

Structure, Conformation and Dynamic Processes of the Stereolabile Atropisomers of Hindered Terphenyl Hydrocarbons

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1,4-Bis-(2-methyl-phenyl)benzene (or 2,2''-dimethyl-*p*-terphenyl), 1.[°]

To a solution of 1-bromo-2-methylbenzene (15 mmol in 100 ml of THF) cooled at -78°C were added 10 ml (16 mmol) of BuLi 1.6 M in hexane. After 2h it was transferred dropwise into a solution of triisopropylborate (45 mmol, 10.3 ml) in 20 ml of THF. When the addition was terminated the reaction was maintained for 1h at this temperature and subsequently 1 h at room temperature. Finally the system was quenched with aqueous HCl and extracted with Et₂O. The crude was crystallized from hexane to yield 1.36 g (10 mmol) of 2-methylphenylboronic acid. To a solution of 1,4-dibromobenzene (1 mmol in 6 ml of benzene), K₂CO₃ (2M solution, 1.25 ml), 2-methylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), and Pd(PPh₃)₄ (0.2 mmol) were added at room temperature. The stirred solution was refluxed for 3h, the reaction being monitored by GC-MS. To the cooled solution a second amount of 2-methylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), K₂CO₃ (2M solution, 1.25 ml) and Pd(PPh₃)₄ (0.2 mmol) was added. After refluxing for 3 h, CHCl₃ and H₂O were added and the extracted organic layer dried (Na₂SO₄) and evaporated. The crude (265 mg 1.02 mmol) was purified by chromatography on silica gel Pet.et./Toluene 10/1. Single crystals suitable for X-ray diffraction were obtained by slow crystallisation from hexane. M.p 145.5-146 °C. ¹H-NMR (300 MHz, CDCl₃, 25°C, TMS): δ=2.48 (s, 6H, CH₃), 7.43 (m, 8H, CH), 7.58 (s, 4H, CH). ¹³C-NMR (300 MHz, CDCl₃, 25°C, TMS): δ=20.8 (CH₃), 126.0 (CH), 127.5 (CH), 129.1 (CH), 130.1 (CH), 130.6 (CH), 135.6 (q), 140.6 (q), 141.9 (q). Anal. Calcd for C₂₀H₁₈ C, 92.98; H, 7.02; found: C, 92.05; H, 7.39

[°] Chaumeil, H; Le Drian, C; Defoin, A. *Synthesis* **2002**, 6, 757-760

1,4-Bis-(2-ethyl-phenyl)benzene (or 2,2''-diethyl-*p*-terphenyl), 2.

To a solution of 1-bromo-2-ethylbenzene (15 mmol in 100 ml of THF) cooled at -78°C were added 10 ml (16 mmol) of BuLi 1.6 M in hexane. After 3h the solution was transferred into a solution of triisopropylborate (45 mmol, 10.3 ml) in 20 ml of THF. When the addition was terminated the reaction was maintained for 2h at this temperature and subsequently 2 h at room temperature. The system was quenched with aqueous HCL and extracted with Et₂O. The crude was crystallized from hexane to obtain 1.55 g (10.5 mmol) of 2-ethylphenylboronic acid. To a solution of 1,4-dibromobenzene (1 mmol in 6 ml of benzene), K₂CO₃ (2M solution, 1.25 ml), 2-ethylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), and Pd(PPh₃)₄ (0.2 mmol) were added at room temperature. The stirred solution was refluxed for 3h, the reaction being monitored by GC-MS. To the cooled solution a second amount of 2-ethylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), K₂CO₃ (2M solution, 1.25 ml) and Pd(PPh₃)₄ (0.2 mmol) was added. After refluxing for 3 h, CHCl₃ and H₂O were added and the extracted organic layer dried (Na₂SO₄) and evaporated. The crude (600 mg 2.1 mmol) was purified by chromatography on silica gel Pet.et./Et₂O 10/1. M.p 163.8-164.4 °C. ¹H-NMR (300 MHz, CDCl₃, 25°C, TMS): δ=1.18 (t J=6.0 Hz, 6H, CH₃), 2.65 (q J=6.1 Hz, 4H, CH₂), 7.2-7.4 (m, 12H, CH). ¹³C-NMR (300 MHz, CDCl₃, 25°C, TMS): δ=16.1 (CH₃), 26.3 (CH₂), 124.8 (CH), 127.5 (CH), 128.4 (CH), 128.7 (CH), 130.5 (CH), 140.5 (q), 141.8 (q), 142.0 (q). Anal. Calcd for C₂₂H₂₂ C, 92.26; H, 7.74; found: C, 92.02; H, 7.92

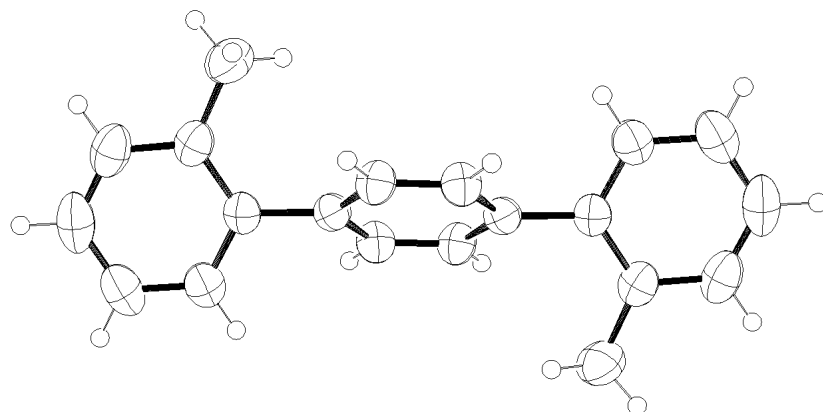
1,4-Bis-(2-isopropyl-phenyl)benzene (or 2,2''-diisopropyl-*p*-terphenyl), 3.

To a solution of 1-bromo-2-isopropylbenzene (15 mmol in 100 ml of THF) cooled at -78°C were added 10 ml (16 mmol) of BuLi 1.6 M in hexane. After 2h the solution was transferred into a solution of triisopropylborate (45 mmol, 10.3 ml) in 20 ml of THF. When the addition was terminated the reaction was maintained for 1h at this temperature and subsequently 1 h at room temperature. The system was quenched with 1 aqueous HCL and extracted with Et_2O . The crude was crystallized in hexane to yield .63 g (10 mmol) of 2-isopropylphenylboronic acid. To a solution of 1,4-dibromobenzene (1 mmol in 6 ml of benzene), K_2CO_3 (2M solution, 1.25 ml), 2-isopropylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), and $\text{Pd}(\text{PPh}_3)_4$ (0.2 mmol) were added at room temperature. The stirred solution was refluxed for 3h, the reaction being monitored by GC-MS. To the cooled solution a second amount of 2-isopropylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), K_2CO_3 (2M solution, 1.25 ml) and $\text{Pd}(\text{PPh}_3)_4$ (0.2 mmol) was added. After refluxing for 3 h, CHCl_3 and H_2O were added and the extracted organic layer dried (Na_2SO_4) and evaporated. The crude (550 mg 2.13 mmol) was purified by chromatography on silica gel n-hexane/ Et_2O 20/1. M.p $171.2\text{-}172.0^{\circ}\text{C}$. $^1\text{H-NMR}$ (300 MHz, CDCl_3 , 25°C , TMS): $\delta=1.38$ (d $J=6.8$ Hz, 12H, CH_3), 3.28 (septet $J=6.7$ Hz, 2H, CH), 7.4-7.6 (m, 12H, CH). $^{13}\text{C-NMR}$ (300 MHz, CDCl_3 , 25°C , TMS): $\delta=24.6$ (CH_3), 29.5 (CH), 125.5 (CH), 125.8 (CH), 127.8 (CH), 129.1 (CH), 130.3 (CH), 140.6 (q), 141.0 (q), 146.6 (q). Anal. Calcd for $\text{C}_{24}\text{H}_{26}$ C, 91.67; H, 8.33; found: C, 92.15; H, 8.06

1,4-Bis-(2-*tert*-butyl-phenyl)benzene (or 2,2''-di-*tert*-butyl-*p*-terphenyl), 4.

A solution of 2-*tert*-butyl-phenylamine (0.1 mol 15.6 ml) in 30 ml of 40 per cent w/w hydrobromic acid was prepared in a 250 ml round-bottomed flask. After cooling to 5°C by immersion in an ice/salt bath, diazotisation was performed by gradual addition of a solution of 15.1 g (0.22 mol) of sodium nitrite in 20 ml of water, stoppering the flask after each addition and shaking until all red fumes were adsorbed. The temperature was kept between 5 and 10°C for 2h. When the diazotisation was completed, 0.4 g of copper powder were added. **The solution was refluxed very cautiously because of evolution of gas.** When the vigorous evolution of nitrogen moderates, the system was kept at 50 °C for 30 minutes and was then diluted with 80 ml of water and extracted with Et₂O. The organic layer was washed with 10% solution of KOH, and the crude purified by chromatography on silica gel (hexane) and distilled at 85°C (3 mm Hg) to obtain 6g (28.3 mmol) of 1-bromo-2-*tert*-butylbenzene. To a solution of 1-bromo-2-*tert*-butylbenzene (15 mmol in 100 ml of THF) kept at –78°C 10 ml (16 mmol) of BuLi (1.6 M in hexane) were added. After 2h the solution was transferred dropwise into a solution of triisopropylborate (45 mmol, 10.3 ml) in 20 ml of THF. When the addition was completed the reaction was maintained for 1h at this temperature and then 1 h at room temperature to be finally quenched with aqueous HCl and extracted with Et₂O. The crude was crystallized from hexane to obtain 0.89 g (5 mmol) of 2-*tert*-butylphenylboronic acid. To a solution of 1,4-dibromobenzene (1 mmol in 6 ml of benzene), K₂CO₃ (2M solution, 1.25 ml), 2-*tert*-butylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), and Pd(PPh₃)₄ (0.2 mmol) were added at room temperature. The stirred solution was refluxed for 5h, the reaction being monitored by GC-MS. To the cooled solution a second amount of 2-*tert*-butylphenylboronic acid (2.5 mmol, suspension in 4 ml of ethanol), K₂CO₃ (2M solution, 1.25 ml) and Pd(PPh₃)₄ (0.2 mmol) was added. After refluxing for 5h, CHCl₃ and H₂O were added and the extracted organic layer dried (Na₂SO₄) and evaporated. The crude (200 mg 0.58 mmol) was purified by chromatography on silica gel (Pet.et./Toluene 10/1) Single crystal suitable for X-ray analysis were obtained by slow crystallisation in hexane. ¹H-NMR (600 MHz, CDCl₃, 25°C, TMS): δ=1.28 (s, 18H, CH₃), 7.15-7.58 (m, 12H, CH). ¹³C-NMR (600 MHz, CDCl₃, 25°C, TMS): δ=32.9 (CH₃), 36.8 (q), 125.0 (CH), 126.8 (CH), 127.3 (CH), 128.5 (CH), 129.0 (CH), 142.1 (q), 143.4 (q), 143.8 (q). Anal. Calcd for C₂₆H₃₀ C, 91.17; H, 8.83; found: C, 91.85; H, 8.30

Crystal Data for 1

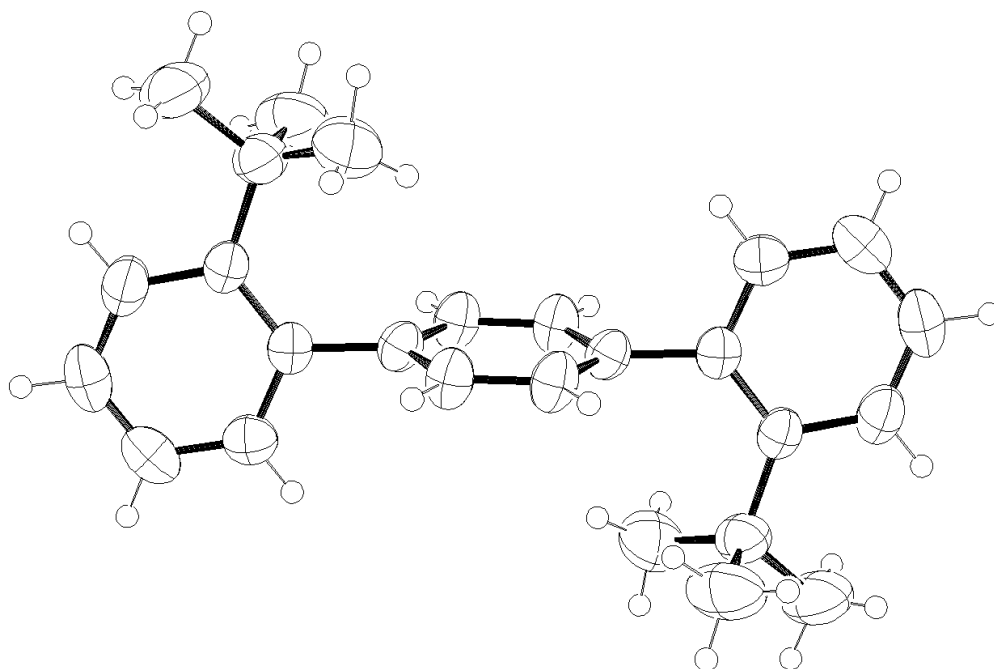


Molecular formula: $C_{20}H_{18}$, $M_r = 258.34$, orthorhombic, space group P_{bca} (No. 61), $a = 10.7905(12)$, $b = 7.6750(8)$, $c = 17.5436(19)$ Å, $V = 1452.9(3)$ Å³, $T = 295(2)$ K, $Z = 4$, $\rho_c = 1.181$ g cm⁻³, $F(000) = 552$, graphite-monochromated $Mo_{K\alpha}$ radiation ($\lambda = 0.71073$ Å), $\mu(Mo_{K\alpha}) = 0.066$ mm⁻¹, colourless block ($0.40 \times 0.40 \times 0.20$ mm³), empirical absorption correction with SADABS (transmission factors: 0.9739 – 0.9868), 2400 frames, exposure time 10 s, $2.99 \leq \theta \leq 28.21$, $-14 \leq h \leq 14$, $-10 \leq k \leq 10$, $-23 \leq l \leq 23$, 14603 reflections collected, 1765 independent reflections ($R_{int} = 0.0239$), 1353 reflections with $I > 2\sigma(I)$ ($R_\sigma = 0.0143$), solution by direct methods (SHELXS^a) and subsequent Fourier syntheses, full-matrix least-squares on F_o^2 (SHELXTL^b), hydrogen atoms refined with a riding model, data / parameters = 1765 / 92, $S(F^2) = 1.073$, $R(F) = 0.0492$ and $wR(F^2) = 0.1038$ on all data, $R(F) = 0.0369$ and $wR(F^2) = 0.0976$ for reflections with $I > 2\sigma(I)$, weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.1543P]$ where $P = (F_o^2 + 2F_c^2)/3$, largest difference peak and hole 0.135 and -0.151 e Å⁻³. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-263239. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

^a SHELXS Ver. 5.10, Bruker Analytical X-ray Systems, 1997

^b SHELXTL Ver. 5.10, Bruker Analytical X-ray Systems, 1997

Crystal Data for 4



Molecular formula: $C_{26}H_{30}$, $M_r = 342.50$, monoclinic, space group $P2_1/c$ (No. 14), $a = 8.206(4)$, $b = 19.137(9)$, $c = 7.029(3)\text{\AA}$, $\beta = 108.955(7)$, $V = 1044.0(8)\text{\AA}^3$, $T = 295(2)\text{ K}$, $Z = 2$, $\rho_c = 1.090\text{ g cm}^{-3}$, $F(000) = 372$, graphite-monochromated $Mo_{K\alpha}$ radiation ($\lambda = 0.71073\text{ \AA}$), $\mu(Mo_{K\alpha}) = 0.061\text{ mm}^{-1}$, colourless plate ($0.20 \times 0.20 \times 0.05\text{ mm}^3$), empirical absorption correction with SADABS (transmission factors: $0.9879 - 0.9970$), 2400 frames, exposure time 20 s, $2.13 \leq \theta \leq 23.75$, $-9 \leq h \leq 9$, $-21 \leq k \leq 21$, $-7 \leq l \leq 7$, 8637 reflections collected, 1576 independent reflections ($R_{int} = 0.0369$), 1137 reflections with $I > 2\sigma(I)$ ($R_\sigma = 0.0286$), solution by direct methods (SHELXS^a) and subsequent Fourier syntheses, full-matrix least-squares on F_o^2 (SHELXTL^b), hydrogen atoms refined with a riding model, data / parameters = 1576 / 122, $S(F^2) = 1.013$, $R(F) = 0.0601$ and $wR(F^2) = 0.1173$ on all data, $R(F) = 0.0423$ and $wR(F^2) = 0.1089$ for reflections with $I > 2\sigma(I)$, weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0700P)^2 + 0.0582P]$ where $P = (F_o^2 + 2F_c^2)/3$, largest difference peak and hole 0.177 and -0.165 e \AA^{-3} . Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-263240. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

^a SHELXS Ver. 5.10, Bruker Analytical X-ray Systems, 1997

^b SHELXTL Ver. 5.10, Bruker Analytical X-ray Systems, 1997

Compound 1: ground state *trans-anti*

B3LYP/6-31G(d) Energy: -772.9913061

C	-0.944558	-0.105233	-3.764601
C	-0.733674	-0.081225	-5.149831
C	0.538072	0.069023	-5.700169
C	1.641609	0.188582	-4.856592
C	1.453281	0.162642	-3.476884
C	0.174892	0.025858	-2.909593
C	-0.790503	0.879666	-0.728540
C	0.061975	0.007106	-1.422894
C	0.852119	-0.870992	-0.662929
C	0.790538	-0.879536	0.728521
C	-0.061947	-0.006982	1.422878
C	-0.852085	0.871122	0.662909
C	-1.641692	-0.188295	4.856525
C	-1.453321	-0.162294	3.476830
C	-0.174882	-0.025753	2.909571
C	0.944568	0.105032	3.764621
C	0.733639	0.080958	5.149849
C	-0.538147	-0.069051	5.700144
C	-2.352286	-0.302764	-3.243613
C	2.352377	0.302289	3.243743
H	-1.591068	-0.194767	-5.809818
H	0.664745	0.084235	-6.779508
H	2.641243	0.303614	-5.267075
H	2.308020	0.268949	-2.814085
H	-1.393185	1.593345	-1.282723
H	1.507000	-1.571704	-1.174239
H	1.393230	-1.593207	1.282704
H	-1.506954	1.571848	1.174215
H	-2.641362	-0.303138	5.266973
H	-2.308065	-0.268380	2.814003
H	1.591044	0.194266	5.809864
H	-0.664853	-0.084321	6.779478
H	-2.837889	0.650135	-2.996526
H	-2.370449	-0.914276	-2.336605
H	-2.974369	-0.793023	-3.999625
H	2.974267	0.793200	3.999495
H	2.838111	-0.650777	2.997539
H	2.370680	0.913076	2.336257

Compound 1: ground state *trans-syn*

B3LYP/6-31G(d) Energy: -772.9913074

C	-0.775020	0.535602	3.746243
C	-0.604370	0.450452	5.134719
C	0.435311	-0.280584	5.706821
C	1.331217	-0.960506	4.882812
C	1.176072	-0.891645	3.500498
C	0.140698	-0.146189	2.911223
C	0.025560	-1.325616	0.696035
C	0.047050	-0.124587	1.423048
C	0.022612	1.076261	0.696041
C	-0.022594	1.076267	-0.696018
C	-0.047034	-0.124574	-1.423038
C	-0.025562	-1.325609	-0.696033
C	-1.331252	-0.960495	-4.882778
C	-1.176083	-0.891623	-3.500468
C	-0.140693	-0.146172	-2.911214
C	0.775026	0.535594	-3.746260
C	0.604350	0.450429	-5.134732
C	-0.435352	-0.280595	-5.706809
C	-1.946747	1.324111	3.201385
C	1.946798	1.324073	-3.201453
H	-1.314636	0.963442	5.779706
H	0.538413	-0.324102	6.787904
H	2.146223	-1.538236	5.310606
H	1.878721	-1.408941	2.852470
H	0.038624	-2.270550	1.232887
H	0.054991	2.023663	1.226338
H	-0.054979	2.023676	-1.226301
H	-0.038637	-2.270539	-1.232892
H	-2.146274	-1.538218	-5.310552
H	-1.878730	-1.408902	-2.852425
H	1.314618	0.963395	-5.779737
H	-0.538471	-0.324124	-6.787890
H	-2.361767	0.868760	2.297400
H	-1.665566	2.352903	2.941410
H	-2.744399	1.389339	3.948713
H	2.744425	1.389263	-3.948812
H	1.665663	2.352879	-2.941488
H	2.361838	0.868723	-2.297477

Compound 1: ground state *cis-anti*

B3LYP/6-31G(d) Energy: -772.9912814

C	0.729325	-0.569777	3.732961
C	0.608551	-0.447312	5.123846
C	-0.408939	0.301297	5.713006
C	-1.332902	0.960850	4.903640
C	-1.227203	0.855027	3.518971
C	-0.214186	0.092268	2.913147
C	-0.174494	-1.184732	0.725629
C	-0.172687	0.033080	1.423643
C	-0.179401	1.216229	0.666957
C	-0.176492	1.184683	-0.725577
C	-0.172633	-0.033125	-1.423600
C	-0.177373	-1.216281	-0.666905
C	-1.331770	-0.962662	-4.903475
C	-1.226142	-0.856562	-3.518825
C	-0.214100	-0.092419	-2.913107
C	0.728552	0.570727	-3.733046
C	0.607882	0.447930	-5.123911
C	-0.408684	-0.302024	-5.712950
C	1.879015	-1.376239	3.167638
C	1.877405	1.378537	-3.167942
H	1.340294	-0.945143	5.756548
H	-0.473209	0.373833	6.795528
H	-2.131628	1.551316	5.344546
H	-1.952418	1.355918	2.883059
H	-0.194235	-2.119478	1.278525
H	-0.179919	2.173665	1.181313
H	-0.197858	2.119398	-1.278456
H	-0.176269	-2.173719	-1.181255
H	-2.129764	-1.554191	-5.344283
H	-1.950703	-1.358309	-2.882841
H	1.339001	0.946569	-5.756699
H	-0.472896	-0.374774	-6.795462
H	2.270988	-0.938519	2.244741
H	1.583024	-2.406668	2.932295
H	2.697361	-1.435624	3.892713
H	2.695642	1.438653	-3.893081
H	1.580333	2.408700	-2.932804
H	2.269908	0.941427	-2.244983

Compound 1: ground state *cis-syn*

B3LYP/6-31G(d) Energy: -772.9912982

C	0.900456	-0.099154	3.716577
C	0.753971	-0.080419	5.110172
C	-0.490755	0.069574	5.719179
C	-1.631820	0.194378	4.927903
C	-1.507592	0.173842	3.540894
C	-0.256980	0.037217	2.914619
C	-1.041923	-0.843495	0.696443
C	-0.212962	0.025532	1.424243
C	0.609005	0.900501	0.696379
C	0.609005	0.900502	-0.696379
C	-0.212962	0.025533	-1.424243
C	-1.041923	-0.843494	-0.696444
C	-1.631819	0.194383	-4.927904
C	-1.507591	0.173848	-3.540894
C	-0.256980	0.037219	-2.914620
C	0.900456	-0.099157	-3.716577
C	0.753971	-0.080422	-5.110172
C	-0.490755	0.069575	-5.719179
C	2.282320	-0.296447	3.130244
C	2.282319	-0.296455	-3.130242
H	1.640720	-0.197779	5.729432
H	-0.567500	0.080797	6.803265
H	-2.611153	0.309734	5.384645
H	-2.391809	0.284691	2.918779
H	-1.680213	-1.540808	1.232777
H	1.234603	1.612393	1.226972
H	1.234603	1.612393	-1.226971
H	-1.680213	-1.540808	-1.232778
H	-2.611151	0.309742	-5.384645
H	-2.391808	0.284699	-2.918780
H	1.640720	-0.197786	-5.729432
H	-0.567499	0.080798	-6.803265
H	2.756948	0.656659	2.863387
H	2.257709	-0.905550	2.221747
H	2.938371	-0.789313	3.855212
H	2.938372	-0.789311	-3.855215
H	2.756944	0.656648	-2.863372
H	2.257705	-0.905569	-2.221753

Compound 1: transition state, 0° degrees

B3LYP/6-31G(d) Energy: -772.980551

Number of imaginary frequencies: 1

C	-0.795443	0.503725	3.800076
C	-0.619422	0.412612	5.187346
C	0.445325	-0.287643	5.751912
C	1.375364	-0.910190	4.920414
C	1.220904	-0.827100	3.538910
C	0.143831	-0.136114	2.957298
C	1.153243	0.288494	0.694606
C	0.054529	-0.096275	1.471341
C	-1.098519	-0.480317	0.770854
C	-1.143746	-0.473274	-0.617548
C	-0.046864	-0.080167	-1.419879
C	1.103981	0.299425	-0.698329
C	-1.597950	-0.556418	-4.867980
C	-1.371978	-0.499602	-3.498623
C	-0.149052	-0.087313	-2.922005
C	0.885199	0.286311	-3.834101
C	0.632717	0.220073	-5.214066
C	-0.582758	-0.192670	-5.746251
C	-1.960414	1.308310	3.263859
C	2.275209	0.765822	-3.463878
H	-1.332772	0.914993	5.837269
H	0.550194	-0.338797	6.832474
H	2.213522	-1.458759	5.341803
H	1.934805	-1.322257	2.885990
H	2.068648	0.604706	1.188160
H	-1.973396	-0.817040	1.319451
H	-2.072644	-0.797407	-1.067840
H	1.996635	0.619306	-1.205755
H	-2.565366	-0.884463	-5.238714
H	-2.195088	-0.792534	-2.861364
H	1.432529	0.507880	-5.891908
H	-0.729620	-0.227079	-6.822231
H	-2.829698	0.675929	3.041504
H	2.844361	0.014878	-2.903848
H	-2.284414	2.049794	4.001521
H	-1.703691	1.834519	2.339792
H	2.843062	0.985133	-4.372823
H	2.258001	1.685056	-2.867211

Compound 1: transition state, 90° degrees

B3LYP/6-31G(d) Energy: -772.9980878

Number of imaginary frequencies: 1

C	0.930489	0.176825	3.754372
C	0.717523	0.158706	5.139382
C	-0.541086	-0.079280	5.689109
C	-1.625003	-0.318289	4.845542
C	-1.432891	-0.308336	3.466024
C	-0.172123	-0.056033	2.899448
C	0.480757	1.024315	0.704477
C	-0.052326	-0.064142	1.412543
C	-0.516252	-1.162522	0.670723
C	-0.444581	-1.174911	-0.721413
C	0.090074	-0.086748	-1.425258
C	0.550354	1.013291	-0.687669
C	1.458617	-0.650539	-4.919965
C	1.333417	-0.613551	-3.530805
C	0.179917	-0.104892	-2.919622
C	-0.876073	0.380068	-3.721865
C	-0.733820	0.335296	-5.114108
C	0.418266	-0.173132	-5.714906
C	2.332518	0.411070	3.233238
C	-2.137586	0.939262	-3.103344
H	1.565919	0.324991	5.799812
H	-0.670359	-0.085252	6.768234
H	-2.613179	-0.508553	5.255804
H	-2.276370	-0.481072	2.802732
H	0.826432	1.898685	1.248318
H	-0.922259	-2.023136	1.195889
H	-0.799864	-2.042381	-1.271916
H	0.964643	1.870174	-1.212887
H	2.361668	-1.049549	-5.374225
H	2.139652	-0.984191	-2.902895
H	-1.544119	0.707221	-5.737313
H	0.499884	-0.195080	-6.798555
H	2.500692	1.460140	2.957702
H	2.543094	-0.189508	2.343256
H	3.072295	0.158110	3.999775
H	-2.846619	1.251841	-3.876259
H	-2.636655	0.201062	-2.464672
H	-1.925983	1.807743	-2.468218

Compound 2: ground state *trans-anti*

B3LYP/6-31G(d) Energy: -851.61622817

C	0.588180	-0.300089	-3.828017
C	0.249362	-0.315188	-5.188246
C	-1.052993	-0.081253	-5.626756
C	-2.054978	0.181985	-4.693856
C	-1.739477	0.197137	-3.336586
C	-0.433203	-0.047787	-2.883069
C	0.222915	-1.172284	-0.712631
C	-0.185761	-0.024780	-1.409377
C	-0.408919	1.146175	-0.668257
C	-0.222943	1.171878	0.713031
C	0.185687	0.024359	1.409793
C	0.408891	-1.146580	0.668659
C	2.054789	-0.183252	4.694276
C	1.739229	-0.198405	3.337012
C	0.433121	0.047333	2.883480
C	-0.588082	0.300464	3.828428
C	-0.249196	0.315576	5.188630
C	1.053022	0.080834	5.627154
C	2.045840	-0.464752	-3.438184
C	-2.045651	0.466057	3.438602
H	1.032544	-0.509131	-5.918454
H	-1.281425	-0.104101	-6.689145
H	-3.076080	0.366300	-5.017004
H	-2.518911	0.384786	-2.602540
H	0.375493	-2.100833	-1.256560
H	-0.716573	2.050696	-1.186604
H	-0.375410	2.100460	1.256930
H	0.716566	-2.051100	1.186997
H	3.075778	-0.368209	5.017415
H	2.518526	-0.386663	2.602977
H	-1.032228	0.510120	5.918834
H	1.281487	0.103693	6.689535
H	2.553828	-1.056393	-4.209860
H	2.139782	-1.025217	-2.503776
H	-2.553768	1.055784	4.211648
H	-2.139403	1.028911	2.505598
C	-2.768854	-0.884035	3.278052
H	-2.308966	-1.481532	2.483694
H	-2.723469	-1.466189	4.205361
H	-3.823703	-0.732211	3.021166
C	2.768958	0.885807	-3.281148
H	2.309441	1.485007	-2.487847
H	3.823996	0.734751	-3.024580
H	2.722873	1.465872	-4.209728

Compound 2: ground state *trans-syn*

B3LYP/6-31G(d) Energy: -851.6163369

C	-0.498636	0.446458	3.819111
C	-0.170783	0.395468	5.181057
C	1.028174	-0.155346	5.631061
C	1.932915	-0.678634	4.708554
C	1.627325	-0.634199	3.349616
C	0.427201	-0.072781	2.884654
C	0.093102	-1.258617	0.691284
C	0.184154	-0.057619	1.409956
C	0.091729	1.144717	0.690515
C	-0.091824	1.144711	-0.690514
C	-0.184139	-0.057630	-1.409960
C	-0.092973	-1.258623	-0.691296
C	-1.932922	-0.678654	-4.708545
C	-1.627324	-0.634218	-3.349609
C	-0.427199	-0.072794	-2.884658
C	0.498628	0.446452	-3.819117
C	0.170768	0.395460	-5.181062
C	-1.028188	-0.155362	-5.631058
C	-1.863701	0.973295	3.415603
C	1.863680	0.973320	-3.415607
H	-0.880759	0.793199	5.903458
H	1.252101	-0.175100	6.694477
H	2.872811	-1.111306	5.040878
H	2.335002	-1.025327	2.623151
H	0.163267	-2.202878	1.225125
H	0.176941	2.090448	1.219345
H	-0.177115	2.090437	-1.219342
H	-0.163056	-2.202887	-1.225142
H	-2.872817	-1.111328	-5.040867
H	-2.334991	-1.025354	-2.623138
H	0.880738	0.793195	-5.903468
H	-1.252123	-0.175121	-6.694472
H	-1.803581	1.536686	2.479949
H	-2.211729	1.677073	4.181870
H	2.211693	1.677096	-4.181883
H	1.803535	1.536727	-2.479963
C	-2.904962	-0.149399	3.252502
H	-3.884371	0.264619	2.985981
H	-2.606063	-0.847858	2.463690
H	-3.016579	-0.719643	4.181655
C	2.904976	-0.149339	-3.252490
H	2.606078	-0.847829	-2.463706
H	3.016653	-0.719558	-4.181652
H	3.884360	0.264711	-2.985923

Compound 2: ground state *cis-anti*

B3LYP/6-31G(d) Energy: -851.6163197

C	0.466205	-0.463662	3.725070
C	0.321189	-0.396867	5.117830
C	-0.803805	0.168477	5.716019
C	-1.818362	0.690642	4.914964
C	-1.695432	0.629545	3.528204
C	-0.571324	0.052938	2.915049
C	-0.533277	-1.192999	0.713005
C	-0.525689	0.018073	1.421761
C	-0.534806	1.210170	0.680964
C	-0.533616	1.192990	-0.712911
C	-0.525751	-0.018084	-1.421666
C	-0.534527	-1.210179	-0.680873
C	-1.818487	-0.690713	-4.914838
C	-1.695546	-0.629578	-3.528082
C	-0.571429	-0.052954	-2.914956
C	0.466081	0.463643	-3.724997
C	0.321057	0.396804	-5.117757
C	-0.803935	-0.168569	-5.715917
C	1.764474	-1.002298	3.152177
C	1.764329	1.002362	-3.152135
H	1.117365	-0.793858	5.744500
H	-0.885523	0.200452	6.799378
H	-2.703081	1.134719	5.363418
H	-2.490479	1.018886	2.897402
H	-0.558038	-2.131617	1.260513
H	-0.544595	2.161018	1.207551
H	-0.558615	2.131598	-1.260427
H	-0.544112	-2.161032	-1.207456
H	-2.703208	-1.134802	-5.363274
H	-2.490578	-1.018917	-2.897259
H	1.117217	0.793800	-5.744445
H	-0.885663	-0.200581	-6.799274
H	1.583102	-1.559578	2.228741
H	2.198240	-1.713428	3.866189
H	2.197768	1.713933	-3.865911
H	1.583001	1.559161	-2.228404
C	2.788030	0.111940	2.865762
H	3.019099	0.676457	3.776177
H	3.723027	-0.309124	2.478175
H	2.400258	0.817298	2.122858
C	2.788221	-0.111749	-2.866446
H	3.723192	0.309362	-2.478846
H	2.400769	-0.817550	-2.123793
H	3.019245	-0.675787	-3.777169

Compound 2: ground state *cis-syn*

B3LYP/6-31G(d) Energy: -851.6163076

C	0.573614	-0.305212	-3.717778
C	0.422925	-0.294588	-5.111370
C	-0.810665	-0.063669	-5.718305
C	-1.933270	0.170162	-4.925571
C	-1.805272	0.159791	-3.537942
C	-0.569842	-0.081909	-2.915862
C	-0.873972	1.064045	-0.697518
C	-0.524512	-0.084926	-1.422199
C	-0.193094	-1.240684	-0.696562
C	-0.193138	-1.240726	0.696372
C	-0.524605	-0.085014	1.422057
C	-0.874017	1.064003	0.697432
C	-1.933510	0.169387	4.925426
C	-1.805512	0.159108	3.537801
C	-0.569980	-0.082102	2.915722
C	0.573546	-0.305012	3.717625
C	0.422863	-0.294481	5.111226
C	-0.810809	-0.064037	5.718159
C	1.965939	-0.466554	-3.135218
C	1.965922	-0.465845	3.135060
H	1.300277	-0.465376	-5.732020
H	-0.892319	-0.066324	-6.802139
H	-2.903248	0.351210	-5.380997
H	-2.679408	0.324265	-2.913150
H	-1.139300	1.970365	-1.235755
H	0.038746	-2.157852	-1.231726
H	0.038703	-2.157912	1.231506
H	-1.139397	1.970285	1.235709
H	-2.903553	0.350046	5.380867
H	-2.679704	0.323281	2.913008
H	1.300280	-0.464984	5.731864
H	-0.892474	-0.066753	6.801992
H	1.939341	-1.064435	-2.219619
H	2.586549	-1.019836	-3.850939
H	1.939392	-1.062881	2.218913
H	2.586488	-1.019762	3.850332
C	2.636834	0.884418	-2.825512
H	2.710811	1.502464	-3.727497
H	2.061935	1.445000	-2.080656
H	3.648412	0.734478	-2.430578
C	2.636799	0.885431	2.826611
H	2.710735	1.502671	3.729152
H	3.648389	0.735889	2.431559
H	2.061891	1.446666	2.082250

Compound 2: transition state

B3LYP/6-31G(d) Energy: -851.6031761

Number of imaginary frequencies: 1

C	-0.521551	0.445202	3.845703
C	-0.360268	0.258607	5.225533
C	0.352629	-0.820408	5.746031
C	0.931608	-1.744159	4.877126
C	0.779036	-1.579235	3.501873
C	0.053270	-0.502406	2.966762
C	1.062690	-0.302811	0.668745
C	-0.069440	-0.409316	1.482383
C	-1.305748	-0.479111	0.824398
C	-1.396291	-0.434339	-0.561548
C	-0.264843	-0.318072	-1.403750
C	0.967345	-0.254043	-0.721784
C	-2.037117	-0.357454	-4.777280
C	-1.733914	-0.384501	-3.422332
C	-0.422300	-0.276039	-2.904510
C	0.625607	-0.143862	-3.868854
C	0.291423	-0.121258	-5.234140
C	-1.011091	-0.221073	-5.705917
C	-1.221809	1.700181	3.356967
C	-0.234477	2.834912	3.026981
C	2.116234	0.014735	-3.597029
C	2.524627	1.447053	-3.202164
H	-0.800743	0.985853	5.904694
H	0.454743	-0.936609	6.821871
H	1.490522	-2.591925	5.264366
H	1.211849	-2.305739	2.818984
H	2.045703	-0.244310	1.129186
H	-2.216754	-0.593834	1.405999
H	-2.393428	-0.500429	-0.975599
H	1.893925	-0.156466	-1.258881
H	-3.071926	-0.446439	-5.096988
H	-2.570095	-0.499059	-2.746972
H	1.102356	-0.020748	-5.951775
H	-1.214928	-0.198855	-6.772920
H	-1.826820	1.491240	2.470181
H	0.369546	3.097149	3.902994
H	-0.770349	3.733544	2.699943
H	0.449062	2.537109	2.224744
H	2.472994	-0.711941	-2.861656
H	2.272983	2.145838	-4.007462
H	2.010879	1.788964	-2.298574
H	3.604843	1.509029	-3.024867
H	-1.915880	2.042827	4.134402
H	2.647784	-0.240812	-4.520821

Compound 3: ground state trans-*anti*

B3LYP/6-31G(d) Energy: -930.2409890

C	0.144713	0.006608	3.894925
C	-0.372086	0.056209	5.199016
C	-1.739783	0.123838	5.452072
C	-2.637136	0.135447	4.384306
C	-2.147054	0.091190	3.082658
C	-0.767316	0.037829	2.813685
C	-0.821582	-0.990527	0.520445
C	-0.346805	0.012283	1.380636
C	0.479297	1.004902	0.830320
C	0.821517	0.990169	-0.520423
C	0.346713	-0.012621	-1.380622
C	-0.479365	-1.005257	-0.830300
C	2.637109	-0.136335	-4.384219
C	2.146992	-0.092031	-3.082585
C	0.767265	-0.038189	-2.813660
C	-0.144711	-0.006497	-3.894933
C	0.372122	-0.056134	-5.199009
C	1.739804	-0.124263	-5.452019
C	1.654267	-0.127135	3.702298
C	2.194646	-1.418715	4.347428
C	2.413029	1.107527	4.225573
C	-1.654212	0.127911	-3.702358
C	-2.194030	1.419630	-4.347680
C	-2.413479	-1.106499	-4.225498
H	0.316580	0.030568	6.039910
H	-2.101358	0.162466	6.476394
H	-3.708075	0.185799	4.562022
H	-2.838481	0.118698	2.244575
H	-1.451615	-1.779488	0.922952
H	0.840075	1.810456	1.464314
H	1.451571	1.779117	-0.922926
H	-0.840113	-1.810832	-1.464283
H	3.708036	-0.187074	-4.561897
H	2.838377	-0.119895	-2.244479
H	-0.316498	-0.030102	-6.039928
H	2.101403	-0.162903	-6.476332
H	1.852023	-0.201715	2.629124
H	2.065444	-1.413873	5.436096
H	3.265971	-1.529306	4.140972
H	1.679561	-2.301819	3.954069
H	2.277901	1.233836	5.306361
H	2.065078	2.026607	3.740532
H	3.488300	1.008501	4.034209
H	-1.851970	0.202719	-2.629201
H	-2.064617	1.414672	-5.436322
H	-3.265357	1.530596	-4.141440
H	-1.678723	2.302587	-3.954279
H	-2.278405	-1.232976	-5.306274
H	-2.065900	-2.025669	-3.740361
H	-3.488709	-1.007015	-4.034142

Compound 3: ground state *trans-syn*

B3LYP/6-31G(d) Energy: -930.2409664

C	0.161622	0.170955	-3.852173
C	-0.289530	0.106391	-5.179716
C	-1.483778	-0.520436	-5.526452
C	-2.262474	-1.114815	-4.533526
C	-1.836584	-1.059581	-3.209831
C	-0.640085	-0.416004	-2.845321
C	-0.140762	0.805349	-0.682216
C	-0.284660	-0.396376	-1.394392
C	-0.141698	-1.596945	-0.682499
C	0.141695	-1.596944	0.682499
C	0.284660	-0.396376	1.394392
C	0.140765	0.805349	0.682215
C	2.262473	-1.114816	4.533525
C	1.836583	-1.059582	3.209830
C	0.640084	-0.416004	2.845321
C	-0.161622	0.170955	3.852173
C	0.289530	0.106391	5.179715
C	1.483778	-0.520437	5.526452
C	1.511936	0.822679	-3.559975
C	1.513392	2.324812	-3.902941
C	2.660197	0.092798	-4.284870
C	-1.511936	0.822679	3.559976
C	-2.660197	0.092799	4.284872
C	-1.513391	2.324812	3.902941
H	0.317142	0.551428	-5.964491
H	-1.800741	-0.548223	-6.565804
H	-3.196081	-1.610741	-4.785484
H	-2.445988	-1.504600	-2.427638
H	-0.262031	1.751592	-1.202785
H	-0.246431	-2.541557	-1.209891
H	0.246426	-2.541557	1.209892
H	0.262036	1.751592	1.202783
H	3.196081	-1.610743	4.785483
H	2.445987	-1.504602	2.427637
H	-0.317141	0.551428	5.964491
H	1.800741	-0.548224	6.565804
H	1.705100	0.731992	-2.487254
H	1.346755	2.492052	-4.973717
H	2.476850	2.778470	-3.641193
H	0.727002	2.860480	-3.359128
H	2.561052	0.161858	-5.374611
H	2.683382	-0.969480	-4.018367
H	3.626188	0.533768	-4.010977
H	-1.705101	0.731993	2.487255
H	-2.561051	0.161860	5.374613
H	-3.626188	0.533769	4.010980
H	-2.683382	-0.969479	4.018369
H	-1.346753	2.492053	4.973717
H	-0.727001	2.860480	3.359127
H	-2.476849	2.778471	3.641194

Compound 3: ground state *cis-anti*

B3LYP/6-31G(d) Energy: -930.2409955

C	0.248858	-0.158299	3.781064
C	0.079775	0.068320	5.155916
C	-1.001295	0.786086	5.661065
C	-1.950459	1.308942	4.782798
C	-1.806222	1.091625	3.415897
C	-0.726783	0.355439	2.894482
C	-0.684437	1.272525	0.554230
C	-0.676877	0.162893	1.414156
C	-0.684423	-1.113656	0.830130
C	-0.684436	-1.272524	-0.554230
C	-0.676877	-0.162892	-1.414155
C	-0.684425	1.113657	-0.830129
C	-1.950459	-1.308943	-4.782796
C	-1.806222	-1.091626	-3.415896
C	-0.726784	-0.355438	-2.894482
C	0.248857	0.158299	-3.781063
C	0.079774	-0.068321	-5.155916
C	-1.001296	-0.786087	-5.661064
C	1.495133	-0.901041	3.302469
C	1.521340	-2.360208	3.796488
C	2.785333	-0.160484	3.706729
C	1.495133	0.901041	-3.302471
C	2.785332	0.160485	-3.706733
C	1.521339	2.360208	-3.796489
H	0.821954	-0.320066	5.849017
H	-1.098528	0.939336	6.732760
H	-2.799726	1.873663	5.158131
H	-2.552132	1.478252	2.726458
H	-0.686042	2.272702	0.979677
H	-0.706029	-1.992622	1.468880
H	-0.686039	-2.272701	-0.979676
H	-0.706032	1.992623	-1.468880
H	-2.799726	-1.873664	-5.158129
H	-2.552132	-1.478253	-2.726456
H	0.821953	0.320065	-5.849017
H	-1.098529	-0.939337	-6.732758
H	1.473824	-0.926523	2.209242
H	1.565034	-2.412900	4.890934
H	2.400529	-2.884328	3.402846
H	0.627931	-2.907901	3.475656
H	2.904606	-0.115885	4.795639
H	2.785007	0.867638	3.328640
H	3.663943	-0.673569	3.297603
H	1.473826	0.926523	-2.209243
H	2.904603	0.115886	-4.795643
H	3.663943	0.673570	-3.297608
H	2.785007	-0.867638	-3.328645
H	1.565031	2.412901	-4.890934
H	0.627930	2.907902	-3.475655
H	2.400529	2.884329	-3.402847

Compound 3: ground state *cis-syn*

B3LYP/6-31G(d) Energy: -930.2409238

C	0.303695	-0.009929	-3.741714
C	0.120265	-0.054762	-5.132568
C	-1.144694	-0.119267	-5.711326
C	-2.275200	-0.132195	-4.894466
C	-2.117011	-0.093170	-3.512472
C	-0.844174	-0.043315	-2.915637
C	-0.134332	-1.037787	-0.696518
C	-0.785665	-0.027750	-1.423068
C	-1.445935	0.975099	-0.696991
C	-1.445935	0.975099	0.696991
C	-0.785665	-0.027751	1.423069
C	-0.134332	-1.037787	0.696518
C	-2.275200	-0.132201	4.894466
C	-2.117011	-0.093174	3.512473
C	-0.844174	-0.043316	2.915637
C	0.303695	-0.009929	3.741714
C	0.120265	-0.054763	5.132568
C	-1.144693	-0.119270	5.711326
C	1.720449	0.122464	-3.185982
C	2.396974	1.421549	-3.667113
C	2.588880	-1.105311	-3.521212
C	1.720448	0.122468	3.185982
C	2.396970	1.421555	3.667112
C	2.588883	-1.105305	3.521211
H	0.992828	-0.028709	-5.780520
H	-1.245837	-0.154509	-6.792995
H	-3.270598	-0.180062	-5.327970
H	-2.991759	-0.122429	-2.868113
H	0.354742	-1.847870	-1.230987
H	-1.953997	1.771403	-1.234703
H	-1.953997	1.771402	1.234704
H	0.354742	-1.847870	1.230986
H	-3.270597	-0.180070	5.327971
H	-2.991759	-0.122434	2.868114
H	0.992829	-0.028708	5.780520
H	-1.245836	-0.154513	6.792995
H	1.650609	0.186011	-2.096275
H	2.533897	1.428934	-4.754860
H	3.386735	1.529718	-3.207339
H	1.799800	2.300161	-3.399887
H	2.721358	-1.220207	-4.603667
H	2.137729	-2.030186	-3.144203
H	3.584981	-1.006026	-3.073319
H	1.650608	0.186014	2.096274
H	2.533894	1.428941	4.754859
H	3.386731	1.529726	3.207337
H	1.799794	2.300165	3.399885
H	2.721362	-1.220200	4.603667
H	2.137734	-2.030181	3.144203
H	3.584983	-1.006017	3.073318

Compound 3: transition state

B3LYP/6-31G(d) Energy: -930.223898

Number of imaginary frequencies: 1

C	0.139840	0.160930	-3.917064
C	-0.247772	-0.010757	-5.255058
C	-1.322022	-0.819404	-5.617365
C	-2.050813	-1.479370	-4.627912
C	-1.682322	-1.326851	-3.294838
C	-0.589288	-0.525336	-2.917394
C	-1.225514	-0.036842	-0.532318
C	-0.267063	-0.447823	-1.463093
C	0.977131	-0.829233	-0.940963
C	1.235702	-0.800355	0.423871
C	0.279168	-0.395419	1.387172
C	-0.960316	-0.004599	0.836403
C	2.416916	-0.908229	4.498343
C	1.915447	-0.877461	3.204117
C	0.629349	-0.398400	2.861106
C	-0.193788	0.031543	3.955189
C	0.344768	0.001201	5.252527
C	1.626784	-0.448543	5.543871
C	1.289379	1.114795	-3.596924
C	0.975267	2.552172	-4.057309
C	2.625019	0.627410	-4.190507
C	-1.630997	0.557498	3.838247
C	-2.489998	0.387076	5.106804
C	-1.640337	2.040957	3.409443
H	0.301954	0.511904	-6.033931
H	-1.590270	-0.928967	-6.664986
H	-2.893602	-2.112905	-4.891306
H	-2.232776	-1.852365	-2.518965
H	-2.203681	0.283901	-0.881580
H	1.758115	-1.173898	-1.613582
H	2.228682	-1.108414	0.720211
H	-1.761409	0.351415	1.458390
H	3.418253	-1.290631	4.677345
H	2.570227	-1.257676	2.433579
H	-0.271822	0.339925	6.076532
H	1.988935	-0.449076	6.568406
H	1.407632	1.149099	-2.510163
H	0.871790	2.615772	-5.146888
H	1.781766	3.233266	-3.760096
H	0.042620	2.914652	-3.611519
H	2.588328	0.589880	-5.285825
H	2.877874	-0.377858	-3.834768
H	3.441051	1.303363	-3.908201
H	-2.145464	-0.041301	3.083666
H	-2.200543	1.073144	5.910569
H	-3.535371	0.607691	4.862252
H	-2.443582	-0.635763	5.495755
H	-1.192647	2.656734	4.198472
H	-1.067960	2.212282	2.493234
H	-2.665331	2.396045	3.245316

Compound 4: ground state trans

B3LYP/6-31G(d) Energy: -1008.844345

C	-0.062987	0.000031	3.983638
C	-0.761938	-0.000049	5.204418
C	-2.153600	-0.000390	5.288085
C	-2.913660	-0.000670	4.124615
C	-2.253705	-0.000588	2.899275
C	-0.851707	-0.000236	2.798739
C	-0.178108	1.199577	0.674636
C	-0.348773	-0.000189	1.380421
C	-0.178080	-1.199965	0.674643
C	0.178096	-1.199965	-0.674646
C	0.348773	-0.000189	-1.380428
C	0.178072	1.199577	-0.674653
C	2.913653	-0.000672	-4.124638
C	2.253707	-0.000587	-2.899291
C	0.851709	-0.000238	-2.798746
C	0.062986	0.000007	-3.983639
C	0.761922	-0.000073	-5.204424
C	2.153584	-0.000403	-5.288103
C	1.490076	0.000405	4.002909
C	-1.490071	0.000399	-4.002897
H	-0.207807	0.000149	6.134087
H	-2.632535	-0.000440	6.263930
H	-3.999649	-0.000947	4.163189
H	-2.831591	-0.000787	1.978808
H	-0.322544	2.145177	1.190380
H	-0.322475	-2.145561	1.190400
H	0.322492	-2.145560	-1.190406
H	0.322489	2.145178	-1.190399
H	3.999642	-0.000940	-4.163222
H	2.831598	-0.000779	-1.978828
H	0.207780	0.000130	-6.134089
H	2.632511	-0.000448	-6.263951
C	2.054522	0.000375	5.441916
H	1.753040	-0.888560	6.007223
H	3.148826	0.000746	5.392907
H	1.752477	0.888940	6.007498
C	2.049680	1.266409	3.310060
H	1.804823	1.300885	2.247468
H	1.656932	2.174805	3.782109
H	3.142884	1.287004	3.400349
C	2.050304	-1.265172	3.309799
H	1.805322	-1.299638	2.247234
H	3.143533	-1.285138	3.399944
H	1.658144	-2.173856	3.781779
C	-2.049596	1.266550	-3.310262
H	-1.804572	1.301279	-2.247714
H	-1.656938	2.174842	-3.782588
H	-3.142816	1.287100	-3.400384
C	-2.050348	-1.265023	-3.309544
H	-3.143548	-1.285128	-3.399985
H	-1.657961	-2.173811	-3.781137
H	-1.805654	-1.299140	-2.246902
C	-2.054521	0.000130	-5.441903
H	-1.752757	0.888769	-6.007524
H	-1.752766	-0.888731	-6.007174
H	-3.148824	0.000155	-5.392885

Compound 4: ground state cis

B3LYP/6-31G(d) Energy: -1008.844498

C	0.118515	-0.000056	-3.871135
C	-0.250604	0.000011	-5.228829
C	-1.576408	0.000281	-5.659999
C	-2.604824	0.000498	-4.725293
C	-2.274642	0.000418	-3.373314
C	-0.943024	0.000139	-2.923087
C	-0.835685	1.199675	-0.697695
C	-0.813011	0.000059	-1.423834
C	-0.836067	-1.199598	-0.697772
C	-0.836078	-1.199639	0.697691
C	-0.813020	-0.000027	1.423835
C	-0.835684	1.199634	0.697775
C	-2.604830	-0.000438	4.725291
C	-2.274644	-0.000378	3.373314
C	-0.943026	-0.000117	2.923087
C	0.118514	0.000045	3.871134
C	-0.250612	-0.000008	5.228829
C	-1.576417	-0.000231	5.659998
C	1.626405	-0.000289	-3.498565
C	1.626407	0.000235	3.498567
H	0.519173	-0.000159	-5.989772
H	-1.794304	0.000320	-6.724977
H	-3.646137	0.000717	-5.036042
H	-3.065660	0.000561	-2.628047
H	-0.865595	2.144943	-1.233049
H	-0.866249	-2.144822	-1.233188
H	-0.866248	-2.144894	1.233054
H	-0.865606	2.144870	1.233184
H	-3.646146	-0.000636	5.036033
H	-3.065661	-0.000515	2.628045
H	0.519162	0.000109	5.989773
H	-1.794313	-0.000257	6.724976
C	2.533341	-0.000581	-4.750015
H	2.381630	0.888354	-5.372257
H	3.581022	-0.000797	-4.430055
H	2.381212	-0.889536	-5.372129
C	1.993287	-1.265526	-2.686066
H	1.489337	-1.297372	-1.718922
H	1.730708	-2.174700	-3.239883
H	3.074043	-1.286557	-2.498699
C	1.993633	1.265040	-2.686358
H	1.489601	1.297261	-1.719267
H	3.074381	1.285783	-2.498905
H	1.731371	2.174149	-3.240427
C	1.993372	1.265777	2.686574
H	1.489420	1.298005	1.719442
H	1.730827	2.174738	3.240754
H	3.074129	1.286832	2.499212
C	1.993557	-1.264791	2.685862
H	3.074307	-1.285525	2.498423
H	1.731238	-2.174106	3.239569
H	1.489550	-1.296625	1.718749
C	2.533358	-0.000076	4.750005
H	2.381530	0.888759	5.372363
H	2.381365	-0.889129	5.372012
H	3.581035	-0.000092	4.430033

Compound 4: transition state
B3LYP/6-31G(d) Energy: -1008.820691
Number of imaginary frequencies: 1

C	-0.068356	0.087658	-4.007243
C	-0.221925	-0.427557	-5.307013
C	-0.232059	-1.792399	-5.591430
C	-0.085532	-2.712045	-4.559847
C	0.068544	-2.236070	-3.261101
C	0.080641	-0.863223	-2.958837
C	-0.820344	-0.523267	-0.613828
C	0.260377	-0.569146	-1.496251
C	1.530390	-0.487341	-0.912211
C	1.698525	-0.330349	0.459331
C	0.619852	-0.253562	1.376636
C	-0.645841	-0.364096	0.761954
C	2.738358	0.155865	4.513736
C	2.256658	-0.004549	3.222219
C	0.888313	-0.076937	2.868232
C	-0.048753	0.028432	3.964886
C	0.477254	0.191920	5.259374
C	1.833120	0.257230	5.557313
C	-0.071959	1.626487	-3.798207
C	-1.599475	-0.019847	3.872060
H	-0.339245	0.254841	-6.138852
H	-0.354591	-2.125637	-6.618851
H	-0.090168	-3.780961	-4.755488
H	0.184593	-2.940729	-2.441863
H	-1.831871	-0.616408	-1.000477
H	2.413511	-0.550881	-1.542583
H	2.724946	-0.277427	0.791333
H	-1.549187	-0.337686	1.339119
H	3.810317	0.200007	4.686354
H	3.011671	-0.075336	2.455238
H	-0.206986	0.274587	6.091359
H	2.161332	0.384667	6.585362
C	-1.247192	2.054337	-2.886226
H	-2.204798	1.718299	-3.301436
H	-1.154301	1.655162	-1.875067
H	-1.279316	3.148296	-2.810360
C	1.266288	2.103187	-3.183147
H	2.112937	1.804636	-3.812798
H	1.272372	3.197836	-3.109600
H	1.429106	1.704268	-2.180834
C	-0.242993	2.393625	-5.128764
H	0.571018	2.189444	-5.833317
H	-1.193756	2.163543	-5.622594
H	-0.234395	3.469340	-4.922045
C	-2.121512	1.201918	3.057223
H	-1.539036	1.437065	2.167511
H	-3.165538	1.050351	2.754885
H	-2.089107	2.093178	3.693906
C	-2.056837	-1.421709	3.363369
H	-2.023794	-2.131202	4.197713
H	-3.092210	-1.387895	3.001073
H	-1.432679	-1.842685	2.576363
C	-2.313583	0.123084	5.242635
H	-2.060295	-0.684316	5.937417
H	-2.107083	1.081966	5.729373
H	-3.395218	0.073811	5.069978