Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Are intramolecular frustrated Lewis pairs also intramolecular catalysts? A theoretical study on H_2 activation.

Lei Liu Zeonjuk,[a] Petko St. Petkov,[a] Thomas Heine,[a] Gerd-Volker Röschenthaler,[a] Johannes Eicher,[b] Nina Vankova,[*a]

[a] Department of Physics & Earth Sciences, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

[b]Solvay Fluor GmbH, Hans-Böckler-Allee 20, 30173 Hannover, Germany

Tables

Table S1. Relative potential energies (ΔE) calculated at different levels of theory for the three conformations of $Mes_2PCH_2CH_2B(C_6F_5)_2$, **1**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the energy of the closed form of **1**).

Level of theory	**1**	*gauche*-**1**	*trans*-**1**
B97D/6-31G* (gas-phase geometry)	0.0	25.7	13.8
SCS-MP2/cc-pVTZ//B97D/6-31G* (gas-phase geometry + solvent corrections)	0.0	39.5	24.4
ωB97XD/6-31+G** (solvent-phase geometry)	0.0	38.7	23.8
SCS-MP2/cc-pVTZ//B97D/6-31+G** (solvent-phase geometry)	0.0	41.6	33.5

Table S2. Relative potential energies (ΔE) calculated at different levels of theory for the stationary points along the reaction coordinate of an *intramolecular* H_2 activation by **1**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the total energy of the closed conformer and an isolated H_2 molecule (**1** + H_2).

Level of theory	*gauche*-**1** + H_2	TS**1**	*gauche*-PD**1**	*trans*-PD**1**
B97D/6-31G* (gas phase)	25.7	80.6	28.1	23.4
B97D/6-31+G** (gas phase)	24.8	68.3	2.1	4.2
B97D/6-31G* (single point solvent phase)	29.6	68.6	–6.4	–17.0
B97D/6-31+G** (solvent phase)	25.4	68.6	–11.2	–15.4
SCS-MP2/cc-pVTZ//B97D/6-31G* (gas phase)	38.9	104.3	19.6	19.9
SCS-MP2/cc-pVTZ//B97D/6-31G* (single point solvent phase)	39.5	104.8	7.3	1.5
SCS-MP2/cc-pVTZ//B97D/6-31+G** (solvent phase)	41.6	102.1	7.7	–2.3

Table S3. Relative Gibbs energies (ΔG) calculated at different levels of theory for the stationary points along the reaction coordinate of an *intramolecular* H_2 activation by **1**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the total energy of the closed conformer and an isolated H_2 molecule (**1** + H_2).

Level of theory	*gauche*-**1** + H_2	TS**1**	*gauche*-PD**1**	*trans*-PD**1**
B97D/6-31G* (gas phase)	15.6	103.8	43.1	43.8
B97D/6-31+G** (gas phase)	17.2	94.7	21.2	26.5
B97D/6-31G* (single point solvent phase)	19.5	91.8	8.5	3.3
B97D/6-31+G** (solvent phase)	15.5	91.4	4.9	4.1
SCS-MP2/cc-pVTZ//B97D/6-31G* (gas phase)	25.4	140.0	56.8	62.3
SCS-MP2/cc-pVTZ//B97D/6-31G* (single point solvent phase)	29.3	128.0	22.2	21.9
SCS-MP2/cc-pVTZ//B97D/6-31+G** (solvent phase)	31.6	124.9	23.8	17.2

Table S4. Relative potential energies (ΔE) calculated at three different density functionals, at the MP2 and at the SCS-MP2 levels of theory for the stationary points along the reaction coordinate of an *intramolecular* H_2 activation by **1**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the total energy of the open *gauche* conformer and an isolated H_2 molecule (*gauche*-**1** + H_2). The tabulated values are derived from gas-phase single point calculations on geometries optimized at the B97D/6-31G* level of theory, without inclusion of the ZPE corrections.

Level of theory	TS**1a**	*gauche*-PD**1**	*trans*-PD**1**
B97D/6-31G*	39.05	-23.15	-27.70
MP2/cc-pVTZ	34.48	-45.27	-49.34
SCS-MP2/cc-pVTZ	49.60	-44.83	-44.37
B97D3/6-31G*	34.65	-23.62	-25.71
M062X/6-31G*	48.25	-35.73	-37.98

Table S5. Relative potential energies (ΔE) calculated at three different density functionals, at the MP2 and at the SCS-MP2 levels of theory for the stationary points along the reaction coordinate of an *intramolecular* H_2 activation by **2**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the total energy of the open *cis* conformer and an isolated H_2 molecule (*cis*-**1** + H_2). The tabulated values are derived from gas-phase single point calculations on geometries optimized at the B97D/6-31G* level of theory, without inclusion of the ZPE corrections.

Level of theory	TS**2**	*gauche*-PD**2**
B97D/6-31G*	45.54	-43.93
MP2/cc-pVTZ	32.58	-58.21
SCS-MP2/cc-pVTZ	45.68	-51.13
B97D3/6-31G*	42.15	-41.46
M062X/6-31G*	34.04	-60.98

Table S6. Relative potential energies (ΔE) calculated at three different density functionals, at the MP2 and at the SCS-MP2 levels of theory for the stationary points along the reaction coordinate of an *intermolecular* H_2 activation by **1**. All energy values are in $kJ \cdot mol^{-1}$, and are referred to the total energy of the open *gauche* conformer and an isolated H_2 molecule (*gauche*-**1** + H_2). The tabulated values are derived from gas-phase single point calculations on geometries optimized at the B97D/6-31G* level of theory, without inclusion of the ZPE corrections.

Level of theory	*trans*-**1**	dimer-**1**	TS**1b**	dimer-PD**1**	TS**1c**	dimer-PD**1'**
B97D/6-31G*	-27.69	-141.40	-104.20	-150.98	-142.81	-249.10
MP2/cc-pVTZ	-38.28	-147.10	-114.62	-162.15	-151.43	-278.87
SCS-MP2/cc-pVTZ	-34.44	-110.73	-71.22	-120.12	-99.83	-226.07
B97D3/6-31G*	-27.82	-132.31	-98.16	-139.07	-129.24	-228.34
M062X/6-31G*	-24.33	-95.70	-66.82	-108.03	-97.36	-217.38

Table S7. Selected distances and bond lengths (in Å), and natural charges (in units of elementary charge) of the P, B and H atoms from H_2, as obtained for the stationary points along the reaction path of the *intramolecular* mechanism of the H_2 activation by **1**. TS and PD denote transition state and hydrogenated product, respectively. H_P and H_B denote the hydrogen atoms that are close or bound to phosphorus and boron, respectively. The equilibrium H−H bond is calculated as d_{HH} = 0.74 Å. All parameters are derived from B97D/6-31G(d,p) calculations in gas phase.

Stationary points along the reaction coordinate	**Distances and bond lengths**				**Natural charges**			
	d_{PB}, Å	d_{PH}, Å	d_{BH}, Å	d_{HH}, Å	P	B	H_P	H_B
1	2.22	–	–	–	+1.16e	+0.39e	–	–
gauche-**1**	3.29	–	–	–	+0.83e	+0.87e	–	–
TS**1a**	3.39	2.01	1.60	0.82	+0.87	+0.63e	+0.13e	0.00e
gauche-PD**1**	3.18	1.40	1.23	2.16	+1.33e	+0.11e	+0.06e	-0.02e
trans-PD**1**	4.09	1.40	1.22	5.10	+1.32e	+0.13e	+0.05e	0.01e

Table S8. Selected distances and bond lengths (in Å), and natural charges (in units of elementary charge) of the P, B and H atoms from H_2, as obtained for the stationary points along the reaction path of the *intramolecular* mechanism of the H_2 activation by **1**. TS and PD denote transition state and hydrogenated product, respectively. H_P and H_B denote the hydrogen atoms that are close or bound to phosphorus and boron, respectively. The equilibrium H−H bond is calculated as d_{HH} = 0.74 Å. All parameters are derived from B97D/6-31G(d,p) calculations in solvent phase (toluene, ε = 2.3741).

Stationary points along the reaction coordinate	**Distances and bond lengths**				**Natural charges**			
	d_{PB}, Å	d_{PH}, Å	d_{BH}, Å	d_{HH}, Å	P	B	H_P	H_B
1	2.20	–	–	–	+1.16e	+0.42e	–	–
gauche-**1**	3.30	–	–	–	+0.82e	+0.87e	–	–
TS**1a**	3.39	2.01	1.60	0.82	+0.87e	+0.63e	+0.13e	0.00e
gauche-PD**1**	3.21	1.40	1.22	2.19	+1.33e	+0.11e	+0.06e	-0.01e
trans-PD**1**	4.10	1.40	1.22	5.12	+1.32e	+0.13e	+0.06e	0.00e

Table S9. Potential energy of dimerization without (ΔE) and with (CP-ΔE) the counterpoise correction (CP) included, as calculated for compound **1**. The values (in kJ·mol^{-1}) are obtained at the SCS-MP2/cc-pVTZ//B97D/6-31G(d) level of theory.

Dimerization reaction	**ΔE**	**CP**	**CP-ΔE**
2*trans*-**1** → dimer-**1**	–76.3	49.8	–26.5
2*trans*-PD**1** → dimer-PD**1'**	–137.2	53.2	–84.1

Table S10. Relative potential energies (ΔE, 0K) and Gibbs energies (ΔG, 298.15K) calculated for the three conformations of $Mes_2PCHPhCH_2B(C_6F_5)_2$, **2**. All energy values are in $kJ \cdot mol^{-1}$, calculated at the SCS-MP2/cc-pVTZ//B97D/6-31G(d) level of theory (gas-phase optimization with single point corrections for toluene), and are referred to the energy of the closed form of **2**.

Relative energy	**2**	*cis*-**2**	*trans*-**2**
ΔE_{sol}	0.0	29.4	30.4
ΔG_{sol}	0.0	23.3	24.7

Table S11. Selected distances and bond lengths (in Å), as obtained for the stationary points along the reaction path of the *intramolecular* mechanism of the H_2 activation by **2**. TS and PD denote transition state and hydrogenated product, respectively. The equilibrium H−H bond is calculated as d_{HH} = 0.74 Å. All parameters are derived from B97D/6-31G(d) calculations in gas phase.

Stationary points along the reaction coordinate	**Distances and bond lengths**			
	d_{PB}, Å	d_{PH}, Å	d_{BH}, Å	d_{HH}, Å
2	2.17	–	–	–
cis-**2**	2.77	–	–	–
TS**2**	3.24	2.17	1.68	0.80
gauche-PD**2**	3.25	1.40	1.22	2.21

Figures

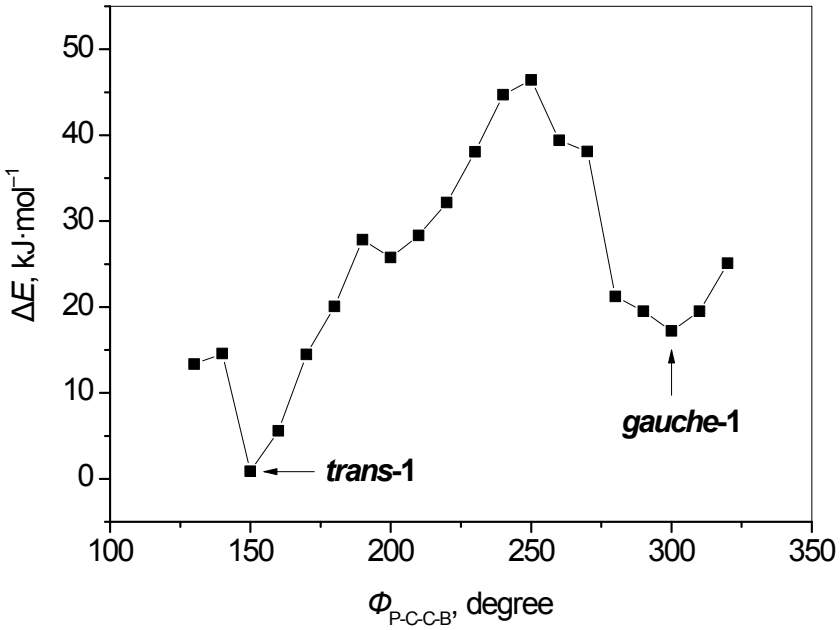

Figure S1. Relaxed scan of the potential energy surface with respect to the PCCB torsion angle in $Mes_2PCH_2CH_2B(C_6F_5)_2$, **1**, for an estimation of the energy required for isomerization of conformer *gauche*-**1** to conformer *trans*-**1**. The values of the potential energy, calculated at the SCS-MP2/cc-pVTZ//B97D/6-31G(d) level of theory, are shown with respect to the energy of *trans*-**1**.

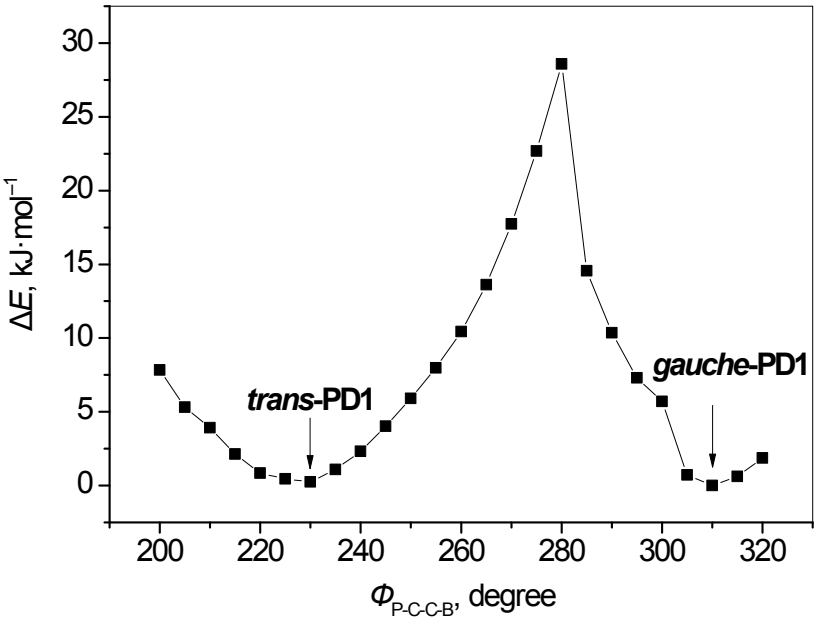

Figure S2. Relaxed scan of the potential energy surface with respect to the PCCB torsion angle in the hydrogenated product of **1**, $Mes_2PH^+CH_2CH_2BH^-(C_6F_5)_2$, for an estimation of the energy required for isomerization of conformer *gauche*-PD**1** to conformer *trans*-PD**1**. The values of the potential energy, calculated at the SCS-MP2/cc-pVTZ//B97D/6-31G(d) level of theory, are shown with respect to the energy of *trans*-PD**1**.

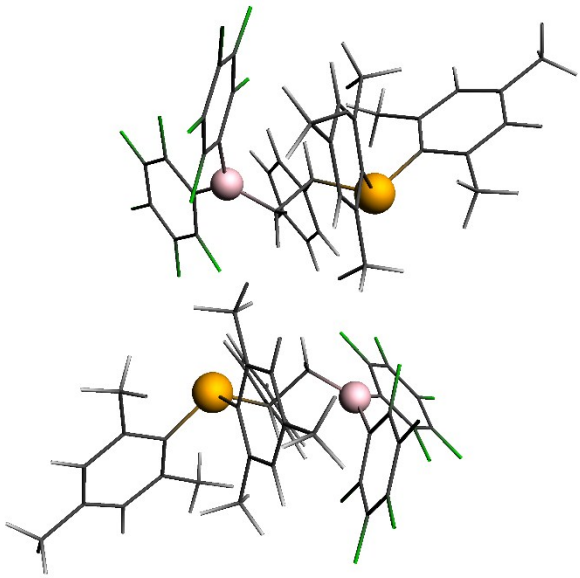

Figure S3. Fully-optimized (B97D/6–31G(d)) structure of two closely lying *trans* monomers of $Mes_2PCHPhCH_2B(C_6F_5)_2$ (**2**). The calculated *intermolecular* P–B' and P'–B distances are of the order of 5.8 Å. Color code: P yellow, B pink, F green, C grey, H white.

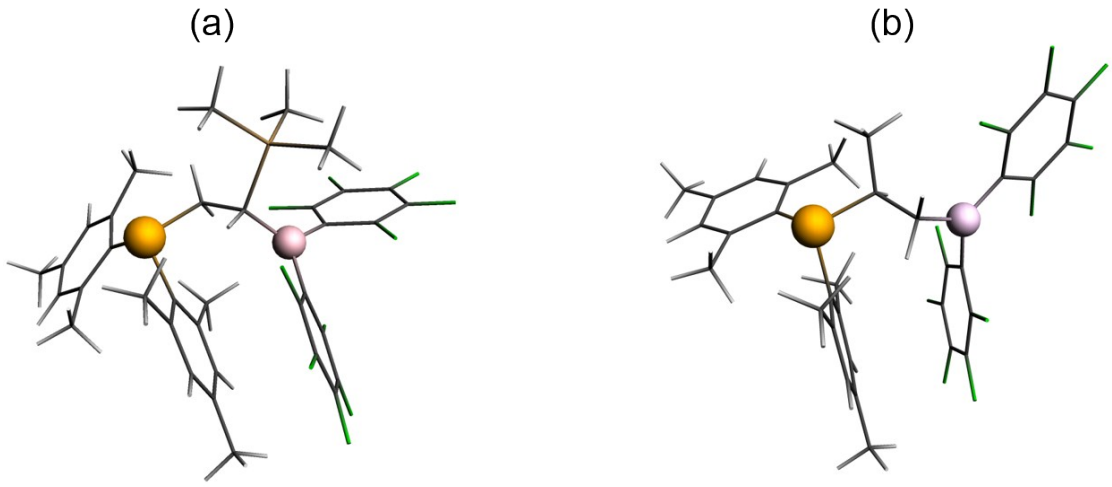

Figure S4. Fully-optimized (B97D/6–31G(d)) structures of the *trans* conformers of $Mes_2PCH_2CH(SiMe_3)B(C_6F_5)_2$, *trans*-**3**, in (a), and $Mes_2PCHMeCH_2B(C_6F_5)_2$, *trans*-**4**, in (b). The calculated *intramolecular* PB distance and PCCB torsion angle are equal to 3.93 Å and 111° in (a), and 4.00 Å and 138° in (b). Color code: P yellow, B pink, F green, C grey, H white, Si (in (a)) orange.

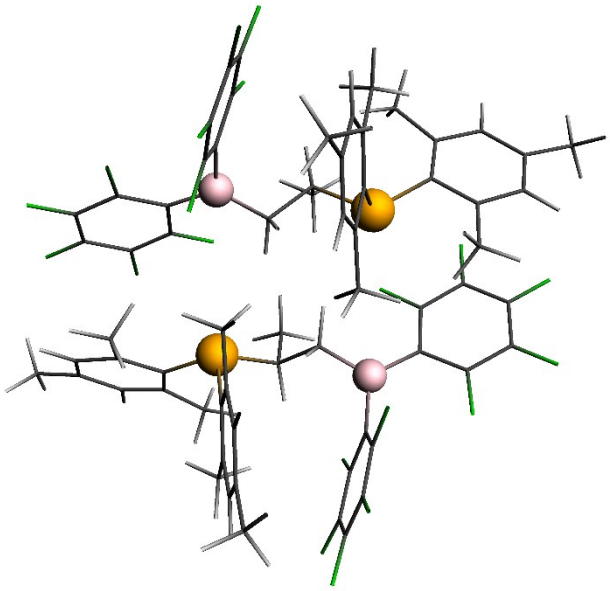

Figure S5. Fully-optimized (B97D/6–31G(d)) structure of dimer-**4** composed of *trans* monomers of $Mes_2PCHMeCH_2B(C_6F_5)_2$ (**4**). The calculated *intermolecular* P–B' and P'–B distances are of the order of 4.5 Å. Color code: P yellow, B pink, F green, C grey, H white.

Optimized Cartesian coordinates

H_2 (optimized at B97D/6-31G* level in gas phase)

H	0.000000	0.000000	-0.002150
H	0.000000	0.000000	0.742150

H_2 (optimized at B97D/6-31+G** level in gas phase)

H	0.000000	0.000000	-0.002150
H	0.000000	0.000000	0.742150

H_2 (optimized at B97D/6-31+G** level in solvent phase)

H	0.000000	0.000000	-0.002150
H	0.000000	0.000000	0.742150

1 (optimized at B97D/6-31G* level in gas phase)

C	0.031935	0.010202	0.047984
C	0.025801	0.001543	1.457026
C	1.308542	-0.069320	2.030005
C	2.490289	-0.181203	1.283134
C	2.427739	-0.207403	-0.111110
C	1.181452	-0.101949	-0.739271
B	-1.374697	-0.171675	2.263054
C	-2.628933	0.703155	1.723163
C	-3.968906	0.309840	1.866971
C	-5.063712	1.063560	1.426075
C	-4.839524	2.324461	0.859794
C	-3.524784	2.792150	0.734394
C	-2.460915	1.986999	1.167527
F	-4.272992	-0.898683	2.417817
F	-6.320250	0.588134	1.542833
F	-5.872843	3.075613	0.441567
F	-3.297887	4.010419	0.206946
F	-1.223506	2.518868	1.028251
F	1.482907	-0.077156	3.376370
F	3.682536	-0.320113	1.898291
F	3.548428	-0.378855	-0.838037
F	1.099106	-0.163620	-2.083558
F	-1.144480	0.045431	-0.637371
P	-1.563619	-2.408735	2.254272
C	0.151186	-3.052073	1.966294
C	1.168527	-3.166779	2.958954
C	2.500659	-3.364432	2.549863
C	2.873243	-3.461007	1.204875
C	1.850667	-3.433240	0.247728
C	0.506618	-3.229730	0.592331
C	0.930408	-3.089310	4.454770
C	4.325503	-3.519622	0.789945
C	-0.502295	-3.209687	-0.540285
C	-1.932697	-1.919657	4.009745
C	-1.438496	-0.446353	3.899563
C	-2.747921	-3.720149	1.697946
C	-2.743213	-4.984378	2.362247
C	-3.658715	-5.968211	1.964814
C	-4.584733	-5.750707	0.929293
C	-4.566875	-4.509133	0.285914
C	-3.668501	-3.484262	0.644152
C	-1.780649	-5.312778	3.486866
C	-5.575627	-6.826883	0.539431
C	-3.761407	-2.203452	-0.164534

H	-1.520769	-2.518509	4.827513
H	-3.027230	-1.960771	4.075234
H	-0.468220	-0.324333	4.390466
H	-2.143437	0.235097	4.402210
H	-3.646554	-6.933654	2.478068
H	-5.271696	-4.321285	-0.528893
H	3.275813	-3.417078	3.318091
H	2.107074	-3.535548	-0.809778
H	-1.930261	-6.345774	3.833624
H	-1.927406	-4.643617	4.349373
H	-0.734326	-5.203396	3.163290
H	-6.054858	-6.598740	-0.424634
H	-5.084720	-7.810522	0.460798
H	-6.372313	-6.920818	1.297779
H	-3.630998	-2.427439	-1.235840
H	-3.019772	-1.450902	0.114412
H	-4.758828	-1.753563	-0.040037
H	1.860620	-3.322757	4.992841
H	0.614548	-2.085894	4.768707
H	0.166680	-3.809008	4.781719
H	4.468122	-4.164726	-0.091355
H	4.963832	-3.889980	1.606635
H	4.673097	-2.508010	0.522075
H	0.017170	-3.220116	-1.509592
H	-1.173198	-4.081287	-0.493721
H	-1.136478	-2.315552	-0.522249

1 (optimized at B97D/6-31+G** level in gas phase)

C	0.000180	0.006953	0.001105
C	0.002174	0.006225	1.410103
C	1.291012	0.004387	1.974182
C	2.473809	-0.045603	1.221611
C	2.404759	-0.078746	-0.173686
C	1.149835	-0.039179	-0.792688
B	-1.390768	-0.193841	2.232625
C	-2.650302	0.700285	1.717254
C	-3.994219	0.319561	1.872078
C	-5.088534	1.103564	1.484788
C	-4.860812	2.373057	0.939396
C	-3.542930	2.826507	0.799279
C	-2.481124	1.997274	1.190612
F	-4.300750	-0.894562	2.413832
F	-6.354192	0.651731	1.635395
F	-5.895611	3.151718	0.566994
F	-3.311045	4.058503	0.297305
F	-1.238117	2.528150	1.051219
F	1.469307	0.044435	3.322812
F	3.680303	-0.078670	1.830897
F	3.530332	-0.159204	-0.912826
F	1.064904	-0.082620	-2.141668
F	-1.184649	0.011821	-0.675957
P	-1.564561	-2.404733	2.255255
C	0.156697	-3.039504	1.977808
C	1.167184	-3.160057	2.977919
C	2.494772	-3.407576	2.577630
C	2.870836	-3.546813	1.235350
C	1.854908	-3.489888	0.271127
C	0.514306	-3.243007	0.608253
C	0.925294	-3.062501	4.472361
C	4.320333	-3.717140	0.838743
C	-0.491922	-3.231749	-0.526045

C	-1.940361	-1.911356	4.004446
C	-1.434150	-0.442968	3.876662
C	-2.737599	-3.721157	1.686834
C	-2.730288	-4.983208	2.356914
C	-3.639308	-5.973568	1.956081
C	-4.560638	-5.764181	0.912910
C	-4.543599	-4.524147	0.263839
C	-3.649793	-3.494460	0.623480
C	-1.772387	-5.303122	3.488374
C	-5.544487	-6.846697	0.522154
C	-3.722714	-2.223736	-0.201170
H	-1.529196	-2.506804	4.823506
H	-3.034475	-1.951673	4.069526
H	-0.457832	-0.328059	4.355769
H	-2.123759	0.253072	4.378717
H	-3.625945	-6.935939	2.473477
H	-5.242782	-4.341874	-0.555984
H	3.262399	-3.479107	3.351055
H	2.109839	-3.624073	-0.782494
H	-1.924247	-6.332480	3.840471
H	-1.923837	-4.628524	4.344166
H	-0.726054	-5.196668	3.167405
H	-6.035448	-6.613066	-0.433229
H	-5.042954	-7.822261	0.427776
H	-6.329272	-6.955152	1.288923
H	-3.474237	-2.445480	-1.250983
H	-3.043565	-1.441236	0.142156
H	-4.745938	-1.820791	-0.181569
H	1.854417	-3.285028	5.013909
H	0.602746	-2.058855	4.775395
H	0.165188	-3.782733	4.803974
H	4.414925	-4.305791	-0.085570
H	4.896179	-4.212641	1.634046
H	4.783109	-2.733259	0.655914
H	0.027289	-3.217207	-1.493777
H	-1.135886	-4.123001	-0.488390
H	-1.153489	-2.359911	-0.495003

1 (optimized at B97D/6-31+G** level in solvent phase)

C	-0.014153	0.011810	-0.027372
C	-0.002740	-0.003361	1.381073
C	1.290621	0.000372	1.934833
C	2.468010	-0.031784	1.173280
C	2.389608	-0.050992	-0.221419
C	1.130035	-0.016172	-0.829794
B	-1.390091	-0.216372	2.215499
C	-2.654258	0.684245	1.713687
C	-3.998575	0.305010	1.868525
C	-5.092212	1.098409	1.499038
C	-4.864776	2.374798	0.971990
C	-3.546965	2.826259	0.833049
C	-2.486114	1.988963	1.207477
F	-4.307547	-0.914310	2.395449
F	-6.359690	0.648783	1.651309
F	-5.900365	3.162831	0.616255
F	-3.313665	4.067152	0.348312
F	-1.241797	2.522476	1.071487
F	1.480348	0.032923	3.282521
F	3.680258	-0.055084	1.773951
F	3.511002	-0.107855	-0.970688
F	1.035310	-0.039607	-2.180031

F	-1.203549	0.020315	-0.697530
P	-1.563605	-2.405608	2.262541
C	0.158745	-3.039042	1.989467
C	1.163975	-3.165464	2.994227
C	2.492329	-3.418791	2.598412
C	2.873053	-3.558231	1.257139
C	1.861566	-3.493860	0.288164
C	0.520716	-3.241617	0.620783
C	0.917058	-3.071856	4.488219
C	4.322699	-3.741866	0.866523
C	-0.481073	-3.227223	-0.517185
C	-1.939639	-1.902987	4.008116
C	-1.418689	-0.441065	3.865118
C	-2.737002	-3.717244	1.686331
C	-2.735275	-4.976909	2.361953
C	-3.642570	-5.968042	1.958180
C	-4.556395	-5.761983	0.907275
C	-4.533825	-4.524082	0.253447
C	-3.641279	-3.493920	0.615324
C	-1.786156	-5.294451	3.501390
C	-5.537183	-6.845702	0.512517
C	-3.706207	-2.227696	-0.216491
H	-1.533820	-2.496252	4.830910
H	-3.033915	-1.933612	4.073527
H	-0.436779	-0.335095	4.334300
H	-2.095287	0.268032	4.366621
H	-3.633440	-6.928211	2.479475
H	-5.226405	-4.344560	-0.572407
H	3.255953	-3.498106	3.375005
H	2.119764	-3.629269	-0.764432
H	-1.943532	-6.321726	3.856377
H	-1.941086	-4.616264	4.353519
H	-0.737413	-5.193331	3.186702
H	-6.026330	-6.611108	-0.443431
H	-5.032942	-7.819814	0.418841
H	-6.322608	-6.956922	1.278089
H	-3.439699	-2.453740	-1.260815
H	-3.035531	-1.441470	0.134323
H	-4.731227	-1.829024	-0.216539
H	1.842206	-3.304535	5.032000
H	0.601470	-2.066930	4.794846
H	0.149723	-3.786509	4.814462
H	4.415124	-4.331970	-0.056965
H	4.890735	-4.240883	1.665054
H	4.795504	-2.762543	0.684201
H	0.041706	-3.211270	-1.482834
H	-1.125435	-4.118265	-0.484035
H	-1.143416	-2.356154	-0.486373

gauche-**1** (optimized at B97D/6-31G level in gas phase)

C	0.366817	0.186101	0.305778
C	0.091562	0.394673	1.665737
C	1.133419	0.948317	2.424895
C	2.383204	1.279697	1.883888
C	2.620041	1.038191	0.522739
C	1.606394	0.484894	-0.274595
B	-1.248407	-0.109640	2.378824
C	-2.654153	0.510042	2.029732
C	-3.860704	0.086385	2.650254
C	-5.130991	0.485538	2.219143
C	-5.248510	1.376212	1.145236

C	-4.092366	1.882320	0.534474
C	-2.836903	1.463414	0.990222
F	-3.854667	-0.724506	3.721176
F	-6.241865	0.022112	2.820184
F	-6.457704	1.761999	0.720584
F	-4.203697	2.769247	-0.468791
F	-1.785461	2.032229	0.372667
F	0.939652	1.199777	3.745762
F	3.348403	1.821832	2.648540
F	3.811379	1.341421	-0.017524
F	1.831938	0.257646	-1.580744
F	-0.585084	-0.332516	-0.502565
C	-0.996875	-1.281938	3.429220
C	-0.172126	-2.454809	2.831328
P	-1.058776	-3.216220	1.329488
C	-0.422721	-4.977367	1.257916
C	0.980756	-5.214152	1.372727
C	1.470095	-6.532000	1.349335
C	0.630727	-7.640013	1.177471
C	-0.728144	-7.385318	0.948536
C	-1.271083	-6.087860	0.960155
C	2.020890	-4.105437	1.451097
C	1.173644	-9.052964	1.206006
C	-2.741226	-5.967341	0.588003
C	-2.805049	-3.332433	1.983925
C	-3.154855	-3.922091	3.229416
C	-4.497188	-3.905557	3.649327
C	-5.512799	-3.323560	2.879224
C	-5.159210	-2.774401	1.638362
C	-3.832550	-2.765006	1.177199
C	-2.146222	-4.578634	4.152526
C	-6.937815	-3.253482	3.381551
C	-3.567849	-2.163284	-0.193134
H	0.060676	-3.204554	3.600739
H	0.778832	-2.054707	2.459905
H	-1.900616	-1.668739	3.902757
H	-0.370286	-0.836440	4.225744
H	-4.752469	-4.360692	4.610638
H	-5.938265	-2.332738	1.011453
H	-3.395199	-5.867612	1.466949
H	-1.395608	-8.224050	0.730170
H	-1.649873	-3.826918	4.789184
H	-2.650443	-5.292035	4.822155
H	-1.365029	-5.113845	3.597635
H	-7.659571	-3.389957	2.560427
H	-7.134546	-2.264701	3.828873
H	-7.131772	-4.017607	4.150026
H	-4.499217	-1.755595	-0.615985
H	-2.819244	-1.361116	-0.155449
H	-3.177495	-2.918211	-0.895657
H	2.991162	-4.480428	1.091603
H	2.169800	-3.739257	2.478990
H	1.743647	-3.240185	0.827768
H	0.586155	-9.720354	0.555636
H	2.224867	-9.084163	0.878199
H	1.135063	-9.472317	2.227360
H	-3.053217	-6.865943	0.033128
H	-2.931211	-5.092573	-0.049974
H	2.548421	-6.689309	1.445930

gauche-**1** (optimized at B97D/6-31+G** level in gas phase)

C	0.356557	0.187110	0.247234
C	0.085763	0.396068	1.609127
C	1.131771	0.959773	2.356761
C	2.374424	1.301986	1.806548
C	2.605330	1.059861	0.444502
C	1.589203	0.497156	-0.342525
B	-1.251085	-0.101103	2.341741
C	-2.655844	0.549532	2.028152
C	-3.855121	0.150662	2.680488
C	-5.127813	0.589671	2.296722
C	-5.255629	1.494917	1.235424
C	-4.105696	1.975528	0.593176
C	-2.848363	1.518445	1.005067
F	-3.833219	-0.661828	3.754251
F	-6.231231	0.164836	2.943370
F	-6.469025	1.922076	0.855531
F	-4.225499	2.878502	-0.399330
F	-1.797567	2.069279	0.361899
F	0.945447	1.218434	3.681767
F	3.342578	1.856081	2.565217
F	3.792895	1.372833	-0.106196
F	1.807253	0.268622	-1.653482
F	-0.599958	-0.334270	-0.557313
C	-1.002286	-1.268112	3.393482
C	-0.159126	-2.440134	2.823769
P	-1.039649	-3.219356	1.329606
C	-0.410567	-4.983813	1.268695
C	0.984735	-5.242110	1.431832
C	1.453169	-6.569322	1.428162
C	0.601558	-7.664753	1.226091
C	-0.744288	-7.387477	0.943861
C	-1.265283	-6.079797	0.934631
C	2.038494	-4.148529	1.538917
C	1.119311	-9.086794	1.277968
C	-2.716471	-5.931436	0.502214
C	-2.787384	-3.342893	1.984058
C	-3.134571	-3.954667	3.220531
C	-4.481932	-3.974832	3.627435
C	-5.505062	-3.406309	2.854088
C	-5.149947	-2.821139	1.628692
C	-3.818178	-2.777646	1.179397
C	-2.118689	-4.594660	4.147320
C	-6.938747	-3.394121	3.338101
C	-3.553174	-2.146806	-0.177683
H	0.068335	-3.178059	3.604620
H	0.792383	-2.042433	2.453069
H	-1.910608	-1.659416	3.852733
H	-0.400183	-0.809116	4.201177
H	-4.735287	-4.451884	4.577718
H	-5.932219	-2.389565	0.999533
H	-3.402940	-5.828846	1.354376
H	-1.416088	-8.213800	0.697186
H	-1.642755	-3.832883	4.786107
H	-2.612904	-5.317544	4.811877
H	-1.324177	-5.113021	3.597351
H	-7.644646	-3.430001	2.495030
H	-7.145157	-2.469596	3.902396
H	-7.142364	-4.245434	4.004270
H	-4.497539	-1.812731	-0.631617
H	-2.876417	-1.285912	-0.103230
H	-3.072416	-2.856430	-0.868413

H	3.013840	-4.543163	1.220715
H	2.152600	-3.772912	2.566351
H	1.797589	-3.289845	0.893963
H	0.548177	-9.743512	0.604629
H	2.181355	-9.134745	0.994153
H	1.029961	-9.500202	2.297075
H	-3.017906	-6.818608	-0.073703
H	-2.863395	-5.048727	-0.134466
H	2.524159	-6.743608	1.561304

gauche-**1** (optimized at B97D/6-31+G** level in solvent phase)

C	0.394448	0.197355	0.259732
C	0.091160	0.418438	1.612120
C	1.106407	1.020473	2.370972
C	2.349875	1.387661	1.840015
C	2.614128	1.133197	0.487040
C	1.629300	0.532643	-0.310433
B	-1.246459	-0.101867	2.329265
C	-2.654973	0.537206	2.013349
C	-3.846862	0.148442	2.684308
C	-5.122891	0.586242	2.311778
C	-5.262219	1.476152	1.239648
C	-4.119926	1.942641	0.575084
C	-2.858864	1.489196	0.977414
F	-3.812592	-0.651652	3.767596
F	-6.219038	0.173535	2.979103
F	-6.479737	1.901293	0.869030
F	-4.250363	2.829870	-0.431796
F	-1.814965	2.023232	0.307276
F	0.886979	1.292723	3.688792
F	3.288744	1.978795	2.609933
F	3.804594	1.470716	-0.045685
F	1.878994	0.292136	-1.615115
F	-0.532518	-0.361093	-0.555889
C	-0.988078	-1.272756	3.372484
C	-0.147542	-2.443111	2.794135
P	-1.038957	-3.233731	1.312273
C	-0.416554	-5.001393	1.261182
C	0.977634	-5.267021	1.425369
C	1.439060	-6.597231	1.422740
C	0.581561	-7.688833	1.221434
C	-0.763385	-7.404717	0.939693
C	-1.277387	-6.093800	0.929752
C	2.037449	-4.179371	1.534122
C	1.092060	-9.113656	1.274064
C	-2.728949	-5.938518	0.500825
C	-2.783187	-3.345266	1.977094
C	-3.125565	-3.951256	3.218130
C	-4.471129	-3.967286	3.631300
C	-5.496576	-3.397570	2.860975
C	-5.145688	-2.815163	1.632838
C	-3.815720	-2.777934	1.176497
C	-2.106142	-4.587575	4.143593
C	-6.928016	-3.382445	3.352034
C	-3.556004	-2.153987	-0.184849
H	0.088334	-3.177489	3.575551
H	0.799791	-2.044310	2.413786
H	-1.891885	-1.666152	3.838619
H	-0.378301	-0.817015	4.176300
H	-4.721294	-4.441548	4.583769
H	-5.929280	-2.381331	1.007045

H	-3.410712	-5.825655	1.355477
H	-1.439658	-8.227810	0.694564
H	-1.622097	-3.822275	4.771775
H	-2.598913	-5.302056	4.818062
H	-1.317300	-5.113655	3.592775
H	-7.637737	-3.386390	2.511613
H	-7.121065	-2.472171	3.943638
H	-7.137759	-4.249166	3.996074
H	-4.498700	-1.798129	-0.624991
H	-2.858164	-1.309074	-0.122015
H	-3.103490	-2.877170	-0.880880
H	3.012789	-4.582189	1.226621
H	2.145039	-3.798237	2.560035
H	1.806983	-3.322937	0.882465
H	0.511332	-9.769193	0.607967
H	2.151703	-9.167906	0.982739
H	1.008362	-9.522658	2.295395
H	-3.038712	-6.827355	-0.067915
H	-2.871947	-5.058358	-0.140434
H	2.509057	-6.777010	1.556237

trans-**1** (optimized at B97D/6-31G level in gas phase)

C	-0.037204	0.079357	0.000164
C	-0.029008	0.061943	1.401554
C	1.228626	0.021752	2.016104
C	2.424603	0.006940	1.293691
C	2.370629	0.000902	-0.106757
C	1.134260	0.027586	-0.763503
B	-1.372113	0.221245	2.236582
C	-1.788705	-0.849971	3.315124
C	-2.783601	-0.608381	4.294255
C	-3.157021	-1.546227	5.264956
C	-2.538827	-2.805128	5.275383
C	-1.556181	-3.106818	4.321494
C	-1.199492	-2.138358	3.374393
F	-3.424158	0.578799	4.354927
F	-4.097726	-1.257765	6.179918
F	-2.887968	-3.716303	6.191283
F	-0.971611	-4.316250	4.327474
F	-0.262240	-2.511973	2.481459
F	1.306623	0.059766	3.371008
F	3.617383	0.065764	1.917786
F	3.511588	0.034465	-0.819767
F	1.089291	0.060222	-2.107428
F	-1.218659	0.132567	-0.659198
C	-2.096635	1.601975	2.006545
C	-1.344226	2.481936	3.071107
P	-1.137501	4.252074	2.410649
C	0.013707	5.216568	3.526741
C	0.238177	4.958761	4.909526
C	1.117160	5.781893	5.634943
C	1.778646	6.874076	5.056471
C	1.493970	7.160879	3.715519
C	0.622352	6.370980	2.945004
C	-0.441515	3.840419	5.681660
C	2.755985	7.712981	5.852547
C	0.376978	6.816341	1.511737
C	-0.013136	3.816665	0.970586
C	-0.577861	3.901085	-0.333407
C	0.207391	3.579791	-1.455177
C	1.551359	3.202547	-1.336251

C	2.095203	3.127404	-0.045854
C	1.346717	3.413735	1.109982
C	-2.010632	4.349229	-0.577578
C	2.084204	3.303959	2.433975
C	2.394334	2.885342	-2.553200
H	-0.355069	2.066419	3.322990
H	-1.935825	2.479754	3.990194
H	-3.175978	1.647096	2.194605
H	-1.893633	1.960938	0.989586
H	3.135499	2.811129	0.071483
H	-0.244849	3.634417	-2.448984
H	1.282615	5.561731	6.693544
H	1.954691	8.035732	3.247596
H	2.931668	2.608939	2.337208
H	2.476587	4.285220	2.745682
H	1.451098	2.953431	3.255740
H	1.762500	2.666922	-3.426976
H	3.040879	2.015498	-2.368860
H	3.047902	3.736712	-2.812173
H	-2.228499	4.361702	-1.656524
H	-2.742939	3.688502	-0.088143
H	-2.186796	5.359758	-0.175037
H	-0.229058	3.939418	6.756675
H	-0.096666	2.843194	5.368200
H	-1.535175	3.867269	5.555686
H	2.801292	8.744611	5.469282
H	2.476870	7.749380	6.917618
H	3.776991	7.295087	5.795101
H	0.674396	7.869176	1.389174
H	-0.685500	6.728832	1.230665
H	0.948184	6.212689	0.789810

trans-**1** (optimized at B97D/6-31+G** level in solvent phase)

C	-0.040057	0.088269	0.055610
C	-0.031729	0.040200	1.457106
C	1.224865	-0.096829	2.061018
C	2.415772	-0.174156	1.332335
C	2.358803	-0.140127	-0.067812
C	1.122380	-0.018376	-0.715213
B	-1.372247	0.212008	2.299871
C	-1.835430	-0.920717	3.297350
C	-2.753442	-0.688817	4.350234
C	-3.181467	-1.684475	5.236388
C	-2.703807	-2.993593	5.080353
C	-1.803204	-3.286266	4.046303
C	-1.386109	-2.260568	3.189504
F	-3.251764	0.550110	4.568579
F	-4.044510	-1.403194	6.232896
F	-3.109503	-3.962564	5.915062
F	-1.354369	-4.547345	3.890010
F	-0.531648	-2.624557	2.205766
F	1.310696	-0.134077	3.419965
F	3.611916	-0.261459	1.953837
F	3.495015	-0.203716	-0.789576
F	1.069318	0.006764	-2.062451
F	-1.223898	0.199989	-0.603125
C	-2.070122	1.612143	2.130309
C	-1.280360	2.501248	3.159945
P	-1.099684	4.255620	2.457094
C	0.040885	5.277666	3.533680
C	0.320005	5.049601	4.912790

C	1.178876	5.927424	5.601262
C	1.768353	7.044233	4.988433
C	1.434466	7.294394	3.649805
C	0.579974	6.449442	2.916448
C	-0.269488	3.902666	5.716135
C	2.725625	7.942472	5.744177
C	0.279126	6.851879	1.481197
C	0.018654	3.811108	1.013628
C	-0.547713	3.878973	-0.291843
C	0.246444	3.571184	-1.412794
C	1.598757	3.217555	-1.290910
C	2.141106	3.148575	0.001399
C	1.385243	3.431615	1.155390
C	-1.985500	4.307374	-0.541196
C	2.122549	3.355644	2.481249
C	2.452556	2.943969	-2.511117
H	-0.285437	2.086797	3.383840
H	-1.840875	2.522809	4.096951
H	-3.142178	1.659054	2.355010
H	-1.905190	1.972856	1.106908
H	3.188713	2.860895	0.121797
H	-0.205000	3.617371	-2.406587
H	1.386962	5.730213	6.656009
H	1.839749	8.180801	3.154999
H	3.009356	2.713498	2.382544
H	2.457241	4.355655	2.796391
H	1.506815	2.968646	3.299317
H	1.840244	2.591035	-3.352897
H	3.222332	2.188788	-2.297833
H	2.970202	3.862710	-2.834562
H	-2.206056	4.290098	-1.617980
H	-2.710072	3.655530	-0.031692
H	-2.165514	5.326307	-0.164723
H	0.004848	4.004147	6.775262
H	0.094804	2.924085	5.372563
H	-1.367869	3.888807	5.657020
H	2.708814	8.967122	5.343963
H	2.474831	7.980338	6.814860
H	3.761164	7.570996	5.660603
H	0.536739	7.909158	1.325157
H	-0.786033	6.719234	1.233929
H	0.850431	6.248090	0.760629

TS**1a** (optimized at B97D/6-31G level in gas phase)

C	0.124305	0.230907	0.091052
C	0.008899	-0.108655	1.464657
C	1.181426	-0.165271	2.273743
C	2.418741	0.171796	1.706376
C	2.540497	0.578950	0.368493
C	1.383846	0.585958	-0.423810
P	-1.602813	-0.334240	2.333814
C	-2.453595	-1.925632	1.892327
C	-3.782203	-2.102398	2.386976
C	-4.482886	-3.281550	2.081248
C	-3.916110	-4.314053	1.323784
C	-2.584763	-4.158044	0.914148
C	-1.830810	-3.002626	1.189411
C	-4.503212	-1.092473	3.266871
C	-4.705161	-5.557100	0.972154
C	-0.378520	-3.017994	0.740935
C	1.159537	-0.610228	3.726361

C	3.889450	0.970173	-0.195202
C	-1.048532	0.182587	-0.870525
C	-2.693230	1.050392	1.671862
C	-1.956277	2.417314	1.655502
B	-1.205189	2.929496	3.013244
C	0.402223	3.060452	2.964101
C	1.096395	3.496469	1.823391
C	2.493513	3.523751	1.739752
C	3.255929	3.109308	2.836461
C	2.612424	2.708952	4.013428
C	1.213453	2.731971	4.061948
F	0.424141	3.933004	0.730705
F	3.110088	3.906676	0.603868
F	4.599006	3.050933	2.741392
F	3.338573	2.289556	5.068315
F	0.640469	2.348945	5.233392
C	-2.002930	3.933991	3.986536
C	-1.545054	5.233464	4.271974
C	-2.248670	6.130231	5.090812
C	-3.460725	5.728213	5.668599
C	-3.956620	4.440347	5.415849
C	-3.226682	3.583679	4.583120
F	-0.391997	5.688653	3.729450
F	-3.741267	2.340199	4.386355
F	-5.117938	4.047001	5.972557
F	-4.147290	6.572235	6.456469
F	-1.776758	7.369100	5.323451
H	-3.086136	0.811122	0.675071
H	-3.542534	1.106481	2.359584
H	-1.227170	2.389897	0.839120
H	-2.710475	3.174258	1.375066
H	1.461482	0.865434	-1.478013
H	-5.499854	-3.397449	2.466583
H	-2.100536	-4.973016	0.369192
H	-1.588286	1.142960	-0.903027
H	-0.691919	-0.027472	-1.890377
H	-1.770383	-0.597577	-0.588701
H	4.487451	0.075265	-0.441005
H	4.462071	1.561616	0.534019
H	3.778959	1.567340	-1.112097
H	2.182740	-0.636976	4.129868
H	0.568845	0.064335	4.361175
H	0.721486	-1.616396	3.832412
H	-5.242958	-1.608941	3.896995
H	-5.050792	-0.347244	2.666866
H	-3.820116	-0.542363	3.932612
H	-5.227308	-5.433101	0.006775
H	-4.047149	-6.435341	0.878944
H	-5.470357	-5.773414	1.734132
H	-0.102949	-4.033503	0.418511
H	0.307098	-2.719812	1.546282
H	-0.190391	-2.335701	-0.099953
H	-1.289044	1.750347	4.021252
H	-1.353364	0.967687	3.740483
H	3.312260	0.136055	2.334190

TS**1a** (optimized at B97D/6-31+G** level in gas phase)

C	0.231251	0.298022	0.128990
C	0.079219	-0.032989	1.502372
C	1.228603	-0.070501	2.344630
C	2.481415	0.271969	1.810154

C	2.640248	0.656711	0.468903
C	1.503752	0.652441	-0.354876
P	-1.555909	-0.338924	2.311628
C	-2.328625	-1.917627	1.685917
C	-3.706461	-2.137559	1.995203
C	-4.348291	-3.296379	1.521385
C	-3.675127	-4.273589	0.775597
C	-2.300583	-4.089288	0.565297
C	-1.603158	-2.951597	1.015924
C	-4.540134	-1.204706	2.860763
C	-4.397104	-5.490110	0.235969
C	-0.100083	-2.947377	0.786136
C	1.172180	-0.524533	3.793238
C	4.004299	1.017682	-0.078914
C	-0.911994	0.229775	-0.866124
C	-2.648984	1.045609	1.639291
C	-1.943444	2.428165	1.646370
B	-1.248728	2.962193	3.016484
C	0.358792	3.105116	3.054429
C	1.108805	3.550684	1.951982
C	2.505071	3.652685	1.961529
C	3.212507	3.299336	3.116263
C	2.509808	2.884836	4.254473
C	1.112518	2.822787	4.205945
F	0.487115	3.960193	0.815008
F	3.176126	4.078583	0.869883
F	4.560163	3.349238	3.129612
F	3.184892	2.543017	5.373713
F	0.480080	2.447319	5.352791
C	-2.084490	3.968427	3.964844
C	-1.634331	5.264001	4.287988
C	-2.370888	6.160816	5.076988
C	-3.614525	5.766892	5.589395
C	-4.106500	4.485703	5.299137
C	-3.342804	3.629995	4.496313
F	-0.449102	5.720575	3.809471
F	-3.860139	2.392705	4.260566
F	-5.301214	4.097143	5.792574
F	-4.334267	6.612428	6.349594
F	-1.900161	7.396694	5.343069
H	-3.008609	0.808375	0.630373
H	-3.517868	1.078794	2.301891
H	-1.186062	2.416980	0.856724
H	-2.703316	3.168408	1.340909
H	1.609089	0.918410	-1.409545
H	-5.403210	-3.443419	1.766628
H	-1.735939	-4.868014	0.046642
H	-1.468006	1.179357	-0.909544
H	-0.521395	0.032182	-1.874460
H	-1.625122	-0.564547	-0.607589
H	4.529063	0.116005	-0.437045
H	4.632711	1.482107	0.694135
H	3.920533	1.715664	-0.923666
H	2.174292	-0.489481	4.242608
H	0.502835	0.095891	4.403016
H	0.798921	-1.558354	3.869901
H	-5.340674	-1.774222	3.353714
H	-5.020201	-0.412618	2.265858
H	-3.942303	-0.717796	3.645707
H	-4.775719	-5.300180	-0.782698
H	-3.726034	-6.360281	0.181673

H	-5.260080	-5.752809	0.865741
H	0.230817	-3.959917	0.514730
H	0.453012	-2.638529	1.682347
H	0.200605	-2.266305	-0.021333
H	-1.386604	1.778858	4.085013
H	-1.412485	1.016036	3.794397
H	3.356881	0.242460	2.462431

TS**1a** (optimized at B97D/6-31+G** level in solvent phase)

C	0.231091	0.297935	0.128826
C	0.079159	-0.033040	1.502241
C	1.228590	-0.070474	2.344416
C	2.481357	0.272062	1.809850
C	2.640087	0.656766	0.468588
C	1.503536	0.652382	-0.355135
P	-1.555909	-0.338924	2.311628
C	-2.328737	-1.917586	1.685999
C	-3.706582	-2.137468	1.995371
C	-4.348505	-3.296203	1.521536
C	-3.675441	-4.273407	0.775611
C	-2.300916	-4.089180	0.565251
C	-1.603380	-2.951552	1.015924
C	-4.540113	-1.204616	2.861075
C	-4.397639	-5.489787	0.235959
C	-0.100313	-2.947448	0.786073
C	1.172290	-0.524504	3.793029
C	4.004049	1.017850	-0.079382
C	-0.912232	0.229639	-0.866194
C	-2.649009	1.045608	1.639341
C	-1.943430	2.428137	1.646360
B	-1.248728	2.962193	3.016484
C	0.358792	3.105099	3.054435
C	1.108780	3.550685	1.951977
C	2.505048	3.652649	1.961479
C	3.212517	3.299237	3.116174
C	2.509843	2.884723	4.254394
C	1.112549	2.822721	4.205914
F	0.487060	3.960253	0.815037
F	3.176076	4.078568	0.869826
F	4.560172	3.349082	3.129471
F	3.184953	2.542844	5.373601
F	0.480135	2.447242	5.352771
C	-2.084504	3.968464	3.964779
C	-1.634372	5.264070	4.287836
C	-2.370955	6.160934	5.076752
C	-3.614593	5.767028	5.589178
C	-4.106540	4.485808	5.299015
C	-3.342814	3.630053	4.496268
F	-0.449139	5.720615	3.809304
F	-3.860133	2.392732	4.260621
F	-5.301249	4.097258	5.792469
F	-4.334354	6.612615	6.349299
F	-1.900255	7.396840	5.342744
H	-3.008708	0.808361	0.630454
H	-3.517846	1.078811	2.302001
H	-1.186032	2.416884	0.856725
H	-2.703265	3.168400	1.340855
H	1.608790	0.918305	-1.409825
H	-5.403409	-3.443204	1.766883
H	-1.736365	-4.867910	0.046505
H	-1.468211	1.179241	-0.909629

H	-0.521715	0.031971	-1.874549
H	-1.625360	-0.564648	-0.607553
H	4.527871	0.116545	-0.439825
H	4.633326	1.480183	0.694215
H	3.920228	1.717667	-0.922613
H	2.174412	-0.489312	4.242365
H	0.502874	0.095816	4.402836
H	0.799187	-1.558384	3.869697
H	-5.340587	-1.774131	3.354136
H	-5.020263	-0.412512	2.266255
H	-3.942162	-0.717726	3.645938
H	-4.780742	-5.297979	-0.780677
H	-3.725418	-6.358740	0.176881
H	-5.257677	-5.755373	0.868556
H	0.230506	-3.960039	0.514751
H	0.452842	-2.638558	1.682232
H	0.200388	-2.266478	-0.021480
H	-1.386604	1.778858	4.085013
H	-1.412485	1.016036	3.794397
H	3.356865	0.242631	2.462071

gauche-PD**1** (optimized at B97D/6-31G level in gas phase)

C	-0.003216	-0.023692	-0.003384
C	-0.012923	0.012069	1.418866
C	1.200746	-0.015243	2.154757
C	2.404231	-0.143523	1.445942
C	2.440712	-0.246531	0.047129
C	1.230323	-0.151316	-0.656707
P	-1.619211	-0.078307	2.248862
C	-2.471574	1.495835	2.630880
C	-3.858251	1.397232	2.967327
C	-4.565435	2.577489	3.249411
C	-3.959551	3.841283	3.216660
C	-2.604574	3.912026	2.861208
C	-1.839845	2.772381	2.558836
C	-4.635146	0.091582	3.053846
C	-4.741281	5.089307	3.563546
C	-0.396412	2.994927	2.140701
C	1.279610	0.093586	3.667034
C	3.745412	-0.476276	-0.680849
C	-1.266166	0.049410	-0.837346
C	-1.573122	-1.247841	3.667349
C	-0.937784	-2.588512	3.230171
B	-1.579482	-3.214854	1.828378
C	-0.841631	-4.641539	1.508170
C	0.475605	-4.629570	1.018730
C	1.211408	-5.787596	0.733016
C	0.619651	-7.040812	0.944974
C	-0.688153	-7.108284	1.442320
C	-1.381629	-5.918084	1.717926
F	1.111969	-3.442102	0.805526
F	2.477338	-5.715017	0.260529
F	1.307190	-8.170936	0.678765
F	-1.258926	-8.313851	1.657395
F	-2.638611	-6.058460	2.215588
C	-3.234528	-3.240382	1.832468
C	-3.963829	-2.945725	0.668061
C	-5.362578	-2.827411	0.619886
C	-6.103352	-3.032056	1.790878
C	-5.431254	-3.351170	2.978531
C	-4.032923	-3.457156	2.966205

F	-3.315943	-2.739673	-0.513142
F	-3.453798	-3.756824	4.161237
F	-6.137372	-3.543756	4.113866
F	-7.446483	-2.919330	1.776973
F	-6.000901	-2.527695	-0.531850
H	-1.081078	-0.748203	4.515453
H	-2.622370	-1.408375	3.945241
H	0.140608	-2.445606	3.060404
H	-1.047174	-3.271510	4.087174
H	3.341026	-0.171693	2.007747
H	-5.626775	2.500252	3.497876
H	-2.122257	4.890741	2.803563
H	1.152952	-0.892311	4.140883
H	2.263402	0.484945	3.964683
H	0.513276	0.763662	4.085925
H	3.728155	-0.031657	-1.687807
H	3.923564	-1.559201	-0.798849
H	4.597394	-0.058128	-0.123000
H	-1.014944	0.212193	-1.895017
H	-1.832608	-0.893050	-0.766947
H	-1.928702	0.871434	-0.518393
H	-5.710727	0.290804	2.946239
H	-4.493385	-0.392105	4.033753
H	-4.363018	-0.648360	2.287670
H	-4.329700	5.973540	3.053392
H	-5.801835	4.985163	3.287594
H	-4.700502	5.283856	4.649560
H	-0.164053	4.069432	2.166942
H	-0.203895	2.628035	1.122099
H	0.316306	2.482507	2.800976
H	-1.261151	-2.464192	0.910936
H	-2.457846	-0.701951	1.321043
H	1.241345	-0.191772	-1.748241

gauche-PD**1** (optimized at B97D/6-31+G** level in gas phase)

C	0.022664	-0.007876	-0.005430
C	0.014375	0.001781	1.418283
C	1.230164	0.011775	2.153130
C	2.438349	-0.031682	1.440142
C	2.478498	-0.084803	0.037014
C	1.261557	-0.050070	-0.663261
P	-1.592296	-0.094674	2.249438
C	-2.444198	1.484879	2.619664
C	-3.840188	1.393872	2.922603
C	-4.549519	2.577641	3.189942
C	-3.937084	3.839692	3.173290
C	-2.572328	3.903461	2.851738
C	-1.804407	2.759686	2.566631
C	-4.624428	0.091968	2.989401
C	-4.720879	5.091192	3.502722
C	-0.348462	2.979415	2.192087
C	1.304981	0.076582	3.667854
C	3.794293	-0.201861	-0.698509
C	-1.243148	0.003409	-0.838592
C	-1.559867	-1.261474	3.670286
C	-0.943553	-2.615524	3.244118
B	-1.604515	-3.254143	1.857362
C	-0.891470	-4.699354	1.533117
C	0.425788	-4.712869	1.041163
C	1.137930	-5.880528	0.737009
C	0.522362	-7.125155	0.929519

C	-0.787313	-7.171269	1.423792
C	-1.455834	-5.971013	1.716176
F	1.085207	-3.532734	0.833082
F	2.407826	-5.826291	0.262166
F	1.188114	-8.267612	0.645659
F	-1.386227	-8.370820	1.617124
F	-2.723242	-6.096908	2.203899
C	-3.262236	-3.271881	1.878076
C	-4.000269	-2.998694	0.713143
C	-5.399173	-2.890995	0.670004
C	-6.133202	-3.067632	1.849659
C	-5.453207	-3.362007	3.038532
C	-4.054736	-3.461605	3.021688
F	-3.356358	-2.814745	-0.477566
F	-3.468425	-3.756497	4.218587
F	-6.155021	-3.526224	4.185723
F	-7.479494	-2.950199	1.842580
F	-6.047311	-2.606072	-0.484855
H	-1.057852	-0.769540	4.515031
H	-2.612739	-1.394930	3.947756
H	0.134295	-2.484718	3.066224
H	-1.051195	-3.287843	4.109274
H	3.375559	-0.026705	2.000555
H	-5.616167	2.504235	3.412170
H	-2.083672	4.878947	2.807871
H	1.184919	-0.923333	4.111027
H	2.283257	0.467194	3.978988
H	0.531897	0.725827	4.103830
H	3.742282	0.272533	-1.689185
H	4.046745	-1.264408	-0.850705
H	4.614554	0.257013	-0.127712
H	-0.999983	0.161006	-1.897447
H	-1.768470	-0.960884	-0.752407
H	-1.938113	0.800838	-0.530571
H	-5.696492	0.296863	2.871870
H	-4.493933	-0.401209	3.964665
H	-4.344031	-0.637865	2.217906
H	-4.291643	5.972735	3.005197
H	-5.773334	4.992409	3.199885
H	-4.704897	5.280591	4.589006
H	-0.117699	4.052768	2.220838
H	-0.123961	2.606940	1.183536
H	0.340253	2.471438	2.878660
H	-1.292445	-2.519094	0.927033
H	-2.428469	-0.724175	1.322821
H	1.271936	-0.066723	-1.754736

gauche-PD**1** (optimized at B97D/6-31+G** level in solvent phase)

C	0.027963	0.040002	-0.010723
C	0.027792	0.015728	1.413397
C	1.247503	0.017694	2.142592
C	2.452122	0.001171	1.421473
C	2.484941	-0.015221	0.016763
C	1.263499	0.023490	-0.676660
P	-1.576718	-0.091420	2.246996
C	-2.435489	1.481591	2.621926
C	-3.833486	1.387400	2.913873
C	-4.547509	2.568871	3.178431
C	-3.936586	3.832214	3.169860
C	-2.568644	3.899059	2.861091
C	-1.796098	2.757343	2.579511

C	-4.614640	0.083802	2.974215
C	-4.725156	5.081345	3.495574
C	-0.336532	2.980478	2.222749
C	1.330753	0.054134	3.657641
C	3.798408	-0.090459	-0.728609
C	-1.243017	0.074394	-0.836522
C	-1.546130	-1.270440	3.657663
C	-0.940499	-2.629488	3.229494
B	-1.605125	-3.276467	1.849556
C	-0.909495	-4.740451	1.551554
C	0.402002	-4.783501	1.045022
C	1.097972	-5.967035	0.765328
C	0.473362	-7.199144	0.998983
C	-0.829829	-7.216653	1.509194
C	-1.481920	-6.002001	1.775713
F	1.073155	-3.619449	0.794984
F	2.363733	-5.940319	0.273767
F	1.124410	-8.357598	0.739016
F	-1.439729	-8.405999	1.743300
F	-2.745660	-6.106363	2.282564
C	-3.263401	-3.286082	1.865940
C	-3.996785	-3.015327	0.697986
C	-5.394803	-2.904596	0.650649
C	-6.133062	-3.075385	1.827680
C	-5.457740	-3.366970	3.019103
C	-4.059972	-3.469078	3.007195
F	-3.349266	-2.838243	-0.492156
F	-3.478354	-3.765608	4.206968
F	-6.164908	-3.530206	4.164921
F	-7.480404	-2.957162	1.815161
F	-6.039865	-2.623313	-0.508701
H	-1.035830	-0.790535	4.503494
H	-2.598805	-1.394183	3.940227
H	0.137698	-2.503713	3.049345
H	-1.045525	-3.297280	4.098893
H	3.392057	0.004797	1.976984
H	-5.615565	2.493160	3.392164
H	-2.080892	4.875134	2.825388
H	1.208040	-0.952159	4.084936
H	2.313161	0.432752	3.969436
H	0.564924	0.700529	4.109631
H	3.732305	0.410887	-1.704921
H	4.067884	-1.143623	-0.913124
H	4.613754	0.364691	-0.148194
H	-1.003806	0.249408	-1.893323
H	-1.778229	-0.885911	-0.766632
H	-1.928443	0.872106	-0.508937
H	-5.686553	0.286633	2.853216
H	-4.485840	-0.410129	3.949312
H	-4.327917	-0.640817	2.200236
H	-4.294643	5.963868	3.001286
H	-5.775820	4.978972	3.188197
H	-4.714300	5.269198	4.582118
H	-0.105359	4.052901	2.268216
H	-0.103645	2.621748	1.211062
H	0.343694	2.462821	2.910430
H	-1.286221	-2.559524	0.908915
H	-2.406735	-0.722141	1.314867
H	1.268139	0.037722	-1.768116

trans-PD**1** (optimized at B97D/6-31G level in gas phase)

C	0.051320	0.288447	0.066559
C	0.029302	0.096578	1.454722
C	1.296828	0.032670	2.057608
C	2.503341	0.175810	1.356407
C	2.466533	0.382823	-0.029273
C	1.228718	0.440037	-0.681846
B	-1.309277	-0.084555	2.393152
C	-1.503007	-1.685133	2.799677
C	-1.804824	-2.128042	4.093033
C	-2.007043	-3.472920	4.436976
C	-1.892982	-4.451529	3.445170
C	-1.612569	-4.066510	2.129972
C	-1.450552	-2.706802	1.837237
F	-2.006572	-1.224995	5.100166
F	-2.388512	-3.830851	5.687120
F	-2.154328	-5.749062	3.733880
F	-1.582816	-5.003542	1.153257
F	-1.271369	-2.396851	0.526516
F	1.395661	-0.185429	3.393627
F	3.695269	0.111286	1.990894
F	3.612425	0.523808	-0.728428
F	1.186046	0.628817	-2.021048
F	-1.111549	0.330711	-0.648002
C	-2.732748	0.368779	1.660112
C	-3.816845	0.506337	2.762768
P	-5.371025	-0.261794	2.176280
C	-5.113594	-2.029631	1.838470
C	-5.067843	-2.936102	2.936480
C	-4.870075	-4.296202	2.668875
C	-4.695653	-4.785780	1.364723
C	-4.733546	-3.869900	0.304479
C	-4.942066	-2.494302	0.502243
C	-5.194599	-2.499416	4.382814
C	-4.436395	-6.256161	1.132730
C	-4.962877	-1.596468	-0.722933
C	-6.937389	0.026954	3.079272
C	-6.987509	0.556081	4.400544
C	-8.246334	0.711733	5.006636
C	-9.444047	0.370627	4.361167
C	-9.368143	-0.133849	3.053843
C	-8.142699	-0.316519	2.395765
C	-5.768131	0.976588	5.199936
C	-10.776776	0.519870	5.061253
C	-8.161922	-0.862091	0.980012
H	-5.594422	0.307919	0.912804
H	-1.161408	0.570672	3.415876
H	-4.017750	1.558511	3.010810
H	-3.523111	0.001664	3.691180
H	-2.676285	1.319365	1.107979
H	-2.992658	-0.406819	0.925042
H	-6.065454	1.255561	6.220510
H	-5.267952	1.847754	4.750611
H	-5.021042	0.175727	5.278259
H	-8.286713	1.116924	6.020352
H	-11.578130	0.761910	4.346358
H	-10.739098	1.307922	5.828428
H	-11.057468	-0.421379	5.565294
H	-9.193443	-1.071629	0.664338
H	-7.579500	-1.792254	0.891903
H	-7.736048	-0.140026	0.262262
H	-10.288621	-0.395618	2.526524

H	-3.588947	-6.589016	1.748469
H	-4.201524	-6.458961	0.078009
H	-5.315390	-6.859517	1.416487
H	-4.825638	-2.199785	-1.630879
H	-4.158335	-0.845790	-0.700724
H	-5.920893	-1.059617	-0.823417
H	-5.054335	-3.359117	5.051332
H	-6.177554	-2.049584	4.592231
H	-4.417918	-1.770251	4.653336
H	-4.801043	-4.987869	3.510328
H	-4.577274	-4.231279	-0.713911

trans-PD**1** (optimized at B97D/6-31+G** level in gas phase)

C	0.065336	0.387770	0.058605
C	0.026353	0.112065	1.432813
C	1.291228	-0.042605	2.027865
C	2.504878	0.076369	1.336157
C	2.483117	0.364929	-0.035380
C	1.250670	0.520787	-0.681178
B	-1.318643	-0.054017	2.372790
C	-1.482196	-1.648256	2.827240
C	-1.725615	-2.061288	4.143724
C	-1.884019	-3.401459	4.529184
C	-1.796908	-4.405058	3.558811
C	-1.566839	-4.050171	2.224328
C	-1.436495	-2.696250	1.892642
F	-1.861110	-1.135726	5.142941
F	-2.161076	-3.738402	5.815333
F	-1.981724	-5.704544	3.897961
F	-1.513029	-5.018833	1.276116
F	-1.270211	-2.415808	0.568277
F	1.377242	-0.337341	3.355455
F	3.693831	-0.081192	1.967502
F	3.639085	0.488584	-0.727433
F	1.220713	0.790898	-2.010597
F	-1.095026	0.528931	-0.655490
C	-2.753375	0.363682	1.646249
C	-3.836336	0.476871	2.752929
P	-5.392541	-0.279054	2.161477
C	-5.133162	-2.047404	1.816952
C	-5.080766	-2.959019	2.910142
C	-4.879156	-4.319414	2.636933
C	-4.715483	-4.803447	1.328592
C	-4.756549	-3.880405	0.272082
C	-4.966260	-2.505672	0.477515
C	-5.208890	-2.525331	4.356636
C	-4.498864	-6.277378	1.074282
C	-4.998374	-1.600978	-0.741792
C	-6.951598	0.014453	3.076990
C	-6.993502	0.546129	4.398307
C	-8.250951	0.716381	5.006493
C	-9.454363	0.386228	4.363697
C	-9.385588	-0.125433	3.057360
C	-8.162121	-0.321632	2.397145
C	-5.769247	0.950671	5.198782
C	-10.784659	0.550806	5.065129
C	-8.188449	-0.873854	0.983851
H	-5.619770	0.294293	0.900212
H	-1.168140	0.627887	3.376235
H	-4.031756	1.522365	3.026004
H	-3.543898	-0.051742	3.668487

H	-2.712595	1.320322	1.104696
H	-3.006311	-0.408402	0.905218
H	-6.062142	1.210964	6.224139
H	-5.271772	1.829094	4.763556
H	-5.023896	0.148386	5.259694
H	-8.284705	1.122417	6.019360
H	-11.576904	0.828282	4.354667
H	-10.729377	1.318840	5.849505
H	-11.086450	-0.395431	5.544210
H	-9.220831	-1.083354	0.675560
H	-7.608706	-1.804699	0.899040
H	-7.766895	-0.155383	0.261861
H	-10.308493	-0.381335	2.532861
H	-3.840808	-6.712350	1.838966
H	-4.046635	-6.446560	0.087757
H	-5.458721	-6.819446	1.109006
H	-4.836291	-2.193421	-1.651186
H	-4.216155	-0.829345	-0.706289
H	-5.969438	-1.091228	-0.845994
H	-5.097227	-3.388894	5.023994
H	-6.183504	-2.057178	4.557960
H	-4.421408	-1.809126	4.629287
H	-4.820889	-5.015898	3.474799
H	-4.603739	-4.235706	-0.748382

trans-PD**1** (optimized at B97D/6-31+G** level in solvent phase)

C	0.081302	0.389232	0.060904
C	0.035901	0.119742	1.436253
C	1.299488	-0.029039	2.034818
C	2.515689	0.085919	1.348008
C	2.499814	0.365902	-0.024634
C	1.269832	0.518082	-0.674492
B	-1.315383	-0.048619	2.373740
C	-1.461503	-1.641740	2.833517
C	-1.679738	-2.055980	4.153830
C	-1.837401	-3.396065	4.539086
C	-1.774112	-4.398525	3.566060
C	-1.563957	-4.042568	2.228751
C	-1.431993	-2.688996	1.897953
F	-1.776549	-1.132293	5.159332
F	-2.079315	-3.734789	5.832343
F	-1.949164	-5.698105	3.908143
F	-1.520148	-5.009990	1.278865
F	-1.273162	-2.407267	0.571325
F	1.384255	-0.313024	3.367059
F	3.703918	-0.067153	1.985982
F	3.659562	0.486065	-0.713677
F	1.245547	0.781477	-2.006981
F	-1.074263	0.528588	-0.659651
C	-2.751173	0.356710	1.647720
C	-3.842089	0.466823	2.748112
P	-5.403901	-0.279939	2.153887
C	-5.140369	-2.049839	1.811814
C	-5.086965	-2.961867	2.904383
C	-4.892116	-4.323820	2.630472
C	-4.737226	-4.808551	1.321362
C	-4.775966	-3.884808	0.264740
C	-4.979182	-2.509199	0.471929
C	-5.212402	-2.529428	4.351449
C	-4.540571	-6.284734	1.062553
C	-5.018568	-1.604179	-0.746686

C	-6.955543	0.014972	3.075082
C	-6.995511	0.545322	4.397470
C	-8.252127	0.716145	5.006353
C	-9.456519	0.387264	4.363158
C	-9.389223	-0.123186	3.056276
C	-8.166217	-0.320214	2.394688
C	-5.770758	0.949098	5.196871
C	-10.785030	0.552407	5.067189
C	-8.194575	-0.871921	0.981492
H	-5.627894	0.292670	0.892607
H	-1.160486	0.639530	3.374027
H	-4.034053	1.511178	3.025877
H	-3.556499	-0.067865	3.662222
H	-2.715396	1.312883	1.104867
H	-2.999889	-0.416568	0.906348
H	-6.062964	1.207297	6.222712
H	-5.274455	1.828472	4.762688
H	-5.026446	0.145750	5.256558
H	-8.284907	1.121717	6.019329
H	-11.593422	0.750765	4.349051
H	-10.748535	1.373255	5.797425
H	-11.045131	-0.368674	5.614782
H	-9.228206	-1.069900	0.670855
H	-7.626493	-1.810180	0.899144
H	-7.763024	-0.158689	0.260600
H	-10.312567	-0.377333	2.532223
H	-3.947060	-6.748000	1.862759
H	-4.031845	-6.454042	0.103829
H	-5.514475	-6.800945	1.026248
H	-4.832874	-2.191299	-1.654846
H	-4.257123	-0.812790	-0.701683
H	-6.000261	-1.117948	-0.859142
H	-5.110000	-3.395261	5.017405
H	-6.183018	-2.053738	4.552787
H	-4.421370	-1.817576	4.625925
H	-4.839775	-5.021115	3.468105
H	-4.632547	-4.240569	-0.756916

dimer-**1** (optimized at B97D/6-31G level in gas phase)

C	0.329936	-0.445988	-0.075757
C	0.382845	-0.100465	1.311107
C	1.617611	-0.255509	2.001054
C	2.718077	-0.817449	1.327660
C	2.659542	-1.217598	-0.013162
C	1.455977	-1.005834	-0.699748
P	-1.185473	0.671607	1.956171
C	-2.427486	-0.737681	1.903865
C	-3.731463	-0.435380	1.417254
C	-4.744432	-1.409095	1.491364
C	-4.510658	-2.686896	2.016255
C	-3.215953	-2.978685	2.470490
C	-2.169221	-2.040396	2.421267
C	-4.078739	0.903604	0.790529
C	-5.607654	-3.728836	2.073204
C	-0.805725	-2.516135	2.890006
C	1.851853	0.192951	3.432814
C	3.860006	-1.815216	-0.713750
C	-0.898665	-0.196713	-0.933735
C	-1.156824	0.831922	3.842618
C	-2.502168	1.494529	4.264934
B	-2.852372	1.086911	5.742727

C	-2.696814	2.079029	6.943636
C	-3.627151	2.118966	8.004268
C	-3.607177	3.113069	8.992272
C	-2.591374	4.081746	8.970269
C	-1.618285	4.056262	7.959791
C	-1.702650	3.081282	6.962581
F	-4.624035	1.211869	8.062812
F	-4.536810	3.144857	9.962681
F	-2.546694	5.022404	9.921708
F	-0.625713	4.959928	7.958996
F	-0.739832	3.104345	6.011764
C	-3.399108	-0.399560	5.866047
C	-4.675102	-0.720298	5.389661
C	-5.116170	-2.039068	5.243067
C	-4.236365	-3.085240	5.555885
C	-2.943685	-2.805584	6.017927
C	-2.558297	-1.469104	6.183976
F	-5.505952	0.285449	5.018217
F	-1.283914	-1.214231	6.584790
F	-2.080626	-3.812773	6.250994
F	-4.615348	-4.362743	5.361651
F	-6.343895	-2.313645	4.767174
C	-1.019203	5.433790	3.538856
P	-2.623450	5.421701	4.527289
C	-3.792585	6.156282	3.254418
C	-4.834716	5.309576	2.767396
C	-5.736011	5.796841	1.805455
C	-5.655907	7.104015	1.303015
C	-4.626967	7.923129	1.783800
C	-3.691763	7.479881	2.738353
C	-5.023429	3.876748	3.238661
C	-6.629839	7.594209	0.253406
C	-2.608762	8.462257	3.141541
C	-1.044197	4.160928	2.639410
B	-0.510251	4.337003	1.171622
C	0.714965	3.548931	0.601399
C	1.819553	3.217382	1.413134
C	2.913869	2.483066	0.948604
C	2.917309	2.032359	-0.378665
C	1.820192	2.292953	-1.211664
C	0.759061	3.060783	-0.721286
F	1.862976	3.631934	2.703160
F	3.945206	2.187468	1.758209
F	3.966157	1.344412	-0.847973
F	1.798830	1.795977	-2.459906
F	-0.285320	3.268190	-1.552640
C	-1.377380	5.342053	0.292243
C	-1.072407	6.702913	0.221131
C	-1.931385	7.642699	-0.360573
C	-3.136675	7.202193	-0.922244
C	-3.476200	5.843323	-0.877261
C	-2.598043	4.945448	-0.262358
F	0.068881	7.157772	0.809392
F	-2.966709	3.643494	-0.177034
F	-4.651762	5.425327	-1.383330
F	-3.991693	8.092173	-1.456052
F	-1.640735	8.956886	-0.336446
C	-2.598068	6.618384	5.956084
C	-1.505568	7.409915	6.409767
C	-1.605832	8.089501	7.639336
C	-2.740520	8.013442	8.453645

C	-3.819196	7.244845	7.991745
C	-3.769500	6.546548	6.777142
C	-0.187813	7.541307	5.669204
C	-2.792768	8.691995	9.804985
C	-4.972012	5.698802	6.403118
H	-1.028584	-0.145625	4.322963
H	-0.333032	1.470747	4.174777
H	-2.439283	2.578382	4.133534
H	-3.320489	1.107680	3.634308
H	-3.012674	-3.967893	2.890184
H	-5.743956	-1.156998	1.127164
H	3.660273	-0.926959	1.870547
H	1.392949	-1.258397	-1.761513
H	-0.239433	-1.750277	3.428846
H	-0.914472	-3.389135	3.551841
H	-0.180846	-2.808594	2.030364
H	-6.602007	-3.260234	2.030995
H	-5.543290	-4.319850	2.997611
H	-5.527404	-4.428976	1.223178
H	-5.132194	0.916165	0.471390
H	-3.922138	1.744025	1.479650
H	-3.448795	1.105162	-0.088494
H	2.886387	-0.027584	3.733408
H	1.182957	-0.306772	4.148083
H	1.704363	1.276950	3.545018
H	3.691678	-2.878525	-0.956816
H	4.062320	-1.289195	-1.660307
H	4.760934	-1.748907	-0.085130
H	-0.681700	-0.427374	-1.987410
H	-1.217236	0.857452	-0.876300
H	-1.756231	-0.809658	-0.614613
H	-0.894263	6.350141	2.951780
H	-0.159064	5.350601	4.212091
H	-0.571773	3.337235	3.179622
H	-2.090007	3.853519	2.447868
H	-4.534194	8.940324	1.393800
H	-6.524655	5.133280	1.440885
H	-0.753769	8.688405	7.973138
H	-4.722600	7.168394	8.603317
H	-2.905736	9.486372	2.869333
H	-2.411137	8.437091	4.219265
H	-1.660564	8.258604	2.616872
H	-7.668640	7.356040	0.534674
H	-6.428922	7.110125	-0.714505
H	-6.547190	8.681856	0.110283
H	-5.902223	3.425976	2.753175
H	-4.151845	3.253483	3.000066
H	-5.160035	3.815931	4.328499
H	0.388559	8.389711	6.068255
H	-0.323573	7.700657	4.592715
H	0.428517	6.636746	5.801654
H	-2.650563	7.952453	10.612469
H	-2.003314	9.453062	9.902995
H	-3.767885	9.176955	9.974643
H	-5.763917	5.795802	7.161188
H	-4.692607	4.633603	6.333066
H	-5.391831	5.984222	5.425931

TS**1b** (optimized at B97D/6-31G level in gas phase)

C	-0.400135	1.456170	0.177978
C	-0.299561	0.685285	1.363678

C	1.026741	0.398002	1.777298
C	2.161361	0.822722	1.077394
C	2.000674	1.575631	-0.095721
C	0.712347	1.893941	-0.551557
B	-1.566256	0.164515	2.130488
C	-3.038027	0.695052	1.843477
C	-4.064913	-0.204870	1.525281
C	-5.410556	0.171464	1.465613
C	-5.757644	1.494551	1.768031
C	-4.763406	2.425500	2.098785
C	-3.426574	2.012521	2.112375
F	-3.756276	-1.500330	1.279905
F	-6.371033	-0.725139	1.179225
F	-7.053239	1.855932	1.801983
F	-5.110066	3.677043	2.454955
F	-2.487148	2.918657	2.492934
F	1.268532	-0.302576	2.905516
F	3.396589	0.526246	1.514432
F	3.073489	1.990318	-0.777361
F	0.563072	2.614097	-1.674997
F	-1.604359	1.788777	-0.324832
C	-1.516103	-0.781518	3.390555
C	-1.311535	0.295465	4.515449
P	-2.123910	-0.267976	6.114377
C	-3.890111	-0.418455	5.544269
C	-4.376840	-1.736755	5.310802
C	-5.667548	-1.909373	4.778560
C	-6.504908	-0.822216	4.491411
C	-6.016677	0.467241	4.750175
C	-4.728400	0.697211	5.261707
C	-3.553232	-2.980508	5.610349
C	-7.893850	-1.020423	3.923336
C	-4.312076	2.138182	5.481399
C	-2.112603	1.055260	7.414560
C	-1.484497	2.331230	7.353575
C	-1.540767	3.172245	8.480990
C	-2.177760	2.803541	9.672126
C	-2.773179	1.536019	9.723775
C	-2.742544	0.653590	8.633294
C	-0.714028	2.858839	6.155364
C	-3.365095	-0.720506	8.822482
C	-2.159066	3.701758	10.888652
F	1.804361	2.491831	7.945420
C	1.329928	1.323048	8.419229
C	1.306308	0.176581	7.615591
C	0.813565	-1.063042	8.052260
C	0.276898	-1.061251	9.353782
C	0.238726	0.069553	10.176701
C	0.794733	1.266403	9.709596
B	0.743295	-2.395372	7.160291
C	1.137970	-3.797531	7.841677
C	2.371287	-3.942323	8.490629
C	2.847903	-5.172092	8.961840
C	2.047634	-6.311430	8.818149
C	0.800814	-6.211265	8.189932
C	0.391321	-4.974308	7.682475
F	3.190242	-2.865769	8.621865
F	4.081753	-5.281685	9.494978
F	2.501966	-7.512285	9.226747
F	0.041229	-7.311058	8.026700
F	-0.791035	-4.946948	7.014898

F	1.763872	0.339785	6.344512
F	0.779341	2.366118	10.480375
F	-0.339696	0.031693	11.390994
F	-0.306606	-2.185091	9.838449
C	0.948363	-2.408776	5.577898
C	2.455852	-2.350664	5.196980
P	2.733998	-3.388114	3.637588
C	2.455424	-5.057151	4.451989
C	1.276141	-5.769567	4.094176
C	1.029826	-7.036642	4.652481
C	1.926767	-7.641662	5.543246
C	3.075656	-6.921917	5.899246
C	3.358821	-5.644241	5.383507
C	0.265969	-5.230344	3.092581
C	1.674887	-9.024002	6.107122
C	4.665955	-5.015683	5.837877
C	4.558271	-3.447087	3.221374
C	5.008146	-4.563711	2.451627
C	6.363649	-4.659494	2.089258
C	7.303290	-3.679272	2.432137
C	6.832464	-2.549455	3.114911
C	5.488781	-2.404900	3.503007
C	4.091137	-5.676869	1.968329
C	5.111637	-1.098793	4.181983
C	8.766334	-3.827817	2.070887
H	-1.729804	1.268526	4.223952
H	-0.239706	0.439114	4.684638
H	-0.712907	-1.524266	3.421718
H	-2.478756	-1.293265	3.515097
H	-6.648450	1.328367	4.518377
H	-6.023572	-2.923856	4.581546
H	-1.043239	4.143654	8.428672
H	-3.253341	1.206991	10.648738
H	-3.321810	2.350979	5.061342
H	-5.026714	2.820329	4.999009
H	-4.260796	2.384417	6.552751
H	-7.980544	-1.993007	3.416391
H	-8.136957	-0.229306	3.199313
H	-8.654122	-0.987532	4.723215
H	-4.123919	-3.886422	5.357303
H	-2.609969	-3.005673	5.042591
H	-3.280362	-3.036366	6.675693
H	-0.238690	3.815970	6.411346
H	-1.358367	3.038159	5.281588
H	0.087200	2.174927	5.849673
H	-1.418247	3.334795	11.618165
H	-1.884783	4.733421	10.620605
H	-3.139843	3.718726	11.390501
H	-3.782230	-0.812169	9.836128
H	-2.614041	-1.517678	8.701071
H	-4.174463	-0.914905	8.101247
H	3.089539	-2.699270	6.023802
H	2.716942	-1.311531	4.999274
H	0.432516	-1.582111	5.082755
H	0.492287	-3.345922	5.223596
H	3.772549	-7.360933	6.618871
H	0.115553	-7.567891	4.374446
H	7.531738	-1.741416	3.349139
H	6.686864	-5.527835	1.507405
H	5.489605	-5.310275	5.166782
H	4.649811	-3.921758	5.836624

H	4.912959	-5.356245	6.855459
H	0.616636	-9.307227	6.006275
H	1.943436	-9.067276	7.172542
H	2.280750	-9.780852	5.578557
H	-0.552460	-5.952568	2.948284
H	-0.175138	-4.274528	3.416803
H	0.737099	-5.036551	2.115351
H	5.953653	-0.391736	4.132960
H	4.858533	-1.237797	5.244321
H	4.249034	-0.622764	3.691813
H	8.893740	-4.438355	1.162774
H	9.237675	-2.846869	1.899258
H	9.328419	-4.324215	2.882247
H	4.561119	-6.209793	1.127058
H	3.119396	-5.287459	1.623727
H	3.876352	-6.410091	2.760655
H	-1.236212	-2.027281	6.920932
H	-0.875406	-2.660543	7.256145

dimer-PD**1** (optimized at B97D/6-31G level in gas phase)

C	-0.799884	-1.674027	0.189570
C	-0.365507	-1.001901	1.354847
C	0.857870	-1.449319	1.907635
C	1.613492	-2.484775	1.351184
C	1.111319	-3.157322	0.225915
C	-0.101583	-2.755565	-0.359707
B	-1.257494	0.039552	2.086075
C	-2.264492	1.049009	1.382823
C	-3.637746	0.780137	1.359409
C	-4.585939	1.736392	0.977847
C	-4.148491	3.020181	0.620131
C	-2.783624	3.334497	0.652861
C	-1.871299	2.338103	1.019702
F	-4.071202	-0.434402	1.774185
F	-5.901470	1.459542	0.998353
F	-5.045793	3.975433	0.311431
F	-2.374295	4.590054	0.393801
F	-0.554531	2.682910	1.120723
F	1.387685	-0.814081	2.976694
F	2.798189	-2.831399	1.865203
F	1.794948	-4.176979	-0.301485
F	-0.567670	-3.406688	-1.438140
F	-1.961720	-1.322251	-0.398695
C	-1.301694	0.116649	3.665602
C	-0.458702	1.295520	4.235389
P	-1.287374	2.007676	5.724544
C	-0.361470	3.191385	6.751122
C	0.888915	3.760832	6.384405
C	1.561019	4.548689	7.331325
C	1.060477	4.767509	8.622528
C	-0.185150	4.212351	8.950224
C	-0.914542	3.427737	8.046291
C	1.580728	3.520578	5.058330
C	1.866134	5.533112	9.646087
C	-2.237228	2.845772	8.502322
C	-2.920284	2.548517	5.127505
C	-4.053883	1.723323	5.392066
C	-5.271455	2.068943	4.780266
C	-5.403202	3.181759	3.935421
C	-4.268611	3.975894	3.699865
C	-3.022463	3.679554	4.270930

C	-4.015091	0.486330	6.272843
C	-1.837180	4.559037	3.915119
C	-6.732446	3.523683	3.299967
C	-3.039476	-3.026801	4.187599
C	-2.638967	-4.129098	5.156008
C	-1.281019	-4.430896	5.458038
C	-0.995117	-5.484452	6.371758
C	-2.058889	-6.181782	6.969836
C	-3.400974	-5.885435	6.693876
C	-3.668078	-4.857444	5.779335
P	0.046859	-3.330475	4.732060
C	1.316426	-4.519270	4.068268
C	2.691392	-4.567957	4.429542
C	3.562757	-5.422486	3.729390
C	3.138921	-6.222163	2.660858
C	1.789410	-6.143004	2.289442
C	0.878123	-5.312937	2.961138
C	0.407833	-5.936302	6.733868
C	-4.513596	-6.657938	7.369481
C	3.303266	-3.697409	5.511177
C	4.097389	-7.134474	1.924707
C	-0.549683	-5.277179	2.445974
C	0.547395	-2.464452	6.332503
C	-0.581274	-1.459086	6.642482
B	-0.742682	-0.922145	8.192762
C	0.511557	-0.046211	8.814510
C	1.475542	0.636541	8.061167
C	2.441799	1.501609	8.592419
C	2.467952	1.722656	9.971469
C	1.527088	1.076041	10.783842
C	0.588023	0.216425	10.195025
F	1.508435	0.527985	6.687340
F	3.328240	2.136340	7.788194
F	3.377015	2.567442	10.512496
F	1.535661	1.297836	12.115782
F	-0.310178	-0.350195	11.037318
C	-1.209977	-2.263423	9.013779
C	-2.549154	-2.676729	8.960619
C	-2.993713	-3.930237	9.397693
C	-2.062312	-4.848650	9.893114
C	-0.711458	-4.489295	9.963466
C	-0.323913	-3.208473	9.543809
F	-3.498440	-1.865526	8.409053
F	-4.296572	-4.281867	9.302371
F	-2.457345	-6.093519	10.247969
F	0.200187	-5.397990	10.382343
F	1.008737	-2.924997	9.598481
H	-0.347336	2.113369	3.513931
H	0.538240	0.944696	4.513885
H	-0.955643	-0.824661	4.106240
H	-2.366845	0.244045	3.918516
H	-4.347535	4.836071	3.031085
H	-6.143041	1.437610	4.966336
H	2.530677	4.969758	7.059197
H	-0.600323	4.378911	9.946529
H	-1.216381	4.100604	3.128332
H	-2.185564	5.524073	3.520374
H	-1.191493	4.758351	4.782972
H	-7.376438	2.635445	3.228033
H	-6.592974	3.935298	2.291123
H	-7.265393	4.280667	3.900976

H	-5.015162	0.037332	6.341433
H	-3.334752	-0.286766	5.885010
H	-3.672755	0.703143	7.294860
H	2.431793	4.207234	4.948941
H	0.915056	3.675090	4.197645
H	1.976309	2.495222	5.017570
H	2.555742	4.844733	10.160404
H	2.471316	6.321335	9.172275
H	1.217146	5.991980	10.407262
H	-2.527287	3.275967	9.471019
H	-2.157345	1.753170	8.632832
H	-3.048398	3.046856	7.784428
H	0.686996	-3.173110	7.156736
H	1.484334	-1.913639	6.194583
H	-0.433318	-0.628120	5.951125
H	-1.561096	-1.903461	6.398172
H	-1.828410	-6.962631	7.698876
H	-4.707237	-4.603939	5.551616
H	4.615276	-5.450013	4.025899
H	1.431199	-6.734736	1.442140
H	0.781543	-6.670885	6.000970
H	1.131670	-5.116259	6.744990
H	0.409649	-6.406032	7.729172
H	-5.472315	-6.123766	7.290838
H	-4.287356	-6.805312	8.435144
H	-4.639490	-7.654350	6.910205
H	-4.122767	-3.059465	3.992812
H	-2.798001	-2.031878	4.590632
H	-2.509184	-3.113046	3.226738
H	4.359537	-3.965402	5.664843
H	2.787001	-3.791280	6.476417
H	3.267999	-2.632691	5.227099
H	3.995623	-7.019562	0.832549
H	5.142083	-6.919479	2.198053
H	3.900257	-8.195506	2.158749
H	-0.636673	-5.852181	1.511088
H	-0.872303	-4.241536	2.243977
H	-1.263239	-5.688106	3.176701
H	-1.552127	0.944795	6.600000
H	-1.702196	-0.137107	8.209141

TS**1c** (optimized at B97D/6-31G level in gas phase)

C	-1.963088	0.973825	1.707715
C	-0.687379	0.597723	2.142825
C	0.306302	0.642808	1.151966
C	0.064753	1.026710	-0.173357
C	-1.234641	1.373227	-0.559284
C	-2.262281	1.346350	0.389166
B	-0.381474	-0.155947	3.578656
C	-1.182192	0.536586	4.858395
C	-1.992951	-0.076838	5.818253
C	-2.602062	0.579046	6.896850
C	-2.375782	1.943089	7.076447
C	-1.542299	2.616004	6.174511
C	-0.987359	1.912949	5.096284
F	-2.201062	-1.439845	5.804217
F	-3.367876	-0.099478	7.786249
F	-2.910586	2.592000	8.134192
F	-1.273018	3.925075	6.376416
F	-0.183954	2.626560	4.271011
F	1.573146	0.242064	1.437716

F	1.054384	1.017470	-1.095788
F	-1.505089	1.672473	-1.851360
F	-3.534123	1.612217	0.009917
F	-3.023986	0.904686	2.567086
C	-0.618542	-1.755549	3.223194
C	-2.062848	-2.217490	2.932417
P	-1.988625	-3.839045	2.002842
C	-3.630056	-4.684648	1.767305
C	-4.876655	-4.294014	2.333772
C	-6.003203	-5.120163	2.152665
C	-5.951398	-6.325042	1.441705
C	-4.713011	-6.709456	0.906167
C	-3.560300	-5.923187	1.055527
C	-5.074582	-3.030435	3.150702
C	-7.181439	-7.186825	1.254254
C	-2.266026	-6.437658	0.450856
C	-1.442521	-3.166850	0.352567
C	-0.094016	-3.410617	-0.031878
C	0.429220	-2.762407	-1.164775
C	-0.339216	-1.879366	-1.936076
C	-1.670459	-1.663188	-1.552496
C	-2.240315	-2.278477	-0.424694
C	0.827372	-4.327022	0.757940
C	-3.675308	-1.908586	-0.093635
C	0.236268	-1.177341	-3.147224
F	1.814699	-5.802932	4.325964
C	1.595133	-6.608102	5.393678
C	0.296303	-6.775320	5.911502
C	0.189035	-7.644344	7.010973
C	1.292816	-8.284428	7.594566
C	2.566056	-8.084976	7.041432
C	2.714828	-7.263417	5.916382
B	-0.946080	-5.895620	5.439055
C	-0.688751	-4.324850	5.535667
C	-0.716321	-3.754964	6.975351
P	0.467245	-2.335714	7.015686
C	2.111122	-3.117213	7.110710
C	2.930741	-3.224748	5.950124
C	4.100853	-4.002245	6.043009
C	4.482285	-4.659549	7.220013
C	3.669410	-4.507720	8.355996
C	2.490568	-3.752933	8.329800
F	3.932401	-7.096441	5.365271
F	3.645626	-8.671548	7.589472
F	1.147477	-9.070301	8.676618
F	-1.018840	-7.842675	7.590371
C	2.617703	-2.585313	4.609162
C	5.720184	-5.526013	7.280256
C	1.667234	-3.666294	9.601968
C	-2.397224	-6.477083	5.225349
C	-2.592957	-7.743345	4.635931
C	-3.847025	-8.215276	4.233744
C	-4.980836	-7.422955	4.465586
C	-4.844046	-6.166692	5.068157
C	-3.568116	-5.720384	5.426435
F	-1.525841	-8.526577	4.364966
F	-3.507517	-4.484154	5.989120
F	-5.929244	-5.402700	5.281939
F	-6.193212	-7.865996	4.106961
F	-3.981427	-9.408881	3.630508
C	0.177317	-0.944804	8.148733

C	-0.778311	-0.962165	9.198958
C	-1.000310	0.227893	9.912950
C	-0.329627	1.420693	9.613430
C	0.624626	1.402698	8.583410
C	0.900602	0.249223	7.840438
C	-1.634654	-2.160589	9.554996
C	-0.636470	2.708489	10.341866
C	1.921284	0.333951	6.725456
H	-0.363321	-4.480390	7.722667
H	-1.722897	-3.430508	7.243314
H	-1.404265	-3.756961	4.938493
H	0.301748	-4.171699	5.089340
H	3.958176	-4.995573	9.290371
H	4.724482	-4.105498	5.153145
H	-1.749777	0.223827	10.707059
H	1.158779	2.321690	8.332385
H	0.767772	-4.302817	9.547313
H	2.256780	-4.017879	10.460588
H	1.334134	-2.639828	9.813545
H	6.282462	-5.486420	6.336634
H	5.443241	-6.575432	7.466898
H	6.384697	-5.206377	8.099561
H	3.524776	-2.563085	3.988787
H	1.863230	-3.162757	4.054834
H	2.239276	-1.556843	4.682468
H	-2.044610	-2.041692	10.568222
H	-1.081607	-3.107952	9.524170
H	-2.486726	-2.232170	8.861957
H	0.277434	3.145133	10.776980
H	-1.055710	3.444131	9.638192
H	-1.367672	2.549738	11.147793
H	2.447226	1.297921	6.765543
H	1.437298	0.268109	5.736186
H	2.674758	-0.467042	6.792127
H	-2.591312	-1.466874	2.337459
H	-2.622847	-2.346873	3.860533
H	-0.184492	-2.427180	3.972970
H	0.001212	-1.912645	2.323358
H	-2.279837	-0.961523	-2.127389
H	1.471982	-2.942009	-1.440007
H	-6.951407	-4.808225	2.597031
H	-4.635862	-7.652412	0.357468
H	-4.188841	-1.555056	-1.000574
H	-4.242100	-2.752507	0.315871
H	-3.722228	-1.081421	0.633158
H	1.335732	-1.161214	-3.110442
H	-0.122320	-0.139755	-3.199234
H	-0.065807	-1.686786	-4.079398
H	1.800198	-4.419204	0.250909
H	1.006319	-3.940420	1.773979
H	0.399855	-5.334998	0.872837
H	-6.147192	-2.855156	3.320309
H	-4.658982	-2.146262	2.651052
H	-4.597205	-3.110058	4.138747
H	-6.954497	-8.245883	1.454318
H	-7.990799	-6.875855	1.931666
H	-7.559399	-7.119386	0.219228
H	-2.433383	-7.398710	-0.058312
H	-1.497596	-6.592238	1.226963
H	-1.845716	-5.727261	-0.278701
H	0.393177	-1.758638	5.743629

H	0.818474	-0.017563	3.830338
H	-0.536409	-5.971559	3.582229
H	-0.837296	-5.418105	3.103375

dimer-PD**1'** (optimized at B97D/6-31G level in gas phase)

C	-1.366607	0.449678	0.521450
C	-0.849619	0.251087	1.806202
C	0.539383	0.058944	1.855101
C	1.369333	0.080548	0.727033
C	0.798872	0.289977	-0.533935
C	-0.585365	0.460732	-0.642731
B	-1.754947	-0.056190	3.144548
C	-3.158720	0.778792	3.302760
C	-4.375280	0.252442	3.752735
C	-5.498147	1.024828	4.082335
C	-5.432977	2.413184	3.946038
C	-4.243089	2.998027	3.495029
C	-3.149163	2.179597	3.188033
F	-4.527411	-1.096234	3.955745
F	-6.613597	0.449835	4.588729
F	-6.481132	3.185367	4.306824
F	-4.149603	4.346742	3.429271
F	-2.011303	2.810450	2.802034
F	1.148592	-0.237186	3.043757
F	2.700441	-0.146530	0.828923
F	1.568574	0.259032	-1.644658
F	-1.151791	0.570830	-1.866115
F	-2.716771	0.551278	0.342731
C	-1.855056	-1.700965	3.161022
C	-2.636281	-2.366358	2.004529
P	-1.803345	-3.955188	1.618119
C	-2.777950	-5.365898	1.002493
C	-4.092049	-5.237771	0.479720
C	-4.793749	-6.411245	0.153016
C	-4.252617	-7.689249	0.342983
C	-2.948240	-7.786497	0.855148
C	-2.193968	-6.656256	1.192655
C	-4.825107	-3.919862	0.320565
C	-5.055435	-8.935424	0.047552
C	-0.812048	-6.858938	1.780318
C	-0.291794	-3.577625	0.668956
C	0.994562	-3.649666	1.284004
C	2.114669	-3.299755	0.512939
C	2.013358	-2.869098	-0.818217
C	0.736910	-2.799212	-1.393292
C	-0.421170	-3.138552	-0.678593
C	1.240630	-4.016022	2.737594
C	-1.760361	-2.976734	-1.372283
C	3.242523	-2.432622	-1.580393
F	1.438468	-6.136533	6.760029
C	0.401656	-6.122418	7.637506
C	-0.919627	-6.049532	7.166768
C	-1.892059	-5.959192	8.170031
C	-1.599535	-5.900173	9.541707
C	-0.264729	-5.970350	9.956029
C	0.745453	-6.094244	8.995436
B	-1.199382	-5.689233	5.578798
C	-0.966715	-4.045367	5.555512
C	-1.969450	-3.187121	6.352407
P	-1.173663	-1.569250	6.690656
C	0.054540	-1.945032	7.984556

C	1.425832	-2.109331	7.635931
C	2.299362	-2.622870	8.610141
C	1.866541	-2.980721	9.895729
C	0.512679	-2.793253	10.214309
C	-0.407976	-2.289081	9.285912
F	2.039677	-6.125976	9.389261
F	0.052563	-5.862446	11.267352
F	-2.578185	-5.705673	10.456977
F	-3.205017	-5.803713	7.828121
C	1.990182	-1.797265	6.259893
C	2.816108	-3.561639	10.918609
C	-1.861359	-2.187310	9.712319
C	-2.599394	-6.312441	4.959261
C	-2.767963	-7.711147	4.983663
C	-3.845864	-8.386240	4.393630
C	-4.851469	-7.647733	3.755146
C	-4.743273	-6.257347	3.705759
C	-3.630957	-5.640202	4.295459
F	-1.828653	-8.484412	5.580053
F	-3.593747	-4.273829	4.134451
F	-5.694446	-5.526457	3.078789
F	-5.898651	-8.273781	3.175237
F	-3.932501	-9.733045	4.427486
C	-2.190439	-0.077396	6.916142
C	-3.601115	-0.115504	7.083477
C	-4.302202	1.103166	7.060370
C	-3.665644	2.337239	6.873642
C	-2.267608	2.345871	6.737277
C	-1.510889	1.168547	6.756239
C	-4.420623	-1.383284	7.238929
C	-4.451679	3.628452	6.833460
C	-0.009776	1.267748	6.570619
H	-2.198570	-3.629008	7.328572
H	-2.911839	-3.048050	5.820280
H	-0.905066	-3.625743	4.547120
H	0.041260	-3.928242	5.987314
H	0.151790	-3.084863	11.202654
H	3.349007	-2.766821	8.344525
H	-5.389536	1.075096	7.156993
H	-1.749247	3.297059	6.595559
H	-2.424180	-3.093410	9.431499
H	-1.926762	-2.102375	10.806716
H	-2.369080	-1.315674	9.275742
H	3.761651	-3.873470	10.452218
H	2.361913	-4.437644	11.402955
H	3.046213	-2.821349	11.704123
H	3.084077	-1.903913	6.269052
H	1.595990	-2.487497	5.497586
H	1.752430	-0.775934	5.928231
H	-5.365937	-1.152559	7.751391
H	-3.906486	-2.161823	7.815341
H	-4.676625	-1.796765	6.252643
H	-4.319526	4.195172	7.771525
H	-4.111367	4.269793	6.006921
H	-5.524504	3.438243	6.694213
H	0.315387	2.314356	6.655381
H	0.278380	0.911644	5.566578
H	0.540591	0.678120	7.321228
H	-2.635157	-1.761310	1.090110
H	-3.672894	-2.554855	2.292458
H	-2.292505	-2.087199	4.083851

H	-0.801746	-2.024269	3.147594
H	0.632867	-2.442470	-2.419858
H	3.100277	-3.343312	0.981277
H	-5.808572	-6.316125	-0.239574
H	-2.506286	-8.773298	1.010793
H	-1.616180	-2.871182	-2.456821
H	-2.424008	-3.837426	-1.202469
H	-2.279034	-2.066441	-1.028272
H	4.088725	-3.112799	-1.394679
H	3.540010	-1.425721	-1.250549
H	3.050218	-2.391798	-2.662508
H	2.310681	-4.212362	2.895868
H	0.962190	-3.178247	3.395136
H	0.689183	-4.900915	3.083238
H	-5.638818	-4.028558	-0.411181
H	-4.178169	-3.099086	-0.011989
H	-5.280817	-3.628490	1.279888
H	-5.428446	-9.368968	0.988957
H	-5.923448	-8.711875	-0.590525
H	-4.437659	-9.699197	-0.450725
H	-0.514596	-7.913562	1.695479
H	-0.792896	-6.600800	2.853254
H	-0.050903	-6.248776	1.269184
H	-0.433438	-1.272237	5.539404
H	-1.093061	0.258692	4.127527
H	-0.293544	-6.172341	4.900753
H	-1.337419	-4.427699	2.845351

2 (optimized at B97D/6-31G level in gas phase)

C	-0.973532	2.616655	-1.460718
C	-0.667260	2.019269	-0.211948
C	0.699083	1.834026	0.159260
C	1.705918	2.371818	-0.650406
C	1.413311	3.092266	-1.820715
C	0.076272	3.154943	-2.228384
P	-1.889360	1.709270	1.128850
C	-2.269512	-0.096818	1.302317
C	-3.048003	-0.504832	2.426263
C	-3.267298	-1.872553	2.655624
C	-2.763274	-2.863721	1.806542
C	-2.059618	-2.444729	0.669397
C	-1.807022	-1.091122	0.381927
C	-3.753076	0.446154	3.370393
C	-2.970355	-4.332808	2.103297
C	-1.106487	-0.814220	-0.939008
C	1.095206	1.033178	1.381349
C	2.504828	3.802782	-2.587940
C	-2.359201	2.679889	-2.077403
C	-3.428343	2.796206	0.921797
C	-3.144076	3.688205	2.169088
B	-1.590069	3.285307	2.589385
C	-0.351792	4.169864	1.993210
C	-0.450377	4.947460	0.821899
C	0.635174	5.569644	0.195039
C	1.906421	5.469579	0.766543
C	2.065217	4.745583	1.952015
C	0.949892	4.126720	2.534808
F	-1.639733	5.092117	0.179013
F	0.478200	6.231741	-0.968975
F	2.968822	6.033293	0.159593
F	3.287799	4.630417	2.506683

F	1.216185	3.410945	3.656653
C	-1.442722	2.932435	4.169027
C	-1.760680	3.958589	5.072814
C	-1.702901	3.814159	6.465658
C	-1.307445	2.582236	7.005251
C	-0.979067	1.526910	6.143686
C	-1.043522	1.726938	4.757795
F	-2.147119	5.169865	4.593663
F	-0.713004	0.661051	3.981027
F	-0.604182	0.336232	6.654027
F	-1.249256	2.412313	8.338819
F	-2.019861	4.835637	7.285442
H	-3.236448	3.398058	0.030239
H	-4.131897	0.487881	-0.458829
H	-3.309957	4.752807	1.955053
H	-3.824763	3.413513	2.987821
H	-0.169073	3.644240	-3.174732
H	-3.860664	-2.163724	3.526326
H	-1.700430	-3.198881	-0.035670
H	-2.788281	3.693114	-2.002747
H	-2.288953	2.440970	-3.150393
H	-3.066527	1.975747	-1.623607
H	3.445480	3.229870	-2.575503
H	2.707655	4.782581	-2.124445
H	2.212448	3.980342	-3.634213
H	2.189935	0.950057	1.445575
H	0.739026	1.486033	2.312982
H	0.671483	0.016464	1.345130
H	-3.803053	0.012539	4.380423
H	-4.782120	0.620247	3.018820
H	-3.271205	1.421237	3.457380
H	-2.972995	-4.931317	1.178979
H	-2.159515	-4.719301	2.745537
H	-3.919658	-4.502872	2.634808
H	-1.080805	-1.736688	-1.538375
H	-0.070808	-0.469621	-0.809420
H	-1.624319	-0.043853	-1.526121
H	2.747392	2.244014	-0.344975
C	-4.789374	2.142293	0.780736
C	-5.911992	2.726545	1.401698
C	-7.187061	2.158073	1.268290
C	-7.364628	0.988791	0.512051
C	-6.256867	0.402290	-0.118230
C	-4.984118	0.976187	0.012910
H	-5.783175	3.632442	1.995307
H	-8.041395	2.628606	1.759686
H	-8.355098	0.539481	0.416125
H	-6.377712	-0.510123	-0.705928

cis-**2** (optimized at B97D/6-31G level in gas phase)

C	0.025905	-0.070718	-0.373724
C	-0.181350	-0.445612	0.988817
C	0.891217	-1.079798	1.691816
C	2.119958	-1.293984	1.046665
C	2.349604	-0.889342	-0.274104
C	1.282160	-0.302993	-0.964505
P	-1.635687	-0.054637	2.085629
C	-2.476565	-1.695932	2.386571
C	-2.772490	-2.046410	3.735083
C	-3.393835	-3.278098	4.007404
C	-3.748904	-4.177063	2.993644

C	-3.460801	-3.814642	1.670262
C	-2.835861	-2.598612	1.345597
C	-2.483408	-1.132602	4.907550
C	-4.449904	-5.480623	3.312548
C	-2.618781	-2.296714	-0.120404
C	0.776051	-1.522453	3.140120
C	3.717877	-1.007372	-0.907059
C	-1.020569	0.569264	-1.266285
C	-2.915020	1.100001	1.274809
C	-2.302785	2.531350	1.427469
B	-1.154107	2.634550	2.563900
C	0.394314	2.405177	2.289309
C	1.015584	2.593035	1.039026
C	2.349367	2.252330	0.783842
C	3.123925	1.696443	1.805910
C	2.567204	1.521028	3.078917
C	1.239691	1.896581	3.298236
F	0.333813	3.129749	-0.000796
F	2.878096	2.403854	-0.444829
F	4.382971	1.298688	1.558115
F	3.292706	0.941469	4.053401
F	0.743911	1.641000	4.531220
C	-1.519215	3.470222	3.886966
C	-1.570782	4.859669	3.689026
C	-1.876399	5.776062	4.702538
C	-2.153001	5.290496	5.989378
C	-2.118027	3.910379	6.232180
C	-1.801361	3.030239	5.185284
F	-1.306671	5.351799	2.448451
F	-1.804464	1.711830	5.473873
F	-2.393155	3.441059	7.463599
F	-2.453819	6.144083	6.982526
F	-1.907363	7.098958	4.459059
H	-3.111744	0.858773	0.223040
H	-4.927245	-0.616803	0.669669
H	-1.887227	2.849515	0.464169
H	-3.118544	3.235384	1.656805
H	1.433772	0.010274	-2.000419
H	-3.610092	-3.534637	5.047914
H	-3.731615	-4.496676	0.859361
H	-1.351311	1.542921	-0.890403
H	-0.604594	0.736839	-2.270525
H	-1.908356	-0.065840	-1.379904
H	4.298056	-1.830192	-0.461416
H	4.283984	-0.074385	-0.749292
H	3.646079	-1.174332	-1.993274
H	1.727967	-1.953383	3.484157
H	0.530905	-0.679382	3.803894
H	-0.014421	-2.277322	3.273956
H	-2.661346	-1.660072	5.857161
H	-3.139589	-0.251439	4.877646
H	-1.450485	-0.759709	4.903536
H	-5.546266	-5.346810	3.316648
H	-4.215718	-6.254448	2.564694
H	-4.161482	-5.856150	4.306790
H	-3.005351	-3.114698	-0.746486
H	-1.556373	-2.149380	-0.358291
H	-3.150937	-1.376863	-0.409441
H	-7.427352	0.050993	4.128046
H	-6.975121	-1.137824	1.970917
H	2.931611	-1.760849	1.610828

C	-4.200907	0.877679	2.055110
C	-4.471965	1.546881	3.263564
C	-5.626923	1.253822	4.004936
C	-6.530620	0.282740	3.549855
C	-6.276840	-0.383734	2.339799
C	-5.124193	-0.086694	1.602774
H	-3.781414	2.305661	3.624864
H	-5.815233	1.785410	4.940192

trans-**2** (optimized at B97D/6-31G level in gas phase)

C	0.049465	-0.009799	0.124890
C	-0.021931	-0.007576	1.523307
C	1.197740	0.009089	2.206873
C	2.433064	0.025772	1.551551
C	2.458901	0.009079	0.150456
C	1.261012	-0.020379	-0.574029
B	-1.437612	0.184125	2.234449
C	-2.082229	-0.921332	3.142283
C	-3.360787	-0.766475	3.739111
C	-3.890871	-1.667160	4.669807
C	-3.150497	-2.803365	5.023463
C	-1.896263	-3.030743	4.437726
C	-1.394733	-2.107011	3.512978
F	-4.148820	0.278249	3.437067
F	-5.094443	-1.456097	5.226342
F	-3.642391	-3.675085	5.911697
F	-1.197410	-4.130469	4.766831
F	-0.191002	-2.405252	2.988925
F	1.200961	0.065688	3.566488
F	3.586727	0.120837	2.241074
F	3.635363	0.083171	-0.499811
F	1.287827	-0.001990	-1.918750
F	-1.101188	0.009970	-0.592658
C	-1.979054	1.659433	2.042440
C	-1.259975	2.463625	3.210773
P	-1.026363	4.258343	2.538419
C	0.131261	5.335568	3.549335
C	0.645566	5.107944	4.856750
C	1.496052	6.061478	5.445614
C	1.861318	7.250038	4.801002
C	1.315399	7.486068	3.533237
C	0.456603	6.570374	2.900713
C	0.318224	3.886827	5.688152
C	2.815916	8.234225	5.443575
C	-0.083491	6.969625	1.536535
C	0.081366	3.832030	1.079538
C	-0.496074	3.918349	-0.221089
C	0.275775	3.590066	-1.350344
C	1.617245	3.198895	-1.244459
C	2.176307	3.132438	0.039237
C	1.443589	3.432343	1.201553
C	-1.932223	4.361971	-0.450321
C	2.187460	3.319668	2.518918
C	2.443855	2.859303	-2.466496
H	-0.270612	2.026633	3.400635
H	-0.804145	0.802501	5.299034
H	-3.058930	1.818671	2.119546
H	-1.638344	2.022548	1.064788
H	3.215005	2.808514	0.146329
H	-0.187710	3.643921	-2.339058
H	1.886451	5.859896	6.447175

H	1.554688	8.418696	3.014276
H	3.078689	2.686713	2.398638
H	2.510111	4.309277	2.877385
H	1.576187	2.884131	3.316407
H	1.801204	2.597356	-3.320315
H	3.112407	2.010082	-2.263664
H	3.073027	3.715430	-2.767118
H	-2.159545	4.379342	-1.527228
H	-2.656153	3.694317	0.041784
H	-2.107493	5.369214	-0.040984
H	0.910023	3.884279	6.616072
H	0.530025	2.947325	5.160417
H	-0.744025	3.864278	5.967824
H	2.593150	9.267418	5.132949
H	2.763663	8.182200	6.542552
H	3.860414	8.022214	5.152930
H	0.134296	8.030054	1.337928
H	-1.175397	6.828159	1.476127
H	0.361425	6.371690	0.726060
C	-2.096751	2.319243	4.469408
C	-3.286372	3.047224	4.656331
C	-4.089004	2.825142	5.784106
C	-3.718131	1.864931	6.739547
C	-2.530176	1.138081	6.564965
C	-1.728081	1.366916	5.438241
H	-3.583198	3.784440	3.907668
H	-5.009457	3.398116	5.914251
H	-4.347447	1.687971	7.613942
H	-2.227939	0.392564	7.303753

TS**2** (optimized at B97D/6-31G level in gas phase)

C	0.084829	-0.006985	-0.161313
C	-0.102077	-0.532780	1.149989
C	0.942062	-1.328893	1.718744
C	2.100171	-1.600046	0.971646
C	2.290882	-1.094526	-0.320168
C	1.269829	-0.303859	-0.860475
P	-1.522117	-0.235034	2.320447
C	-2.387299	-1.873699	2.448328
C	-2.635256	-2.375330	3.757652
C	-3.291862	-3.610349	3.905809
C	-3.714406	-4.367995	2.805781
C	-3.454665	-3.863359	1.522506
C	-2.802529	-2.636372	1.321545
C	-2.236510	-1.633281	5.021725
C	-4.452407	-5.676906	2.992573
C	-2.586051	-2.171675	-0.102005
C	0.884847	-1.877789	3.133907
C	3.578125	-1.335240	-1.077255
C	-0.914483	0.873027	-0.886482
C	-2.849417	0.992607	1.674395
C	-2.514769	2.504230	2.030179
B	-1.291621	2.917909	3.010039
C	0.202354	2.496032	2.572369
C	0.678333	2.873741	1.307594
C	1.909458	2.465064	0.786937
C	2.743908	1.659763	1.569467
C	2.338094	1.296365	2.856979
C	1.102401	1.741765	3.342255
F	-0.077852	3.683791	0.517235
F	2.283483	2.808956	-0.459390

F	3.919830	1.226882	1.083583
F	3.122711	0.497692	3.605050
F	0.781755	1.348234	4.601425
C	-1.461122	4.239771	3.906904
C	-0.515809	5.287770	3.914715
C	-0.688340	6.470799	4.650079
C	-1.838410	6.636956	5.432821
C	-2.804317	5.620797	5.467122
C	-2.599422	4.463406	4.706912
F	0.612785	5.213682	3.176217
F	-3.556690	3.507490	4.799471
F	-3.905436	5.766391	6.226015
F	-2.014351	7.759346	6.146440
F	0.237234	7.445886	4.610497
H	-2.953847	0.906025	0.589374
H	-4.901258	-0.284906	0.413138
H	-2.292719	3.022245	1.083865
H	-3.443948	2.957911	2.402376
H	1.400762	0.117004	-1.860648
H	-3.478919	-3.986948	4.915028
H	-3.771844	-4.438424	0.647903
H	-1.214807	1.741640	-0.292021
H	-0.473032	1.256381	-1.817907
H	-1.824560	0.316955	-1.157947
H	4.047347	-2.285170	-0.777235
H	4.297793	-0.526137	-0.868419
H	3.406151	-1.356676	-2.164902
H	1.817296	-2.410095	3.372592
H	0.763569	-1.067302	3.869080
H	0.045360	-2.576405	3.272748
H	-2.397467	-2.271465	5.904211
H	-2.841500	-0.722532	5.149149
H	-1.181949	-1.322333	5.003497
H	-5.543379	-5.529268	2.904294
H	-4.159981	-6.414006	2.227611
H	-4.255618	-6.108379	3.986199
H	-3.094597	-2.842781	-0.810528
H	-1.517725	-2.135827	-0.361215
H	-2.987482	-1.158677	-0.248861
H	-1.571862	1.904366	4.323314
H	-1.497503	1.208298	3.944794
H	2.887340	-2.203208	1.431040
C	-4.165113	0.524864	2.278484
C	-4.457636	0.701006	3.644523
C	-5.646924	0.205264	4.196605
C	-6.569771	-0.476752	3.389614
C	-6.296887	-0.646412	2.023242
C	-5.107214	-0.147407	1.476469
H	-3.750175	1.226708	4.279825
H	-5.849721	0.352171	5.259628
H	-7.495178	-0.866063	3.818756
H	-7.010313	-1.167709	1.381398

gauche-PD**2** (optimized at B97D/6-31G level in gas phase)

C	0.084829	-0.006985	-0.161313
C	-0.102077	-0.532780	1.149989
C	0.942062	-1.328893	1.718744
C	2.100171	-1.600046	0.971646
C	2.290882	-1.094526	-0.320168
C	1.269829	-0.303859	-0.860475
P	-1.522117	-0.235034	2.320447

C	-2.387299	-1.873699	2.448328
C	-2.635256	-2.375330	3.757652
C	-3.291862	-3.610349	3.905809
C	-3.714406	-4.367995	2.805781
C	-3.454665	-3.863359	1.522506
C	-2.802529	-2.636372	1.321545
C	-2.236510	-1.633281	5.021725
C	-4.452407	-5.676906	2.992573
C	-2.586051	-2.171675	-0.102005
C	0.884847	-1.877789	3.133907
C	3.578125	-1.335240	-1.077255
C	-0.914483	0.873027	-0.886482
C	-2.849417	0.992607	1.674395
C	-2.514769	2.504230	2.030179
B	-1.291621	2.917909	3.010039
C	0.202354	2.496032	2.572369
C	0.678333	2.873741	1.307594
C	1.909458	2.465064	0.786937
C	2.743908	1.659763	1.569467
C	2.338094	1.296365	2.856979
C	1.102401	1.741765	3.342255
F	-0.077852	3.683791	0.517235
F	2.283483	2.808956	-0.459390
F	3.919830	1.226882	1.083583
F	3.122711	0.497692	3.605050
F	0.781755	1.348234	4.601425
C	-1.461122	4.239771	3.906904
C	-0.515809	5.287770	3.914715
C	-0.688340	6.470799	4.650079
C	-1.838410	6.636956	5.432821
C	-2.804317	5.620797	5.467122
C	-2.599422	4.463406	4.706912
F	0.612785	5.213682	3.176217
F	-3.556690	3.507490	4.799471
F	-3.905436	5.766391	6.226015
F	-2.014351	7.759346	6.146440
F	0.237234	7.445886	4.610497
H	-2.953847	0.906025	0.589374
H	-4.901258	-0.284906	0.413138
H	-2.292719	3.022245	1.083865
H	-3.443948	2.957911	2.402376
H	1.400762	0.117004	-1.860648
H	-3.478919	-3.986948	4.915028
H	-3.771844	-4.438424	0.647903
H	-1.214807	1.741640	-0.292021
H	-0.473032	1.256381	-1.817907
H	-1.824560	0.316955	-1.157947
H	4.047347	-2.285170	-0.777235
H	4.297793	-0.526137	-0.868419
H	3.406151	-1.356676	-2.164902
H	1.817296	-2.410095	3.372592
H	0.763569	-1.067302	3.869080
H	0.045360	-2.576405	3.272748
H	-2.397467	-2.271465	5.904211
H	-2.841500	-0.722532	5.149149
H	-1.181949	-1.322333	5.003497
H	-5.543379	-5.529268	2.904294
H	-4.159981	-6.414006	2.227611
H	-4.255618	-6.108379	3.986199
H	-3.094597	-2.842781	-0.810528
H	-1.517725	-2.135827	-0.361215

H	-2.987482	-1.158677	-0.248861
H	-1.571862	1.904366	4.323314
H	-1.497503	1.208298	3.944794
H	2.887340	-2.203208	1.431040
C	-4.165113	0.524864	2.278484
C	-4.457636	0.701006	3.644523
C	-5.646924	0.205264	4.196605
C	-6.569771	-0.476752	3.389614
C	-6.296887	-0.646412	2.023242
C	-5.107214	-0.147407	1.476469
H	-3.750175	1.226708	4.279825
H	-5.849721	0.352171	5.259628
H	-7.495178	-0.866063	3.818756
H	-7.010313	-1.167709	1.381398

dimer-**2** (optimized at B97D/6-31G level in gas phase)

C	0.880467	-0.917597	-1.402452
C	0.816430	-0.473363	-0.076101
C	2.042101	-0.298588	0.574666
C	3.271605	-0.528953	-0.053869
C	3.287870	-0.967252	-1.384148
C	2.083436	-1.175707	-2.067218
B	-0.595933	0.036306	0.469690
C	-1.455161	-0.727157	1.532896
C	-2.816570	-0.408414	1.753942
C	-3.554400	-0.900080	2.832597
C	-2.935517	-1.768501	3.743946
C	-1.598789	-2.148634	3.552762
C	-0.894099	-1.643529	2.452817
F	-3.480409	0.391861	0.897509
F	-4.845558	-0.563415	3.004049
F	-3.624191	-2.244237	4.788054
F	-1.014869	-2.990120	4.422747
F	0.388452	-2.037001	2.335448
F	2.072515	0.173028	1.849817
F	4.432692	-0.274286	0.579877
F	4.460946	-1.131624	-2.023551
F	2.097235	-1.568532	-3.353608
F	-0.277210	-1.078739	-2.094531
C	-0.949206	1.479323	-0.067786
C	-0.218456	2.454225	0.945347
P	0.056600	4.087908	-0.055237
C	1.283615	5.278476	0.716759
C	1.763726	5.300068	2.055624
C	2.676081	6.294120	2.451983
C	3.134341	7.289579	1.579022
C	2.617374	7.290049	0.277424
C	1.699902	6.322690	-0.168979
C	1.332930	4.304903	3.110324
C	4.152830	8.318480	2.022776
C	1.194332	6.461691	-1.596007
C	1.123419	3.307607	-1.399185
C	0.522558	3.125146	-2.679668
C	1.216320	2.423099	-3.681165
C	2.502349	1.905383	-3.469595
C	3.094111	2.123230	-2.217877
C	2.439381	2.810395	-1.178422
C	-0.862573	3.650609	-3.006877
C	3.217316	2.989842	0.112373
C	3.238051	1.147871	-4.554830
H	0.759658	2.040885	1.215621

H	0.229112	1.219162	3.315879
H	-2.006002	1.754096	-0.090677
H	-0.536401	1.585737	-1.076679
H	4.094713	1.724438	-2.030863
H	0.732999	2.275869	-4.651185
H	3.038701	6.284195	3.483793
H	2.926804	8.074272	-0.419474
H	4.051822	2.275039	0.156113
H	3.627333	4.009386	0.183590
H	2.604669	2.842473	1.007694
H	2.533726	0.659825	-5.245356
H	3.890097	0.374482	-4.123986
H	3.873277	1.828045	-5.149158
H	-1.120036	3.454682	-4.057987
H	-1.639457	3.187062	-2.381566
H	-0.929028	4.734171	-2.833740
H	1.856779	4.497509	4.058824
H	1.548019	3.266712	2.820553
H	0.253214	4.364704	3.304477
H	4.025959	9.267069	1.477292
H	4.069695	8.523619	3.101835
H	5.182474	7.965755	1.833447
H	1.484105	7.440249	-2.008089
H	0.095541	6.382443	-1.645881
H	1.600207	5.678741	-2.255256
C	-1.078840	2.525168	2.197732
C	-2.300439	3.221543	2.219787
C	-3.140850	3.161439	3.343001
C	-2.771083	2.393655	4.458604
C	-1.551452	1.697440	4.449583
C	-0.714722	1.766394	3.327783
H	-2.595177	3.807364	1.348566
H	-4.082520	3.709595	3.342182
H	-3.427282	2.341783	5.329887
H	-1.251370	1.100355	5.313532
C	-4.604844	5.078889	-4.028519
C	-5.750618	4.916933	-3.243106
C	-7.011738	7.392705	1.467671
C	-7.271321	7.675999	0.117748
C	-6.765794	6.824638	-0.873077
F	-5.026003	4.395032	1.203125
F	-5.990783	5.995651	3.100590
F	-7.490582	8.195908	2.424419
F	-7.997916	8.758969	-0.205730
F	-7.057025	7.165074	-2.142375
F	-8.118045	4.641674	-3.232652
F	-8.227285	4.725389	-5.958042
C	-6.965426	4.833964	-3.929324
F	-5.928926	5.029177	-7.418330
F	-3.504923	5.264262	-6.141167
F	-3.399969	5.158856	-3.409902
C	-5.058735	3.153995	-1.420545
C	-6.397463	2.295385	-1.432554
P	-5.873543	0.534584	-2.033322
C	-7.300231	-0.578505	-2.528246
C	-8.688220	-0.416810	-2.258637
C	-9.601263	-1.389934	-2.703935
C	-9.203506	-2.536525	-3.403357
C	-7.048833	4.885746	-5.325037
C	-7.831557	-2.709861	-3.624133
C	-6.875923	-1.771593	-3.196807

C	-9.262645	0.752420	-1.488841
C	-10.216395	-3.542334	-3.908620
C	-5.418521	-2.101322	-3.477999
C	-5.235075	1.054058	-3.727484
C	-3.823206	1.033872	-3.921860
C	-3.278825	1.475767	-5.140984
C	-4.086088	1.923999	-6.194945
C	-5.474408	1.913490	-6.000472
C	-5.873868	5.041187	-6.073195
C	-6.068526	1.492491	-4.796533
C	-2.860155	0.543966	-2.857321
C	-7.584424	1.517608	-4.742800
C	-3.489019	2.398177	-7.503004
H	-7.094312	2.720899	-2.165858
H	-8.459572	3.885335	-0.693534
H	-4.527718	2.955410	-0.484879
H	-4.413129	2.862412	-2.258895
H	-6.122696	2.269395	-6.805613
H	-2.192522	1.468348	-5.263936
C	-4.637441	5.147693	-5.424474
H	-10.663843	-1.239089	-2.493234
H	-7.483199	-3.609857	-4.138998
H	-7.982460	2.179087	-5.525787
H	-7.999665	0.509414	-4.895510
H	-7.972158	1.868991	-3.781153
H	-2.446005	2.722431	-7.368244
H	-4.062259	3.241356	-7.914562
H	-3.495938	1.590492	-8.255889
H	-1.820317	0.665056	-3.189357
H	-2.983486	1.084588	-1.910193
B	-5.571359	4.629972	-1.682891
H	-3.024589	-0.521173	-2.630246
H	-10.362095	0.703523	-1.479959
H	-8.979821	1.722161	-1.920301
H	-8.918144	0.754997	-0.445540
H	-9.789663	-4.557460	-3.939955
H	-11.113481	-3.561456	-3.269733
H	-10.547015	-3.293393	-4.932903
H	-5.322222	-3.147309	-3.806689
H	-4.792090	-1.965428	-2.580629
H	-4.994418	-1.455597	-4.262630
C	-6.008595	5.660471	-0.584675
C	-7.031456	2.396496	-0.054321
C	-6.543716	1.668778	1.045956
C	-7.064746	1.879274	2.330435
C	-8.087156	2.819838	2.534550
C	-8.596886	3.535226	1.439233
C	-8.070775	3.322820	0.157258
H	-5.745588	0.945328	0.900665
H	-6.659769	1.312301	3.169877
H	-8.488572	2.988688	3.535900
H	-9.399842	4.261916	1.581939
C	-5.759566	5.444241	0.792563
C	-6.244588	6.270395	1.809515

trans-**3** (optimized at B97D/6-31G level in gas phase)

C	-0.989888	0.573610	-0.583799
C	-0.557927	0.350605	0.736562
C	0.730747	-0.206277	0.858330
C	1.531711	-0.539042	-0.236956
C	1.044413	-0.319176	-1.531054

C	-0.224356	0.243912	-1.708370
B	-1.407488	0.711289	2.026437
C	-1.376119	-0.379993	3.206824
C	-1.242090	-0.149439	4.587606
C	-1.327355	-1.157868	5.556695
C	-1.575638	-2.477794	5.157488
C	-1.720624	-2.767232	3.794252
C	-1.600029	-1.730390	2.859824
F	-0.990337	1.093105	5.068261
F	-1.175977	-0.871867	6.861437
F	-1.672839	-3.453827	6.071005
F	-1.963313	-4.028467	3.398738
F	-1.769230	-2.085838	1.561336
F	1.275727	-0.384982	2.084840
F	2.788009	-0.995160	-0.064926
F	1.816903	-0.586449	-2.596116
F	-0.675907	0.498963	-2.949851
F	-2.210892	1.106092	-0.832277
C	-2.366538	1.949466	2.038273
C	-2.094772	3.085664	3.086502
P	-1.492182	4.635508	2.164255
C	-0.540674	5.686258	3.394846
C	-0.866512	5.765789	4.780880
C	-0.092466	6.576942	5.630709
C	0.979314	7.348962	5.164612
C	1.233095	7.329986	3.787001
C	0.492233	6.537411	2.893459
C	-2.051049	5.053928	5.416684
C	1.785913	8.224504	6.100999
C	0.835859	6.671367	1.417562
C	-0.114660	3.824817	1.175336
C	-0.228728	3.872205	-0.242252
C	0.795740	3.336982	-1.041457
C	1.947210	2.760690	-0.486597
C	2.032879	2.693738	0.910376
C	1.023088	3.194345	1.752493
C	-1.430890	4.476900	-0.949255
C	1.206323	2.958242	3.240522
C	3.060005	2.227288	-1.363497
H	-1.361092	2.779498	3.829078
H	-3.006437	3.363848	3.631818
Si	-4.186988	1.315264	2.250018
H	-2.356917	2.391624	1.032453
H	2.900919	2.209526	1.366536
H	0.687742	3.369249	-2.129049
H	-0.349470	6.611663	6.693506
H	2.029297	7.962270	3.382902
H	2.274583	2.837447	3.476791
H	0.807091	3.770501	3.857521
H	0.705289	2.026838	3.548170
H	2.687977	1.961281	-2.364130
H	3.523094	1.332529	-0.921090
H	3.855652	2.981834	-1.492876
H	-1.311193	4.398848	-2.040776
H	-2.365039	3.964736	-0.670958
H	-1.566267	5.538440	-0.688061
H	-2.265091	5.491733	6.403319
H	-1.873283	3.977993	5.565830
H	-2.959607	5.158590	4.803214
H	1.387603	9.254537	6.126295
H	1.760632	7.835802	7.131177

H	2.837775	8.288992	5.779653
H	1.340792	7.633759	1.240131
H	-0.063525	6.638952	0.782943
H	1.501391	5.866676	1.070442
H	-5.061887	3.673296	2.498801
H	-3.928276	1.399844	4.762931
H	-3.911296	-0.974106	1.204803
C	-5.297612	2.809567	1.855716
H	-5.161622	3.130499	0.809353
H	-6.363812	2.563291	1.997857
C	-4.572289	-0.107774	1.049741
H	-5.611644	-0.453217	1.185135
H	-4.455662	0.211581	0.002729
C	-4.451130	0.743493	4.048155
H	-5.523425	0.751123	4.307538
H	-4.077138	-0.280822	4.201898

trans-**4** (optimized at B97D/6-31G level in gas phase)

C	0.129415	-0.014841	0.288439
C	0.059852	0.105112	1.683280
C	1.280106	0.209544	2.357172
C	2.514246	0.190779	1.699648
C	2.537866	0.063155	0.304206
C	1.339653	-0.054057	-0.410792
B	-1.367309	0.285294	2.371403
C	-1.961271	-0.788423	3.361139
C	-3.284956	-0.713560	3.868723
C	-3.834343	-1.658037	4.745139
C	-3.058468	-2.753651	5.149185
C	-1.748920	-2.892168	4.668668
C	-1.232107	-1.928310	3.792999
F	-4.112512	0.291197	3.517211
F	-5.093957	-1.531961	5.194998
F	-3.567660	-3.665327	5.985393
F	-1.008809	-3.946571	5.049101
F	0.024821	-2.153208	3.368653
F	1.280538	0.385414	3.705496
F	3.667323	0.356973	2.375932
F	3.709487	0.111521	-0.356053
F	1.364646	-0.147572	-1.752618
F	-1.020137	-0.096105	-0.425951
C	-2.024801	1.673768	2.007664
C	-1.465757	2.629045	3.139236
P	-0.964582	4.302512	2.378696
C	0.193053	5.232892	3.513817
C	0.715816	4.864444	4.792120
C	1.510722	5.789326	5.498720
C	1.837029	7.056342	5.001258
C	1.335567	7.400027	3.739678
C	0.518467	6.531089	2.998982
C	0.551110	3.508912	5.465216
C	2.679606	8.024769	5.804165
C	0.034896	7.026741	1.644498
C	0.106856	3.820124	0.917411
C	-0.535516	3.845510	-0.357825
C	0.181529	3.469058	-1.508595
C	1.533915	3.107041	-1.456883
C	2.164583	3.128825	-0.205420
C	1.485891	3.464565	0.978559
C	-1.983485	4.276051	-0.541856
C	2.284575	3.413138	2.263078

C	2.300632	2.707898	-2.699575
H	-0.590688	2.174472	3.627785
C	-2.561738	2.891442	4.197818
H	-3.118793	1.726405	1.997976
H	-1.659308	1.982535	1.020955
H	3.215902	2.837019	-0.138688
H	-0.334753	3.465804	-2.472336
H	1.907894	5.493285	6.473846
H	1.578860	8.378233	3.315298
H	3.231439	2.877761	2.105314
H	2.514397	4.420246	2.641320
H	1.734680	2.892200	3.053071
H	1.618839	2.386748	-3.501446
H	2.992244	1.880633	-2.481436
H	2.899885	3.552126	-3.083486
H	-2.249414	4.270156	-1.610167
H	-2.687724	3.615906	-0.012357
H	-2.148707	5.290008	-0.144532
H	1.038811	3.523380	6.451499
H	1.020195	2.693586	4.895099
H	-0.494980	3.226316	5.630934
H	2.044128	8.722768	6.377836
H	3.320623	7.493544	6.525198
H	3.322973	8.633019	5.148395
H	0.341221	8.072434	1.489322
H	-1.063741	6.972764	1.562826
H	0.444849	6.424365	0.818009
H	-2.754029	1.988514	4.796302
H	-3.498740	3.179265	3.698341
H	-2.291350	3.709269	4.882312

dimer-**4** (optimized at B97D/6-31G level in gas phase)

C	0.129415	-0.014841	0.288439
C	0.059852	0.105112	1.683280
C	1.280106	0.209544	2.357172
C	2.514246	0.190779	1.699648
C	2.537866	0.063155	0.304206
C	1.339653	-0.054057	-0.410792
B	-1.367309	0.285294	2.371403
C	-1.961271	-0.788423	3.361139
C	-3.284956	-0.713560	3.868723
C	-3.834343	-1.658037	4.745139
C	-3.058468	-2.753651	5.149185
C	-1.748920	-2.892168	4.668668
C	-1.232107	-1.928310	3.792999
F	-4.112512	0.291197	3.517211
F	-5.093957	-1.531961	5.194998
F	-3.567660	-3.665327	5.985393
F	-1.008809	-3.946571	5.049101
F	0.024821	-2.153208	3.368653
F	1.280538	0.385414	3.705496
F	3.667323	0.356973	2.375932
F	3.709487	0.111521	-0.356053
F	1.364646	-0.147572	-1.752618
F	-1.020137	-0.096105	-0.425951
C	-2.024801	1.673768	2.007664
C	-1.465757	2.629045	3.139236
P	-0.964582	4.302512	2.378696
C	0.193053	5.232892	3.513817
C	0.715816	4.864444	4.792120
C	1.510722	5.789326	5.498720

C	1.837029	7.056342	5.001258
C	1.335567	7.400027	3.739678
C	0.518467	6.531089	2.998982
C	0.551110	3.508912	5.465216
C	2.679606	8.024769	5.804165
C	0.034896	7.026741	1.644498
C	0.106856	3.820124	0.917411
C	-0.535516	3.845510	-0.357825
C	0.181529	3.469058	-1.508595
C	1.533915	3.107041	-1.456883
C	2.164583	3.128825	-0.205420
C	1.485891	3.464565	0.978559
C	-1.983485	4.276051	-0.541856
C	2.284575	3.413138	2.263078
C	2.300632	2.707898	-2.699575
H	-0.590688	2.174472	3.627785
C	-2.561738	2.891442	4.197818
H	-3.118793	1.726405	1.997976
H	-1.659308	1.982535	1.020955
H	3.215902	2.837019	-0.138688
H	-0.334753	3.465804	-2.472336
H	1.907894	5.493285	6.473846
H	1.578860	8.378233	3.315298
H	3.231439	2.877761	2.105314
H	2.514397	4.420246	2.641320
H	1.734680	2.892200	3.053071
H	1.618839	2.386748	-3.501446
H	2.992244	1.880633	-2.481436
H	2.899885	3.552126	-3.083486
H	-2.249414	4.270156	-1.610167
H	-2.687724	3.615906	-0.012357
H	-2.148707	5.290008	-0.144532
H	1.038811	3.523380	6.451499
H	1.020195	2.693586	4.895099
H	-0.494980	3.226316	5.630934
H	2.044128	8.722768	6.377836
H	3.320623	7.493544	6.525198
H	3.322973	8.633019	5.148395
H	0.341221	8.072434	1.489322
H	-1.063741	6.972764	1.562826
H	0.444849	6.424365	0.818009
H	-2.754029	1.988514	4.796302
H	-3.498740	3.179265	3.698341
H	-2.291350	3.709269	4.882312