000
C	2.6518500000	-0.9824000000	0.3609100000
C	3.9035700000	-0.5885400000	-0.1736000000
C	2.4977900000	-2.3241900000	0.7925200000
C	4.8864500000	-1.5572200000	-0.3859100000
C	3.5133500000	-3.2507400000	0.5547600000
C	4.7062100000	-2.8980500000	-0.0635100000
C	1.4290600000	1.7600100000	-0.1743500000
C	1.5200600000	2.9310700000	0.6084500000
C	1.3926200000	1.8823500000	-1.5829600000
C	1.5023200000	4.1807900000	-0.0140500000
C	1.3832100000	3.1514900000	-2.1579800000
C	1.4088300000	4.3153400000	-1.3942600000
C	-3.2047000000	-1.1965100000	1.5402000000

C	-2.8382300000	1.9362200000	0.0820200000
Al	-2.0466300000	0.1736900000	0.6274000000
C	-0.1330300000	0.4346500000	3.1211000000
C	-1.4407100000	-1.9877300000	-1.7092200000
C	-1.6515200000	-3.3606200000	-1.8876700000
C	-2.3782300000	-1.0933300000	-2.2411800000
C	-2.7901900000	-3.8237400000	-2.5364800000
C	-3.5174100000	-1.5555400000	-2.8949700000
C	-3.7299700000	-2.9225700000	-3.0377300000
C	1.4027800000	0.7075900000	-2.5312400000
C	1.3248000000	5.6712900000	-2.0447300000
C	1.6557200000	2.9233600000	2.1153200000
C	1.2895100000	-2.8222500000	1.5512000000
C	5.7741400000	-3.9229300000	-0.3457000000
C	4.2994600000	0.8392200000	-0.4842400000
C	-4.2461100000	-1.8331400000	0.6021800000
C	-3.9692600000	-0.5238400000	2.6968500000
C	-2.3449600000	-2.3328600000	2.1158300000
C	-2.0022000000	2.6645800000	-0.9805000000
C	-4.2520300000	1.7019700000	-0.4820700000
C	-2.9590300000	2.8717600000	1.2999300000
O	-1.0947300000	0.7835400000	2.5212500000
O	0.6194100000	0.1479900000	3.9598100000
H	0.6831700000	-2.0024800000	-1.2377100000
H	5.8393000000	-1.2416600000	-0.8060500000
H	3.3683700000	-4.2773900000	0.8854900000
H	1.5653000000	5.0748500000	0.6029100000
H	1.3528300000	3.2323400000	-3.2429500000
H	-0.9218100000	-4.0664000000	-1.4980700000
H	-2.1909800000	-0.0242200000	-2.1732800000
H	-2.9480000000	-4.8918400000	-2.6531700000
H	-4.2335100000	-0.8444200000	-3.2964500000
H	-4.6178800000	-3.2878700000	-3.5444100000
H	1.9421200000	-0.1522000000	-2.1287800000
H	0.3857900000	0.3747700000	-2.7622200000
H	1.8815700000	0.9951200000	-3.4725600000
H	1.8641900000	5.6928500000	-2.9970100000
H	0.2794700000	5.9291800000	-2.2529000000
H	1.7365000000	6.4524700000	-1.3986700000
H	0.6727500000	2.8980300000	2.6016200000
H	2.2350100000	2.0737000000	2.4840700000
H	2.1503500000	3.8394400000	2.4517300000
H	0.9046700000	-2.0726100000	2.2489700000
H	0.4630600000	-3.0906900000	0.8874500000
H	1.5538800000	-3.7088000000	2.1347900000
H	5.7815500000	-4.7104100000	0.4144300000
H	5.6056000000	-4.4045100000	-1.3166200000

H	6.7681900000	-3.4660500000	-0.3738200000
H	3.8514100000	1.2126000000	-1.4087800000
H	4.0118200000	1.5309900000	0.3110600000
H	5.3856900000	0.8998000000	-0.5979100000
H	-4.8846500000	-1.0870400000	0.1144100000
H	-3.7803600000	-2.4345300000	-0.1848400000
H	-4.9087400000	-2.5038300000	1.1744800000
H	-4.6465400000	0.2619300000	2.3391500000
H	-4.5891600000	-1.2640700000	3.2289100000
H	-3.3013600000	-0.0696600000	3.4396100000
H	-1.8150900000	-2.8755100000	1.3240000000
H	-1.5919200000	-1.9768900000	2.8332400000
H	-2.9719200000	-3.0628000000	2.6539100000
H	-1.0159300000	2.9425600000	-0.5972200000
H	-1.8388700000	2.0651100000	-1.8859400000
H	-2.5053400000	3.5933500000	-1.2979500000
H	-4.7031500000	2.6559000000	-0.8014100000
H	-4.2503000000	1.0372300000	-1.3561600000
H	-4.9254100000	1.2594400000	0.2618500000
H	-3.5346500000	2.4228600000	2.1192000000
H	-1.9746100000	3.1464700000	1.6994400000
H	-3.4673800000	3.8086300000	1.0181000000

4PAl[a]

Total number of atoms = 85

C	-0.8280753310	1.1963060250	1.1963582970
C	-0.6597883300	0.2180829390	0.2839564820
P	0.9917905240	0.0215331470	-0.3678756610
C	1.9459054130	1.5794776880	-0.3049448200
C	2.8530886730	1.8486623920	0.7478547070
C	1.7130970080	2.5578992010	-1.2981824250
C	3.5707219910	3.0428891330	0.7202837490
C	2.4623546260	3.7339060330	-1.2730635670
C	3.4136820490	3.9864723510	-0.2914878260
C	1.9559485470	-1.3659460950	0.3410947520
C	3.1839575710	-1.7039627940	-0.2721019730
C	1.5129035810	-2.1007543350	1.4733448960
C	3.8958565370	-2.8072620720	0.2073428660
C	2.2655802330	-3.1925916600	1.8942120270
C	3.4488252810	-3.5793248590	1.2677658860
C	-3.4605623840	0.3923425530	-1.6737522900
C	-2.3709718920	-2.7270582860	-0.6256912430
Al	-1.9805120170	-0.7761999720	-0.9577224630
C	0.5990050860	-0.5415689650	-2.1707916250

C	-2.0885425170	1.5011833470	1.8886203990
C	-2.3231452920	2.7999296310	2.3583348590
C	-3.0608311220	0.5196071690	2.1089930070
C	-3.5182817410	3.1199784100	2.9904674830
C	-4.2524223070	0.8356821500	2.7517942250
C	-4.4879739020	2.1376976100	3.1858256300
C	0.3051431800	-1.7622152120	2.3177408180
C	4.2117819000	-4.7863632870	1.7448224070
C	3.8533290100	-0.9488645320	-1.3992472890
C	0.6770723090	2.4202056090	-2.3866166500
C	4.2416920110	5.2442664470	-0.3108401740
C	3.0801432200	0.9466479900	1.9403916320
C	-4.8164065750	0.0799454180	-1.0159565240
C	-3.5818627390	0.1085811280	-3.1850992490
C	-3.1954487610	1.8959246820	-1.5033903650
C	-3.1635593800	-2.9867552540	0.6654013260
C	-3.2098554830	-3.2420112460	-1.8122923270
C	-1.0847040880	-3.5704910110	-0.5958553920
O	-0.6372597570	-0.8342231080	-2.2899136070
O	1.4756676870	-0.5901319090	-3.0056332940
H	0.0031415310	1.8453562050	1.4924453230
H	4.2692088070	3.2477116310	1.5284652160
H	2.2828896070	4.4790011510	-2.0446280020
H	4.8373762720	-3.0582548610	-0.2761545640
H	1.9183219770	-3.7586735810	2.7551734120
H	-1.5671233790	3.5662241560	2.2039954130
H	-2.8766330280	-0.5015521020	1.7894205510
H	-3.6943660490	4.1350672160	3.3333836880
H	-4.9979119900	0.0624138740	2.9114282940
H	-5.4208945860	2.3848260420	3.6833370910
H	0.4083879690	-0.7873988340	2.8058769670
H	-0.6189222860	-1.7261579320	1.7408901940
H	0.1842393090	-2.5151154310	3.1008649920
H	4.3523254110	-4.7612586220	2.8307140960
H	3.6648725280	-5.7059353000	1.5072166900
H	5.1963111840	-4.8510188680	1.2733643780
H	3.7306736820	-1.4829317730	-2.3449967780
H	3.4672408200	0.0558658060	-1.5584476330
H	4.9243303670	-0.8672224700	-1.1855940540
H	1.0632374730	1.8540515310	-3.2396399720
H	-0.2305592870	1.9232237280	-2.0354886070
H	0.3789375590	3.4095993580	-2.7436684800
H	4.4615063580	5.5927008420	0.7030395220
H	5.2000161850	5.0652499010	-0.8126233630
H	3.7331096480	6.0503683020	-0.8478311750
H	2.1434864780	0.5668044750	2.3579554070
H	3.7034756670	0.0821736310	1.6943873360

H	3.5829393020	1.5078894960	2.7326993180
H	-5.0899029660	-0.9782725920	-1.1041972700
H	-4.8242362520	0.3380506850	0.0494487300
H	-5.6217415460	0.6615457740	-1.4959296780
H	-3.8214643950	-0.9407058350	-3.3952283930
H	-4.3866997700	0.7200254740	-3.6272213200
H	-2.6548811570	0.3446860160	-3.7220550770
H	-3.1113084010	2.1885718880	-0.4509240110
H	-2.2772081990	2.2125341760	-2.0131316620
H	-4.0192166180	2.4842956960	-1.9420025310
H	-2.5863093910	-2.7360768480	1.5663643540
H	-4.0992717000	-2.4122381040	0.6995414600
H	-3.4351023820	-4.0522441740	0.7548212110
H	-3.4008560310	-4.3234690560	-1.7071712410
H	-4.1864443600	-2.7495301470	-1.8823513340
H	-2.6949149530	-3.0958649790	-2.7705575510
H	-0.5029014720	-3.4543229320	-1.5185471740
H	-0.4252088520	-3.3179927390	0.2408564020
H	-1.3253523240	-4.6426670880	-0.4961482500