π-Stacking Effect on Levoglucosenone Derived Internal Chiral Auxiliaries. A Case of Complete Enantioselectivity Inversion on the Diels-Alder Reaction.

Deleted: case

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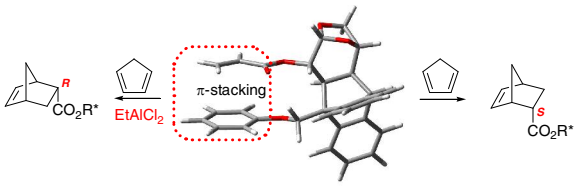
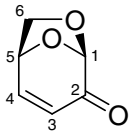


General Information: The melting points were taken on a Leitz Wetzlar Microscope Heating Stage Model 350 apparatus and are uncorrected. Optical rotations were recorded with a Jasco DIP 1000 polarimeter. Infrared spectra were obtained on an IRPrestige-21 Fourier Transform Spectrophotometer Shimadsu. High resolution mass spectrometry measurements were performed using a Waters AutoSpect equipment or Applied Biosystems MS. HPLC analyses were performed with a chromatograph Varian ProStar equipped with UV-V detector ProStar 320 at 270 nm. HPLC was performed on a Beckman C-18, 25 cm column. Acetonitrile and water HPLC grade was used as eluent in a mixture 80:20 respectively. Flow rate was 1 mL/min. Nuclear magnetic resonance spectra were recorded on a Bruker AC-200 or a Bruker Avance-300 DPX spectrometers with tetramethylsilane as internal standard and deuterochloroform as solvent. The NMR assignments were corroborated by NOE measurements, H,H- and H,C-correlations.

The reactions were monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plates (60F254) that were developed using UV light and anisaldehyde-sulfuric acid-acetic acid with subsequent heating. Flash column chromatography were performed using Merck silica gel 60H, by gradient elution created by mixtures of hexanes and increasing amounts of ethyl acetate. All reactions were carried out under argon atmosphere with dry, freshly distilled solvents under anhydrous conditions unless otherwise noted. Yields refer to chromatographically and spectroscopically (^{1}H NMR) homogeneous materials, unless otherwise stated.

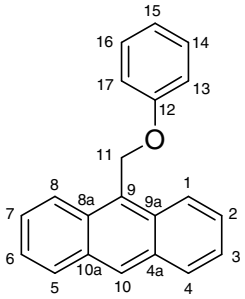


1

Levoglucosenone (1)

Levoglucosenone was synthesized according to the procedure described in literature.[1]

1: Yellow oil; $[\alpha]_D^{25}$ = -562,3 (*c* 1,04, $CHCl_3$); IR (film) 3631, 2966, 2899, 1712 (C=O), 1693, 1379, 1107, 972, 891, 854, 831 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.27 (dd, $J_{3\text{-}4}$= 9.9 Hz, $J_{4\text{-}5}$= 4.6 Hz, 1 H, H-4), 6.12 (dd, $J_{3\text{-}4}$= 9.9 Hz, $J_{1\text{-}3}$=1.7 Hz, 1 H, H-3), 5.36 (d, $J_{1\text{-}3}$=1.7 Hz, 1 H, H-1), 5.00 (dd, $J_{4\text{-}5}$= $J_{5\text{-}6exo}$= 4.8 Hz, 1 H, H-5), 3.90 (dd, $J_{5\text{-}6exo}$= 4.8 Hz, J_{gem}= 6.9 Hz, 1 H, H-6*exo*), 3.77 (d, J_{gem}= 6.9 Hz, 1 H, H-6*endo*); ^{13}C NMR (50 MHz, $CDCl_3$) δ = 188.6 (C, C-2), 148.1 (CH, C-4), 126.5 (CH, C-3), 101.4 (CH, C-1), 71.5 (CH, C-5), 66.3 (CH_2, C-6).



2

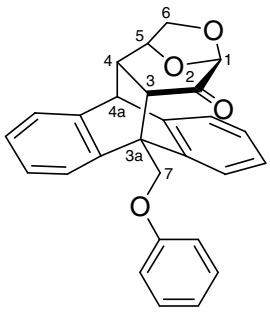
9-(Phenoxymethyl)anthracene (2)

Anthracen-9-ylmethanol 97% (2.50 g, 11.67 mmol) was dissolved in dry CH_2Cl_2 (2,5 mL) and dry benzene (15 mL) under argon. $SOCl_2$ was added (0.99 mL, 13.60 mmol) and the solution was stirred at reflux overnight under argon. The reaction mixture was poured into ice-water (25 mL). The organic phase was washed with water (3x10 mL), dried (Na_2SO_4) and concentrated. The residual solid was dried azeotropically with dry benzene and dissolved in dry acetone (80 mL). Phenol (4.14 g, 44.05 mmol) and anhydrous K_2CO_3 (6.10 g, 44.22 mmol) were incorporated and the solution was stirred at reflux for 24 hours under argon. The solvent was evaporated under reduced pressure. Water (300 mL) and CH_2Cl_2 (300 mL) were added. The aqueous phase was extracted with CH_2Cl_2 (3 x 100 mL). The organic phase was washed with saturated Na_2CO_3 (2 x 150 mL), brine (2 x 150

[1] a) A. M. Sarotti, R. A. Spanevello, A. G. Suárez, A. G. *Green Chemistry,* **2007**, *9*, 1137-1140.
b) Z. J. Witczak (Ed.), *Levoglucosenone and Levoglucosans: Chemistry and Applications*, ATL Press, Mount Prospect, 1994. Chapter 2. (C. Morin)

mL), dried (Na_2SO_4) and concentrated. The residual solid was purified by flash chromatography to afford **2** (3.16 g, 11.11 mmol, 95%).

2: Orange solid; mp 117-118 ºC (EtOH); IR (KBr) 3031, 2886, 1597, 1585, 1494, 1476, 1236, 989, 879, 731 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 8.49 (s, 1 H, H-10), 8.29-8.24 (m, 2 H, H-1 and H-8), 8.04-7.99 (m, 2 H, H-4 and H-5), 7.55-7.00 (m, 9 H, H-2, H-3, H-6, H-7, H-13, H-14, H-15, H-16 and H-17), 5.92 (s, 2 H, H-11); ^{13}C NMR (50 MHz, $CDCl_3$) δ 159.1 (C, C-12), 131.4 (C, C-9), 130.9 (C, C-4a and C-10a), 129.5 (CH, C-4 and C-5), 129.0 (CH, C-1 and C-8), 128.9 (C, C-8a and C-9a), 126.8 (CH, C-14 and C-16), 126.4 (CH, C-2 and C-7), 124.9 (CH, C-3 and C-6), 123.9 (CH, C-10), 121.1 (CH, C-15), 114.7 (CH, C-13 and C-17), 62.5 (CH_2, C-11).

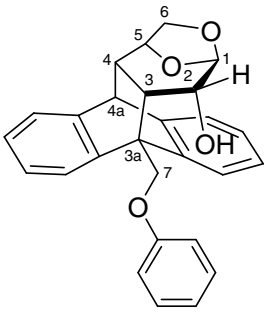


3

Ketone 3

Levoglucosenone (0.57 g, 4.52 mmol) and 9-phenoxymethylanthracene (3.16 g, 11.11 mmol) were dissolved in toluene (14 mL) at room temperature. The solution was heated under reflux during 10 days and evaporated under vacuum. The solid residue was purified by flash chromatography to give **3** (1.67 g, 4.07 mmol, 90%). The excess of the diene was recovered quantitatively and reused.

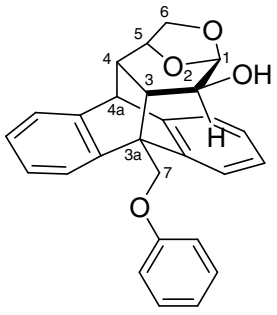
3: White crystalline solid; mp 249-250 ºC (hexane/chloroform); $[\alpha]^{19}_D$ -64.1 (*c* 0.88, $CHCl_3$); IR (KBr) 3068, 3040, 2969, 2899, 1717 (C=O), 1599, 1497, 1464, 1241, 1115, 750 cm^{-1} ; ^1H NMR (200 MHz, $CDCl_3$) δ 7.47-7.00 (m, 13 H, aromatics), 5.56 (d, J_{gem}=9.3 Hz, 1 H, H-7), 5.23 (d, J_{gem}=9.3 Hz, 1 H, H-7), 4.83 (d, $J_{5\text{-}6exo}$=4.3 Hz, 1 H, H-5), 4.57 (s, 1 H, H-1), 4.35 (d, $J_{4\text{-}4a}$=1.5 Hz, 1 H, H-4a), 3.78 (dd, J_{gem}=7.3 Hz, $J_{5\text{-}6exo}$=4.3 Hz, 1 H, H-6 *exo*), 3.71 (dd, J_{gem}=7.3 Hz, $J_{5\text{-}6endo}$=1.0 Hz, 1 H, H-6 *endo*), 3.25 (d, $J_{3\text{-}4}$=9.7 Hz, 1 H, H-3), 2.37 (dd, $J_{3\text{-}4}$=9.7 Hz, $J_{4\text{-}4a}$=1.5 Hz, 1 H, H-4); ^{13}C NMR (50 MHz, $CDCl_3$) δ 198.8 (C, C-2), 158.6 (C, aromatic), 145.1 (C, aromatic), 140.8 (C, aromatic), 140.7 (C, aromatic), 140.1 (C, aromatic), 129.5 (CH, 2C, aromatic), 126.4 (CH, aromatic), 126.1 (CH, aromatic), 126.0 (CH, aromatic), 125.9 (CH, aromatic), 125.1 (CH, aromatic), 124.2 (CH, aromatic), 122.2 (CH, aromatic), 121.6 (CH, aromatic), 121.1 (CH, aromatic), 114.9 (CH, 2C, aromatic), 99.7 (CH, C-1), 77.1 (CH, C-5), 68.8 (CH_2, C-6), 66.2 (CH_2, C-7), 50.3 (CH, C-4a), 49.6 (C, C-3a), 44.8 (CH, C-4), 44.3 (CH, C-3); HRMS calc. for $C_{27}H_{22}O_4$ $[M]^+$ 410.1518. Found 410.1500.



4

Reduction of ketone 3: Alcohols 4 and 5

Ketone **3** (1,67 g, 4.07 mmol) was dissolved in a CH_2Cl_2: MeOH 95:5 mixture (65 mL), cooled at 0 ºC and $NaBH_4$ (333 mg, 8.80 mmol) was incorporated. The mixture was stirred during 4 h and then water (100 mL) was added. The solution was extracted with CH_2Cl_2 (100 mL) and then with AcOEt (3x100 mL). The combined organic extracts were dried (Na_2SO_4) and concentrated. The residue was purified by flash chromatography to afford **4** (640 mg, 1.55 mmol, 38%) and **5** (950 mg, 2.30 mmol, 56%).



5

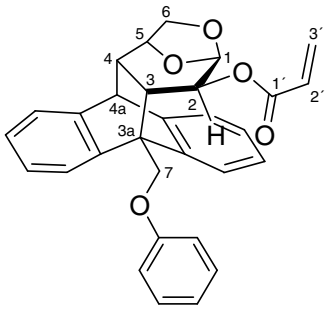
4: White cristalline solid; mp 252-253 ºC (hexane/chloroform); $[\alpha]_D^{20}$ = +63.7 (*c* 0.82, $CHCl_3$); IR (KBr) 3557 (OH), 3061, 2953, 2884, 1603, 1587, 1499, 1477, 1456, 1244, 1223, 1132, 1028, 752 cm^{-1}; ^1H NMR

(200 MHz, $CDCl_3$) δ 7.45–7.00 (m, 13 H, aromatics), 5.49 (d, J_{gem}=9.2 Hz, 1 H, H-7), 5.29 (d, J_{gem}=9.2 Hz, 1 H, H-7), 4.98 (s, 1 H, H-1), 4.68 (d, $J_{5\text{-}6exo}$=3.6 Hz, 1 H, H-5), 4.17 (s, 1 H, H-4a), 3.88 (dd, $J_{2\text{-}OH}$=13.3 Hz, $J_{2\text{-}3}$=8.2 Hz, 1 H, H-2), 3.75 (d, J_{gem}=6.7 Hz, 1 H, H-6*endo*), 3.69 (dd, J_{gem}=6.7 Hz, $J_{5\text{-}6exo}$=3.6 Hz, 1 H, H-6*exo*), 2.93 (dd, $J_{3\text{-}4}$=12.0 Hz, $J_{2\text{-}3}$=8.2 Hz, 1 H, H-3), 2.07 (d, $J_{3\text{-}4}$=12.0 Hz, 1 H, H-4), 0.69 (d, $J_{2\text{-}OH}$=13.3 Hz, 1 H, OH); ^{13}C NMR (50 MHz, $CDCl_3$) δ 158.9 (C, aromatic), 147.1 (C, aromatic), 143.6 (C, aromatic), 142.0 (C, aromatic), 141.1 (C, aromatic), 129.5 (CH, 2 C, aromatic), 125.8 (CH, 2 C, aromatic), 125.7 (CH, aromatic), 125.6 (CH, aromatic), 125.1 (CH, aromatic), 123.5 (CH, aromatic), 122.9 (CH, aromatic), 121.8 (CH, aromatic), 121.1 (CH, aromatic), 114.7 (CH, 2 C, aromatic), 102.2 (CH, C-1), 76.3 (CH, C-5), 72.1 (CH_2, C-7), 68.2 (CH, C-2), 66.3 (CH_2, C-6), 50.9 (CH, C-4a), 49.6 (C, C-3a), 45.1 (CH, C-4), 34.5 (CH, C-3); HRMS calc. for $C_{27}H_{24}O_4$ $[M]^+$ 412.1675. Found 412.1664.

5: Colorless oil; $[\alpha]_D^{21}$ = -7.8 (*c* 1.69, $CHCl_3$); IR (film) 3432 (OH), 3040, 2951, 1599, 1244, 1048 , 909, 752, 732 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.46–7.00 (m, 13 H, aromatics), 5.15 (d, J_{gem}=9.9 Hz, 1 H, H-7), 5.02 (d, J_{gem}=9.9 Hz, 1 H, H-7), 4.96 (d, $J_{1\text{-}2}$=3.2 Hz, 1 H, H-1), 4.68 (d, $J_{5\text{-}6exo}$=4.7 Hz, 1 H, H-5), 4.19 (d, $J_{4\text{-}4a}$=0.6 Hz, 1 H, H-4a), 3.74 (dd, J_{gem}=7.1 Hz, $J_{5\text{-}6exo}$=4.7 Hz, 1 H, H-6*exo*), 3.65 (dd, J_{gem}=7.1 Hz, $J_{5\text{-}6endo}$=0.6 Hz, 1 H, H-6*endo*), 3.02–2.93 (m, 1 H, H-2), 2.28 (dd, $J_{3\text{-}4}$=10.5 Hz, $J_{2\text{-}3}$=5.9 Hz, 1 H, H-3), 2.12 (d, $J_{3\text{-}4}$=10.5 Hz, 1 H, H-4), 1.94 (d, $J_{2\text{-}OH}$=10.5 Hz, 1 H, OH); ^{13}C NMR (50 MHz, $CDCl_3$) δ 158.6 (C, aromatic), 146.2 (C, aromatic), 141.2 (C, aromatic), 141.0 (C, aromatic), 140.4 (C, aromatic), 129.6 (CH, 2 C, aromatic), 126.3 (CH, aromatic), 125.8 (CH, 2 C, aromatic), 125.7 (CH, aromatic), 125.1 (CH, aromatic), 124.0 (CH, aromatic), 123.3 (CH, aromatic), 121.9 (CH, aromatic), 121.2 (CH, aromatic), 114.8 (CH, 2 C, aromatic), 99.9 (CH, C-1), 76.6 (CH, C-5), 70.2 (CH_2, C-7), 68.8 (CH, C-2), 66.7 (CH_2, C-6), 50.4 (CH, C-4a), 50.3 (C, C-3a), 47.8 (CH, C-4), 42.2 (CH, C-3); HRMS calc. for $C_{27}H_{25}O_4$ $[M+H]^+$ 413.1753. Found 413,1761.

Oxidation of alcohol 4

Alcohol **4** (725 mg, 1.75 mmol) was dissolved in dry CH_2Cl_2 (14 mL) and PCC (1019 mg, 4.74 mmol) was added in one portion and stirred overnight under argon atmosphere. The reaction mixture was diluted with CH_2Cl_2 and filtered through Florisil® contained in a sintered glass funnel. The filtrate was concentrated to give pure ketone **3** (705 mg, 1.72 mmol, 98%).



6

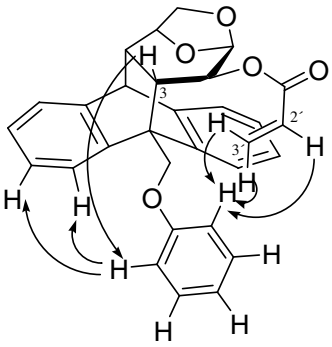
Preparation of acrylate 6

Alcohol **5** (939 mg, 2.28 mmol) was dried azeotropically with dry benzene, dissolved in dry CH_2Cl_2 (32 mL) and cooled at 0 ºC. Dry triethylamine (1.09 mL, 7.84 mmol) and acryloyl chloride (0.39 mL, 2.78 mmol) were added and stirred for 0.5 h under argon atmosphere. The mixture was diluted with water (50 mL) and extracted several times with 50 mL portions of CH_2Cl_2. The combined organic extracts were dried (Na_2SO_4) and concentrated. The residue was purified by flash chromatography to give **6** (892 mg, 1.91 mmol, 84%).

6: Colorless oil; $[\alpha]_D^{20}$ = -13.4 (*c* 1.20, $CHCl_3$); IR (film) 3061, 3023, 2965, 1716 (C=O), 1599, 1499, 1477, 1405, 1243, 1191, 1051, 1015 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$) δ 7.45–6.94 (m, 13 H, aromatics), 6.12 (d, J_{vec}=16.8 Hz, 1 H, H-3´*cis*), 5.62 (dd, J_{vec}=16.8 Hz, J_{vec}=10.1 Hz, 1 H, H-2´), 5.43 (d, J_{vec}=10.1 Hz, 1 H, H-3´*trans*), 5.11 (d, $J_{1\text{-}2}$=3.2 Hz, 1 H, H-1), 4.99 (d, J_{gem}=9.7 Hz, 1 H, H-7), 4.73–4.70 (m, 1 H,

H-5), 4.66 (d, J_{gem}=9.7 Hz, 1 H, H-7), 4.37 (dd, J_{2-3}=6.4 Hz, J_{1-2}=3.2 Hz, 1 H, H-2), 4.25 (s, 1 H, H-4a), 3.78–3.76 (m, 2 H, H-6*endo* y H-6*exo*), 2.91 (dd, J_{3-4}=10.5 Hz, J_{2-3}=6.4 Hz, 1 H, H-3), 2.29 (d, J_{3-4}=10.5 Hz, 1 H, H-4); ^{13}C NMR (50 MHz, $CDCl_3$) δ 165.4 (C, C-1´), 158.4 (C, aromatic), 146.0 (C, aromatic), 141.0 (C, aromatic), 140.7 (C, aromatic), 140.4 (C, aromatic), 130.7 (CH_2, C-3´), 129.4 (CH, 2 C, aromatic), 127.0 (CH, C-2´), 126.5 (CH, aromatic), 126.1 (CH, aromatic), 125.9 (CH, aromatic), 125.9 (CH, aromatic), 125.1 (CH, aromatic), 124.1 (CH, aromatic), 122.6 (CH, aromatic), 122.0 (CH, aromatic), 120.9 (CH, aromatic), 114.3 (CH, 2 C, aromatic), 97.1 (CH, C-1), 76.7 (CH, C-5), 70.6 (CH, C-2), 70.4 (CH_2, C-7), 65.4 (CH_2, C-6), 50.6 (CH, C-4a), 49.7 (C, C-3a), 47.5 (CH, C-4), 36.5 (CH, C-3); HRMS calc. for $C_{30}H_{26}O_5$ $[M]^+$ 466.1780. Found 466.1759.

Selected NOE experiments of acrylate 6



General procedure for the cycloaddition reaction of 6 and cyclopentadiene

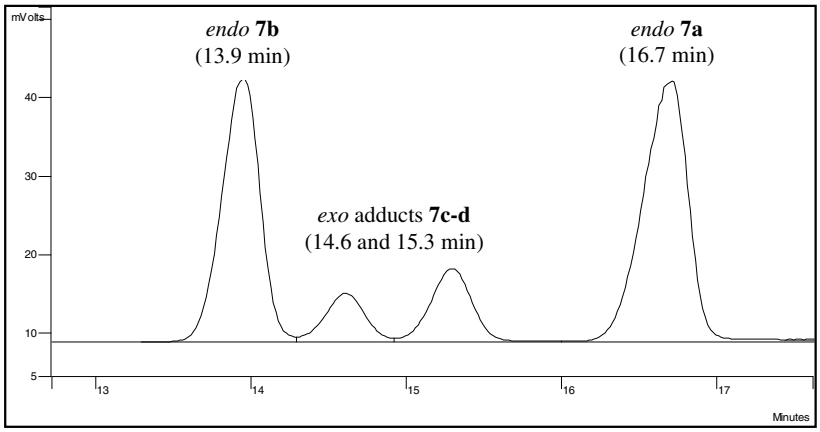
Acrylic ester **6** (46.9 mg, 0.1 mmol) was dried azeotropically with dry benzene and dissolved in the corresponding amount of solvent to give a 0.2 M solution. When the reaction was promoted by Lewis acid the appropriate amount was added under nitrogen and stirred for 20 minutes at the corresponding temperature. Freshly distilled cyclopentadiene (82 μL, 1 mmol) was added dropwise and the mixture was stirred at the temperature and time indicated in Table 1. The cycloaddition reactions carried out without Lewis acid were concentrated after completion to afford a solid residue. The reactions promoted by Lewis acids were quenched by the addition of water (10 mL) and HCl 0.1N (10 mL), then extracted with CH_2Cl_2 (3x30 mL). The combined organic extracts were dried (Na_2SO_4) and concentrated. The solid residue was purified by flash chromatography to separate the excess of cyclopentadiene and the mixture of adducts **8a-d** were collected together to obtain an accurate yield. *Endo/exo* and *endo R/S* ratios were determined by HPLC as shown in Figure 1.

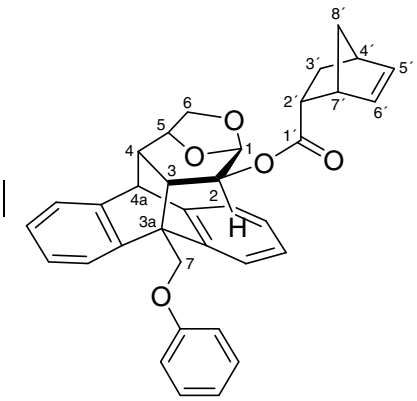
Diels-Alder reactions between acrylate **6** and cyclopentadiene

Entry	Lewis Acid (eq.)	Solv.	T (ºC)	t (h)	Yield (%)	*endo/exo*	*endo R/S*	d.e. (*endo*)
1	-	PhMe	110	1,5	88	69 : 31	21 : 79	58%
2	-	PhMe	25	48	92	73 : 27	16 : 84	68%
3	-	CH_2Cl_2	25	48	91	78 : 22	13 : 87	74%
4	Et_2AlCl (2)	CH_2Cl_2	0	1	84	92 : 8	96 : 4	92%

5	Et_2AlCl (2)	CH_2Cl_2	- 40	1	81	95 : 5	97 : 3	94%
6	Et_2AlCl (2)	CH_2Cl_2	-80	1	82	96 : 4	97 : 3	94%
7	$EtAlCl_2$ (2)	CH_2Cl_2	0	1	92	93 : 7	92 : 8	86%
8	$EtAlCl_2$ (2)	CH_2Cl_2	-40	1	93	95 : 5	94 : 6	88%
9	$EtAlCl_2$ (2)	CH_2Cl_2	-80	1,5	85	97 : 3	95 : 5	90%
10	$AlCl_3$ (1,5)	CH_2Cl_2	0	1	88	92 : 8	91 : 9	82%
11	$AlCl_3$ (1,5)	CH_2Cl_2	-40	1	89	95 : 5	94 : 6	88%
12	$AlCl_3$ (1,5)	CH_2Cl_2	-80	1	88	96 : 4	96 : 4	92%
13	$TiCl_4$ (0,5)	CH_2Cl_2	0	1	72	93 : 7	90 : 10	80%
14	$TiCl_4$ (0,5)	CH_2Cl_2	-40	3	24	95 : 5	88 : 12	76%
15	$TiCl_4$ (0,5)	CH_2Cl_2	-80	3	10	95 : 5	83 : 17	66%
16	$BF_3.OEt_2$ (0.5)	CH_2Cl_2	25	24	-	-	-	-
17	$BF_3.OEt_2$ (1.0)	CH_2Cl_2	25	24	-	-	-	-
18	$LiClO_4$ 5M	Et_2O	25	3	78	82 : 18	45 : 55	10%

HPLC Chromatogram of the mixtures of adducts



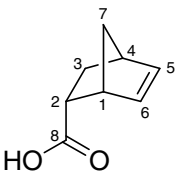


7b

A second purification by flash chromatography can provide pure *endo* **7b** in the more polar fraction and a mixture of adducts **7a**, **7c** and **7d** in the less polar fraction.

7b: Colorless oil; $[\alpha]_D^{22}$ = +11.0 (*c* 1.45, $CHCl_3$); IR (film): 3064, 2970, 1725 (C=O), 1599, 1499, 1478, 1244, 1029, 753, 733 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$) δ 7.43-6.99 (m, 13 H, arom), 6.05 (dd, $J_{5´-6´}$=5.6 Hz, $J_{4´-5´}$=3.0 Hz, 1 H, H-5´), 5.90 (dd, $J_{5´-6´}$=5.6 Hz, $J_{6´-7´}$=2.6 Hz, 1 H, H-6´), 5.00 (d, J_{gem}=9.7 Hz, 1 H, H-7), 4.94 (d, J_{1-2}=3.2 Hz, 1 H, H-1), 4.71 (d, J_{gem}=9.7 Hz, 1 H, H-7), 4.66 (dd, J_{5-6exo}=2.8 Hz, $J_{5-6endo}$=2.8 Hz, 1 H, H-5), 4.27 (dd, J_{2-3}=6.4 Hz, J_{1-2}=3.2 Hz, 1 H, H-2), 4.21 (d, J_{4-4a}=1.3 Hz, 1 H, H-4a), 3.72-3.71 (m, 2

H, H-6*endo* y H-6*exo*), 2.74 (sa, 3 H, H-3, H-4´ y H-7´), 2.31-2.21 (m, 2 H, H-4 y H-2´), 1.70 (td, J_{gem}=10.7 Hz, $J_{2´-3´exo}$=10.7 Hz, $J_{3´exo-4}$=3.5 Hz, 1 H, H-3´*exo*), 1.28-1.10 (m, 2 H, H-3´*endo* y H-8´*syn*), 0.96 (da, J_{gem}=8.4 Hz, 1 H, H-8´*anti*); ^{13}C NMR (50 MHz, $CDCl_3$) δ 174.3 (C, C-1´), 158.5 (C, aromatic), 145.9 (C, aromatic), 141.1 (C, aromatic), 140.6 (C, aromatic), 140.5 (C, aromatic), 137.1 (CH, C-5´), 133.0 (CH, C-6´), 129.5 (CH, 2C, aromatic), 126.4 (CH, aromatic), 126.0 (CH, aromatic), 125.9 (CH, aromatic), 125.8 (CH, aromatic), 125.0 (CH, aromatic), 124.0 (CH, aromatic), 122.7 (CH, aromatic), 122.0 (CH, aromatic), 121.1 (CH, aromatic), 114.4 (CH, 2C, aromatic), 97.0 (CH, C-1), 76.6 (CH, C-5), 70.3 (CH_2, C-6), 70.0 (CH, C-2), 65.6 (CH_2, C-7), 50.6 (CH, C-4a), 49.8 (C, C-3a), 49.1 (CH_2, C-8´), 47.5 (CH, C-4), 44.8 (CH, C-7´), 43.3 (CH, C-2´), 42.2 (CH, C-4´), 36.6 (CH, C-3), 30.2 (CH_2, C-3´); HRMS calc. for $C_{35}H_{32}O_5Na$ $[M+Na]^+$ 555.2147. Found 555.2171.



8

Hydrolysis of adduct 7b

Adduct **7b** (170 mg, 0.32 mmol) was dissolved in THF-H_2O 2:1 (30 mL) and LiOH.H_2O (80.4 mg, 1.92 mmol) was added. The reaction was stirred at room temperature for 15 days at 25 ºC. The solution was neutralized with HCl 0.1 N to reach pH=4 and extracted with ether (5x40 mL). The combined organic extracts were dried (Na_2SO_4) and the solvent was evaporated. The resulting residue was purified by flash chromatography to obtain the chiral auxiliary **5** (131 mg, 0.32 mmol, 100%) and 2-norbornene-5-carboxylic acid (**8**) (38.2 mg, 0.28 mmol, 88%). The optical rotation of **8** was $[\alpha]_D$ +149.9 (*c* 1.42, $CHCl_3$) [lit.[2] –151.6 (*c* 2.0, Cl_3CH)], indicating that cycloadduct **7b** was the (2-*R*) enantiomer.

NMR spectra of 6 with Et_2AlCl

Complexation of **6** with Lewis acids: for the ^{1}H NMR experiments the acrylic ester **6** (30 mg, 0.074 mmol) was dissolved in dry $CDCl_3$ (0.4 mL) in a NMR tube under nitrogen. The appropriate amount of Et_2AlCl (1.8 M in toluene) was added to the solution. Compound **6** showed to be stable during the time required for the acquisition of the spectra.

[2] H. Chang, L. Zhou, R. D. McCargar, T. Mahmud, I. Hirst, *Org. Process Research & Development*, **1999**, *3*, 289-291.

^{1}H NMR (200 MHz, $CDCl_3$) Spectra of compound **1**

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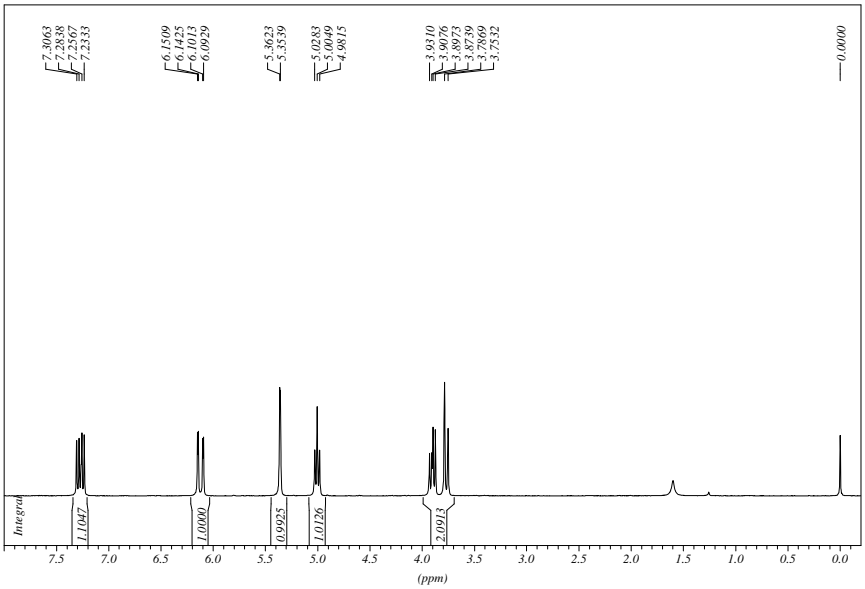

^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **1**

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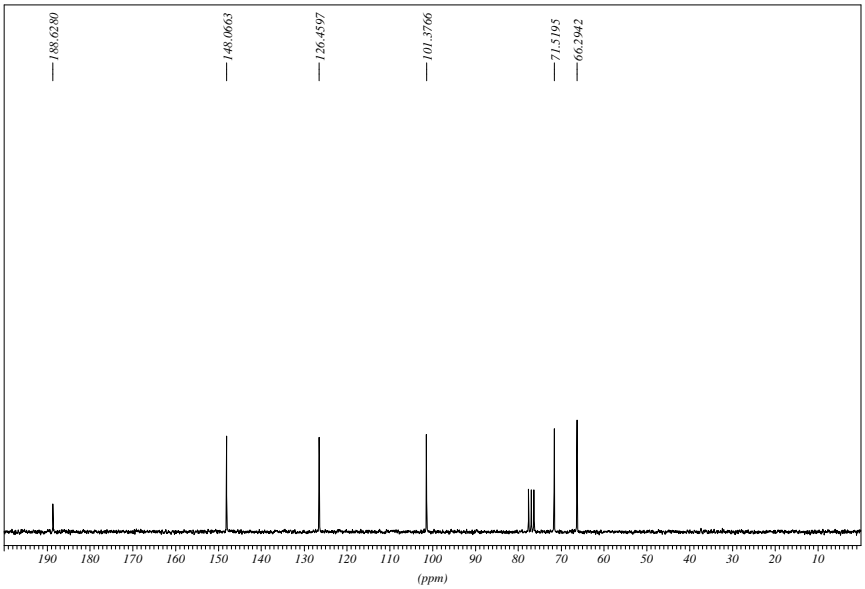

^{1}H NMR (200 MHz, $CDCl_3$) Spectra of compound **2**

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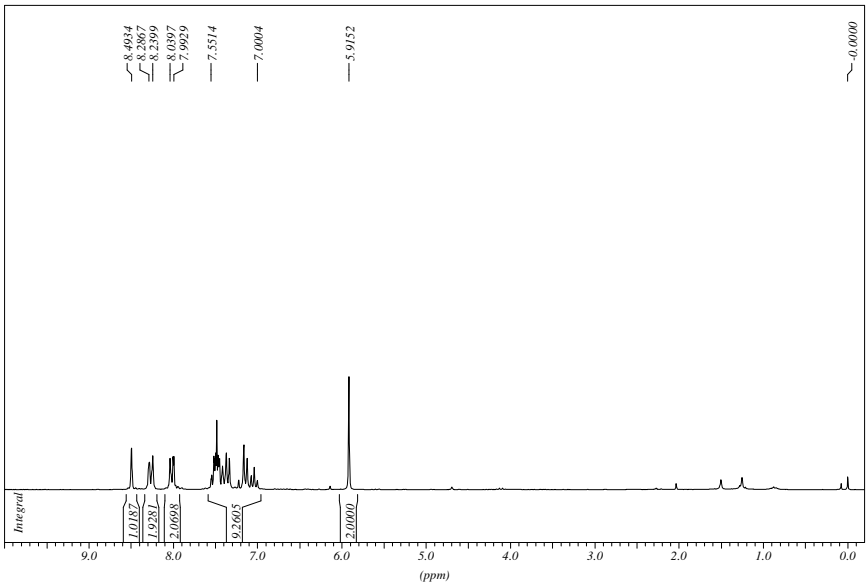
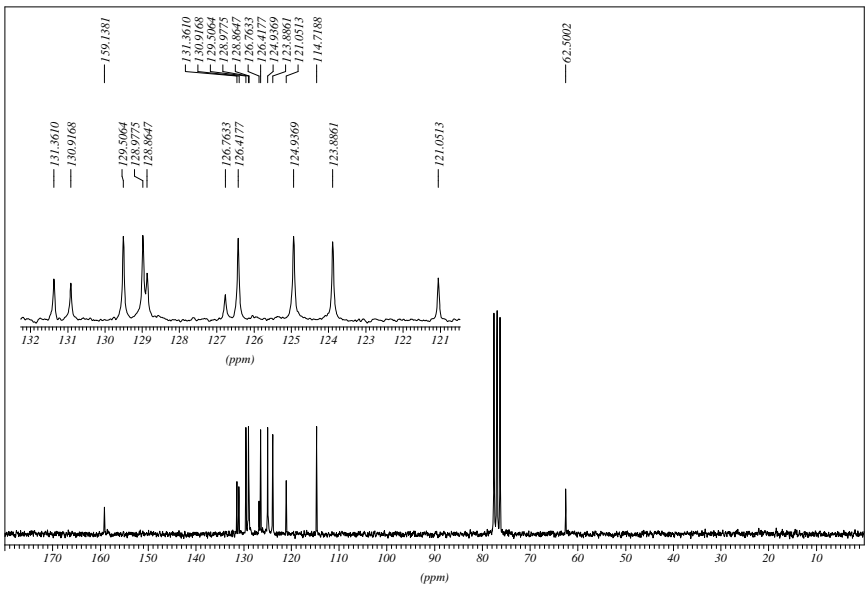


^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **2**



^{1}H NMR (200Hz, $CDCl_3$) Spectra of compound **3**

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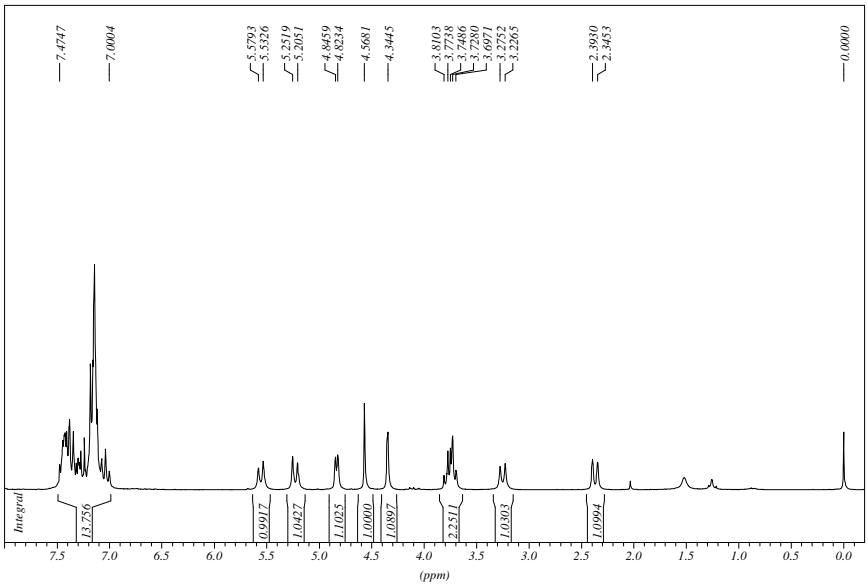

^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **3**

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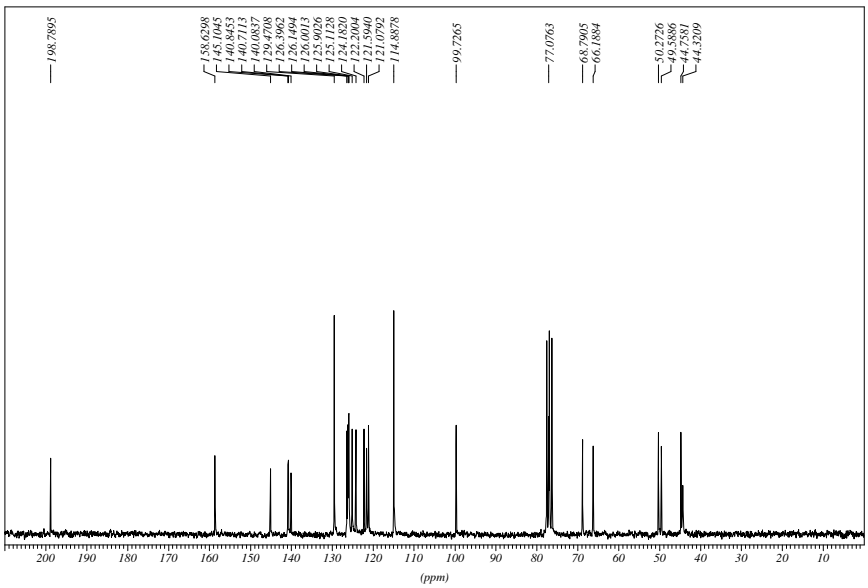

^{1}H NMR (200 MHz, $CDCl_3$) Spectra of compound **4**

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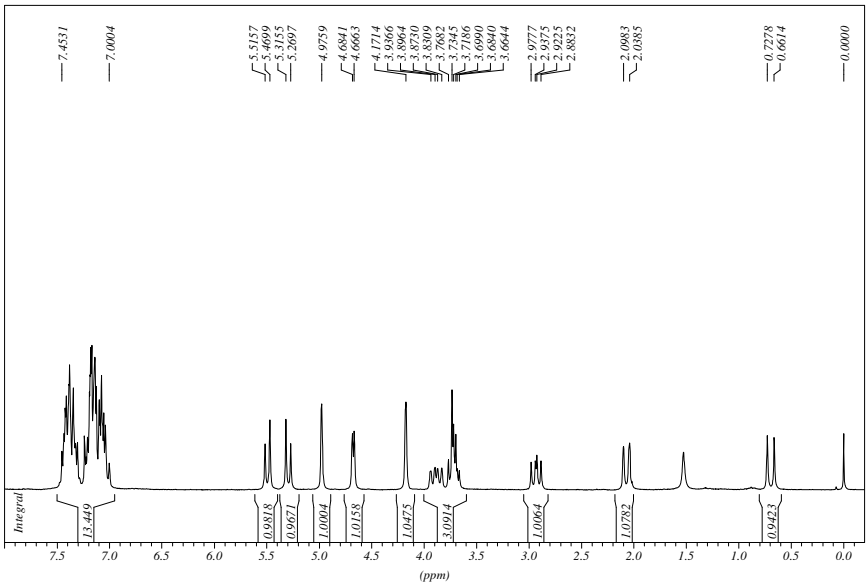

^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **4**

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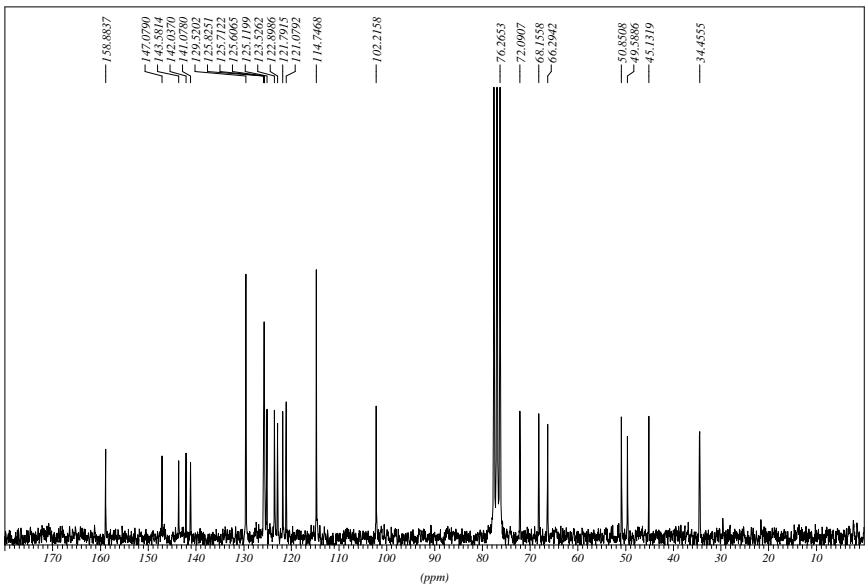

^{1}H NMR (200MHz, $CDCl_3$) Spectra of compound **5**

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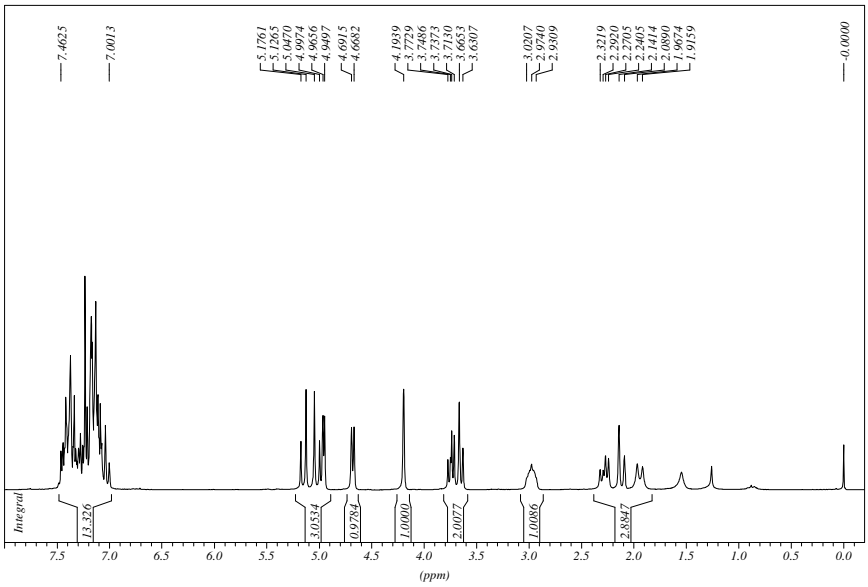
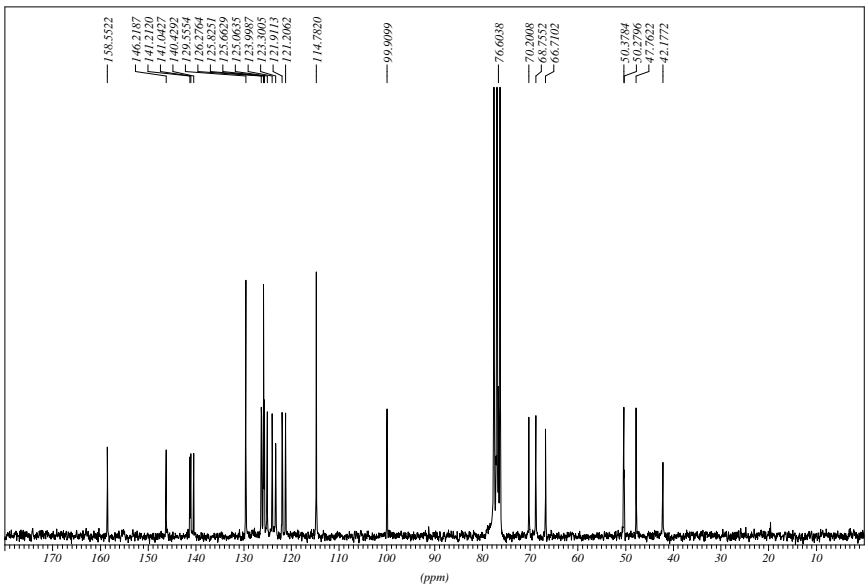


^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **5**



^{1}H NMR (200 MHz, $CDCl_3$) Spectra of compound **6**

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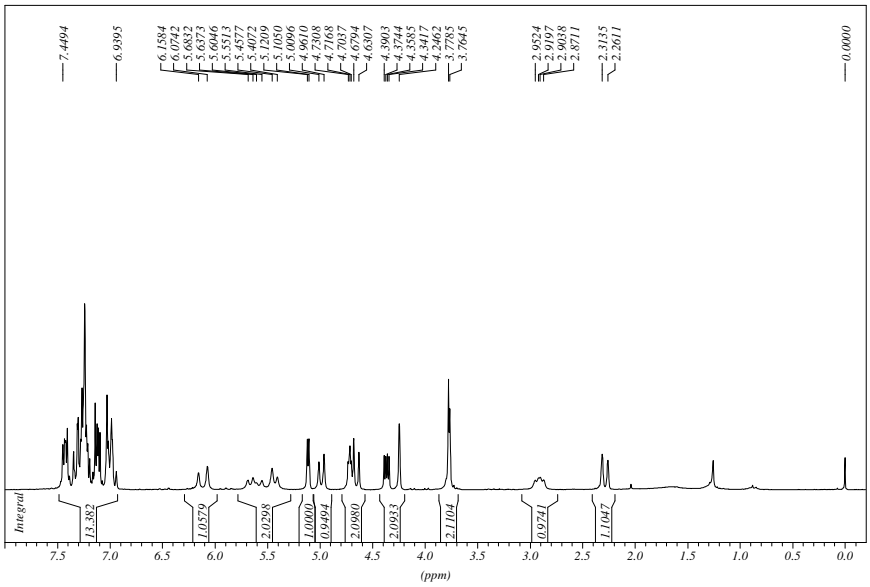
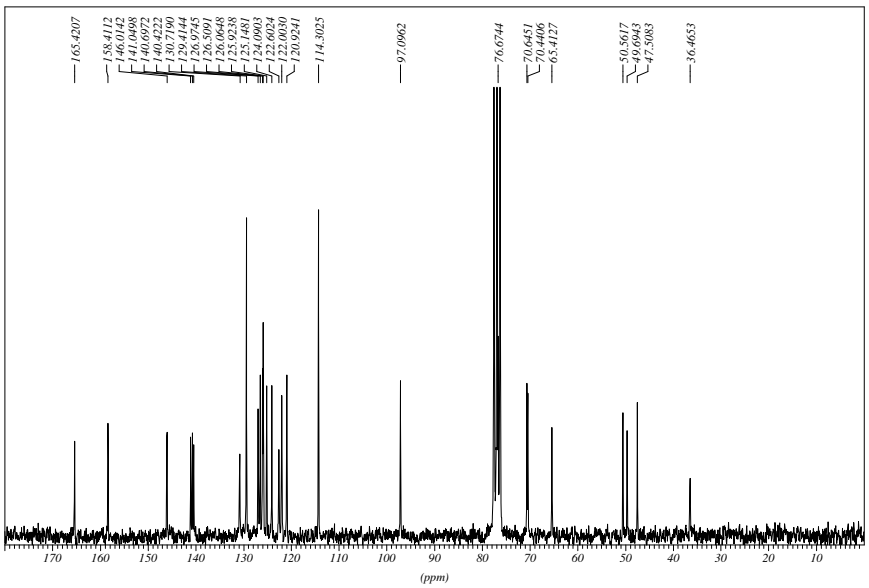


^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **6**



^{1}H NMR (200 MHz, $CDCl_3$) Spectra of compound **7b**

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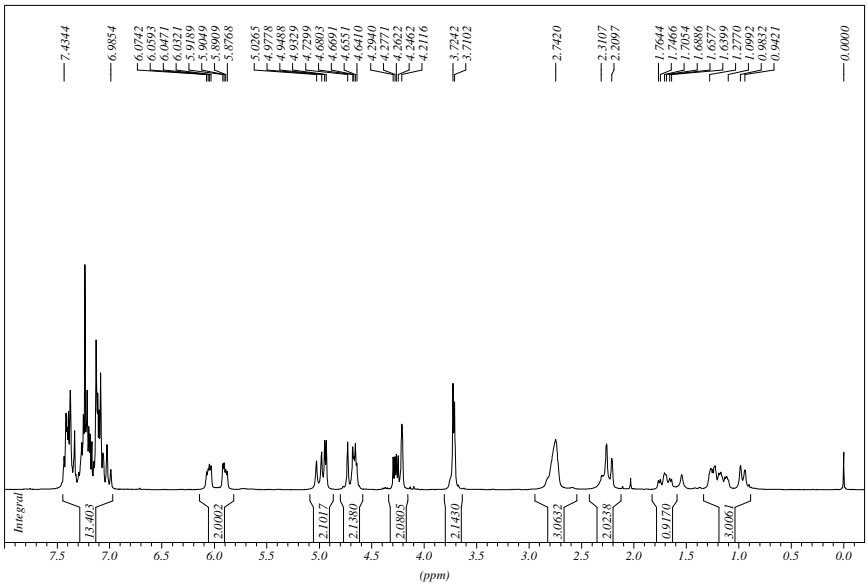
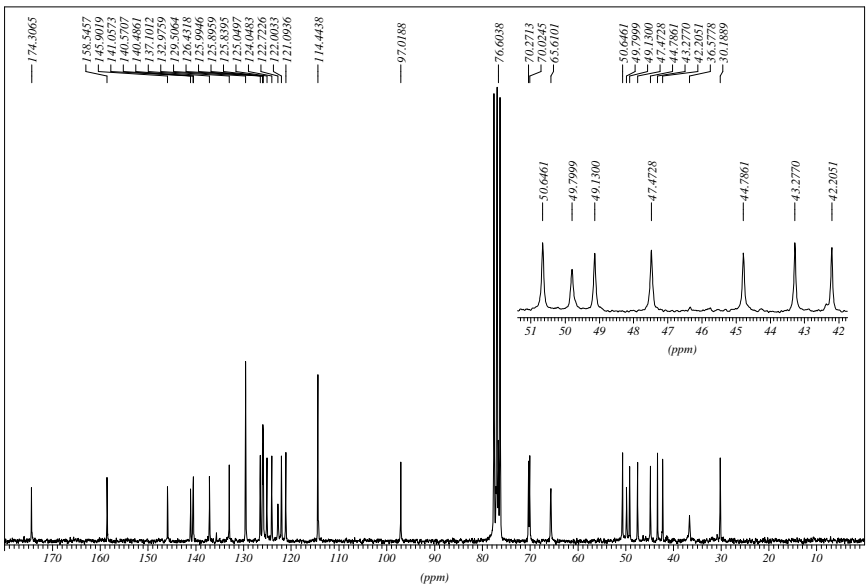


^{13}C NMR (50 MHz, $CDCl_3$) Spectra of compound **7b**



^{1}H NMR (200 MHz, $CDCl_3$) Spectra of related acrylates[3,4]

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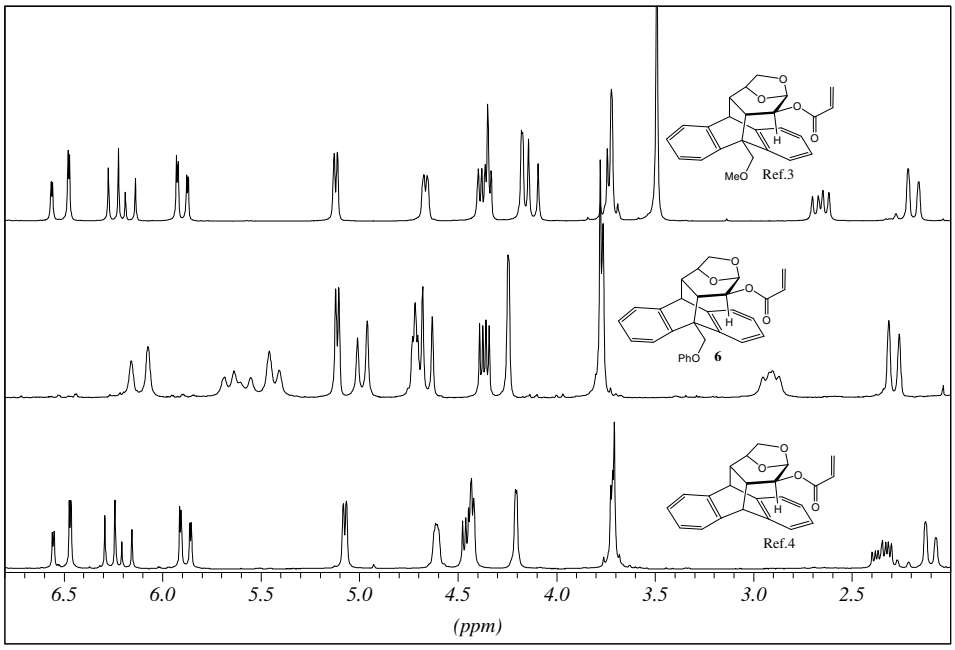

[3] A. M. Sarotti, R. A. Spanevello, A. G. Suárez. *Org. Lett.* **2006**, *8*, 1487-1490.
[4] A. M. Sarotti, R. A. Spanevello, C. Duhayon, J-P. Tuchagues, A. G. Suárez. *Tetrahedron*, **2007**, *63*, 241-251.

Variable temperature ^{1}H NMR (300 MHz, $CDCl_3$) Spectra of **6**

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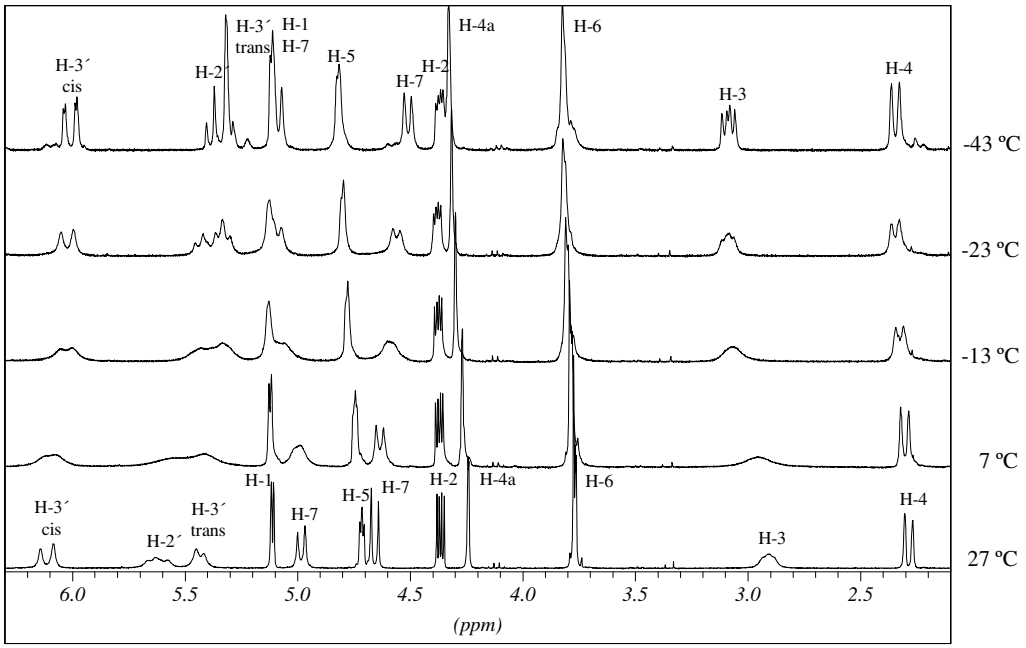

^{1}H NMR (300 MHz, $CDCl_3$) Spectra of **6** with Et_2AlCl recorded at 300 K

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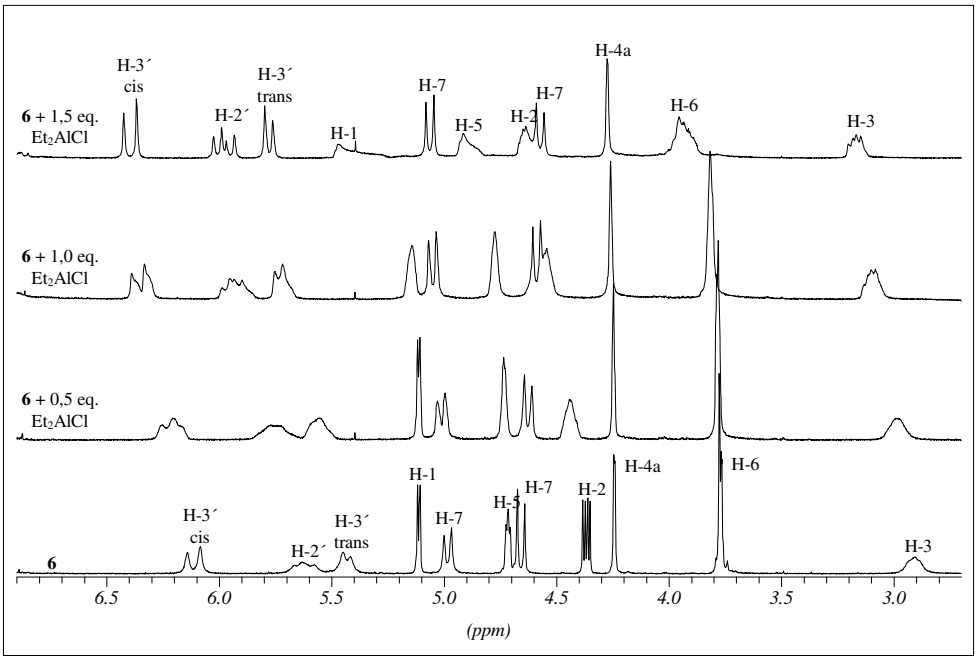

^{1}H NMR (300 MHz, $CDCl_3$) Spectra of **6** with Et_2AlCl recorded at 230 K

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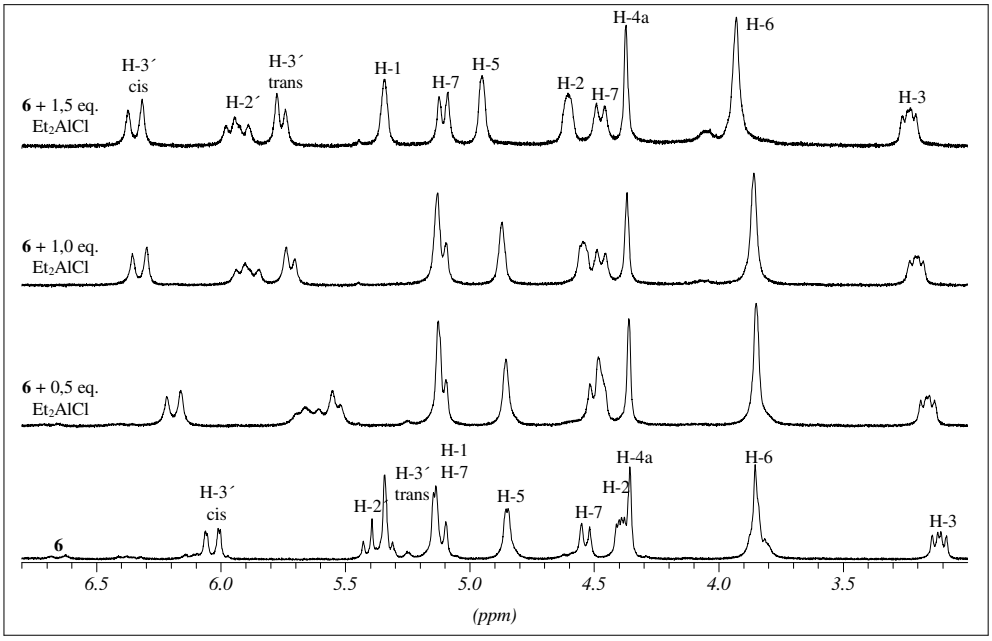
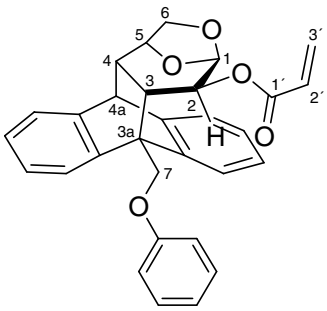


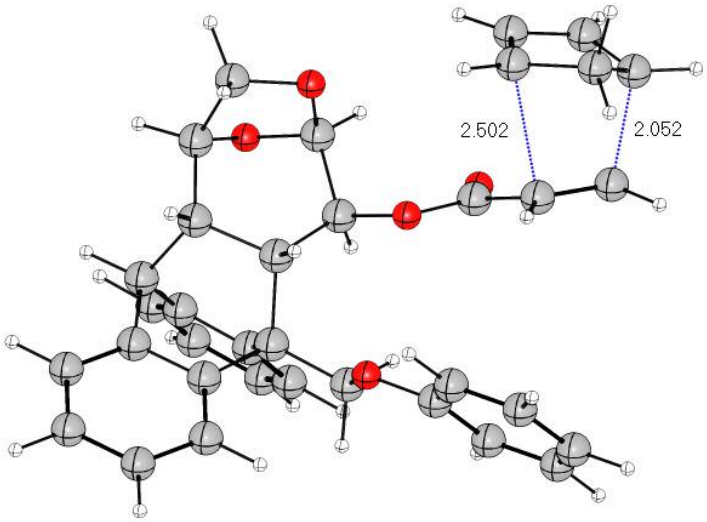
Selected ^{1}H NMR (300 MHz, $CDCl_3$) chemical shifts (ppm) for **6** recorded in the presence of Et_2AlCl at different temperatures.

Atom	300 °K		230 °K	
	-	1.5 eq. Et_2AlCl	-	1.5 eq. Et_2AlCl
H-1	5.11	5.47	5.14	5.34
H-2	4.37	4.65	4.39	4.60
H-3	2.91	3.18	3.11	3.23
H-4a	4.25	4.27	4.35	4.37
H-5	4.72	4.91	4.84	4.95
H-6	3.77	3.96	3.84	3.93
H-7a	4.99	5.06	5.11	5.10
H-7b	4.66	4.57	4.53	4.47
H-2´	5.62	5.98	5.38	5.93
H-3´*cis*	6.12	6.40	6.03	6.34
H-3´*trans*	5.43	5.78	5.32	5.76

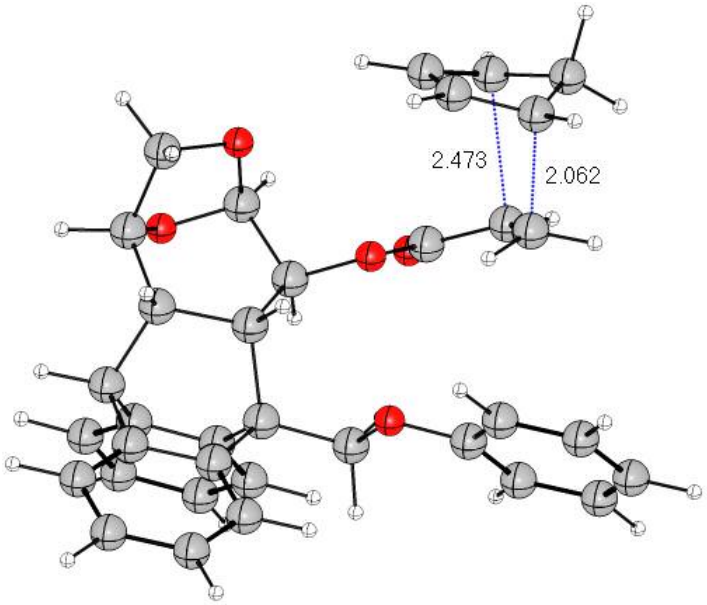


6

Ball and stick representations of the TS's corresponding to the reaction of **6-s-*cis*** and **6-s-*trans*** with cyclopentadiene to yield *S*- and *R*- cycloadducts, respectively. All structures correspond to fully optimized B3LYP/def2-SVP geometries. Bond distances are given in Å. Unless otherwise stated, white, gray, and red colors denote hydrogen, carbon, and oxygen atoms, respectively.



TS 6-s-*cis* → *S*-adduct



TS 6-s-*trans* → *R*-adduct

Full list of authors for reference [15]: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al–Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian03, Revision E.01, Gaussian, Inc., Wallingford CT, (2004).

Cartesian coordinates (in Å) and total energies of all the stationary points discussed in the text. All calculations have been performed with the programs TURBOMOLE (see ref. 8 in the text) and Gaussian 03.

RI-MP2/def2-SVP calculations:

6-s-cis, E = -1529.201967

C	-2.146898000	-0.517740000	-1.348455000
C	-0.700126000	-0.319456000	-0.792624000
C	-0.010430000	-1.593121000	-0.276554000
C	-2.519324000	-1.984883000	-1.558648000
O	-2.035597000	-2.799188000	-0.492245000
C	-0.663216000	-2.870751000	-0.784153000
C	-1.783529000	-2.602288000	-2.749205000
O	-0.535066000	-2.981571000	-2.187117000
C	-0.736816000	0.758549000	0.354691000
C	-1.617572000	0.157968000	1.435285000
C	-2.914646000	-0.157522000	0.985637000
C	-3.158133000	0.239375000	-0.441290000
C	-2.791347000	1.691495000	-0.584001000
C	-1.467683000	1.967745000	-0.192198000
C	-0.953539000	3.262919000	-0.331563000
C	-1.777329000	4.276774000	-0.840917000
C	-3.097274000	4.000814000	-1.223130000
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C	-3.459236000	-1.078648000	3.151772000
C	-2.170583000	-0.767174000	3.604511000
C	-1.241520000	-0.159907000	2.747250000
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C	2.325793000	-1.782696000	0.199719000
O	2.126385000	-1.945315000	1.387455000
C	3.652475000	-1.765947000	-0.459872000
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O	1.475659000	1.423962000	-0.225444000
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C	5.626252000	1.322800000	0.134517000
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H	3.665158000	-1.649015000	-1.544323000
H	5.760024000	-1.875408000	-0.199504000
H	4.710628000	-1.997697000	1.352919000
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H	0.604406000	1.887676000	1.610280000
H	2.855499000	1.192041000	2.129917000
H	5.319839000	1.123730000	2.266970000

H	6.716019000	1.298448000	0.204776000
H	5.597606000	1.545205000	-2.022111000
H	3.094279000	1.591049000	-2.160248000

6-s-trans, E = -1529.201143

C	-1.998690000	-0.538282000	-1.409239000
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O	1.464717000	-1.495460000	-0.437191000
C	2.318586000	-1.796774000	0.569918000
O	1.970623000	-2.021370000	1.712898000
C	3.728630000	-1.808462000	0.121527000
C	4.104725000	-1.667757000	-1.161170000
C	0.601856000	1.127898000	0.973431000
O	1.449254000	1.543599000	-0.080663000
C	2.795619000	1.450918000	0.102943000
C	3.411518000	1.184949000	1.335245000
C	4.810727000	1.101584000	1.400290000
C	5.595030000	1.286453000	0.259629000
C	4.969851000	1.561897000	-0.965859000
C	3.580269000	1.647941000	-1.045433000
H	-2.002594000	-0.023512000	-2.384840000
H	0.086818000	0.094984000	-1.502649000
H	-0.097192000	-1.624164000	0.921225000
H	-3.370105000	-2.173402000	-1.854501000
H	-0.073759000	-3.735322000	-0.249607000
H	-1.207769000	-1.827601000	-3.600763000
H	-1.885269000	-3.459077000	-3.271333000
H	-4.100958000	-0.074567000	-0.942083000
H	-0.018745000	3.532941000	0.023902000
H	-1.502242000	5.287525000	-0.936335000
H	-3.781305000	4.706063000	-1.750400000
H	-4.600348000	2.343270000	-1.603042000
H	-4.835315000	-1.168256000	1.249192000
H	-4.302614000	-1.668441000	3.644296000
H	-2.095414000	-1.012858000	4.592643000
H	-0.404348000	0.119789000	3.181522000
H	4.452213000	-1.962946000	0.923855000
H	5.159668000	-1.694218000	-1.439379000
H	3.361284000	-1.524704000	-1.946524000
H	1.019087000	0.244866000	1.479871000
H	0.494098000	1.929212000	1.729006000
H	2.823007000	1.049506000	2.242923000
H	5.283844000	0.895392000	2.363967000
H	6.683453000	1.221064000	0.322445000
H	5.570441000	1.714947000	-1.866285000
H	3.070930000	1.858009000	-1.988455000

[6-Al-*s-cis*]$^{+}$, E = -1850.461079

C	3.078994000	-1.964679000	1.198577000
C	2.096617000	-2.336427000	0.266671000
C	2.424683000	-3.155197000	-0.825383000
C	3.756782000	-3.558160000	-0.999272000
C	4.749140000	-3.155049000	-0.101488000
C	4.400466000	-2.364201000	1.007036000
O	0.846987000	-1.840038000	0.506813000
C	-0.152374000	-2.006357000	-0.481772000
C	-1.283051000	-1.054384000	-0.129831000
C	-0.728550000	0.390638000	0.174714000
C	-1.894264000	1.256361000	0.762687000
C	-3.248278000	0.542349000	0.478032000
C	-3.293403000	0.064408000	-0.946493000
C	-2.276986000	-0.862165000	-1.258620000
C	-0.148401000	1.026587000	-1.090331000
C	-0.133700000	2.548195000	-1.009369000
O	-1.454398000	2.948428000	-0.990890000
C	-1.849203000	2.735925000	0.374441000
C	-3.184352000	-0.674015000	1.366356000
C	-2.077258000	-1.497168000	1.087649000
O	0.411406000	3.031610000	0.270184000
C	-0.718946000	3.464321000	1.083682000
C	-4.244456000	0.426751000	-1.904377000
C	-4.184705000	-0.144482000	-3.182994000
C	-3.183744000	-1.074363000	-3.493715000
C	-2.218236000	-1.427665000	-2.538912000
C	-1.814909000	-2.612691000	1.891946000
C	-2.682074000	-2.908959000	2.953285000
C	-3.791867000	-2.095416000	3.218895000
C	-4.040325000	-0.962008000	2.432215000
O	1.082922000	0.418871000	-1.563880000
C	2.245440000	0.511705000	-0.966090000
C	3.306074000	-0.218425000	-1.649500000
C	4.580126000	-0.165124000	-1.211025000
Al	2.231976000	2.829798000	0.947372000
C	2.027737000	2.471730000	2.851267000
O	2.427129000	1.188034000	0.065247000
C	3.338189000	4.120423000	-0.002911000
H	-1.785369000	1.240275000	1.859687000
H	0.068078000	0.294562000	0.926519000
H	-0.820445000	0.831734000	-1.938045000
H	-2.823082000	3.223718000	0.515622000
H	0.414430000	3.033030000	-1.831202000
H	-0.543604000	3.146778000	2.116686000
H	-0.811398000	4.556201000	1.009376000
H	-4.097861000	1.196489000	0.730589000
H	-0.943049000	-3.243914000	1.710167000
H	-2.489385000	-3.783806000	3.578558000
H	-4.462092000	-2.342443000	4.045392000
H	-4.897920000	-0.316015000	2.641285000
H	-5.033068000	1.141507000	-1.652298000
H	-4.929333000	0.124560000	-3.935564000
H	-3.152634000	-1.527809000	-4.487179000
H	-1.448160000	-2.157185000	-2.801324000
H	3.018280000	-0.765005000	-2.547012000
H	5.377913000	-0.675037000	-1.751344000
H	4.841290000	0.394702000	-0.311254000
H	0.255713000	-1.769153000	-1.476340000
H	-0.524810000	-3.046117000	-0.505625000
H	1.660034000	-3.498168000	-1.523791000
H	4.011698000	-4.203269000	-1.843697000
H	5.782137000	-3.480892000	-0.241678000
H	5.163130000	-2.075100000	1.734644000
H	2.781395000	-1.353606000	2.053813000
H	4.407385000	3.976593000	0.217908000
H	3.093615000	5.154426000	0.287065000
H	3.225265000	4.056948000	-1.096709000

H	1.703636000	3.351860000	3.428662000
H	2.988829000	2.157451000	3.288681000
H	1.310321000	1.659330000	3.050559000

[6-Al-*s-trans*]$^{+}$, E = -1850.459276

C	3.216973000	-1.892760000	1.268105000
C	2.212823000	-2.339197000	0.394547000
C	2.517001000	-3.232554000	-0.640672000
C	3.849122000	-3.634573000	-0.823561000
C	4.860390000	-3.179282000	0.029339000
C	4.534725000	-2.317299000	1.086071000
O	0.970314000	-1.808152000	0.608522000
C	-0.009636000	-2.014692000	-0.389341000
C	-1.180577000	-1.102713000	-0.077035000
C	-0.698205000	0.373804000	0.194737000
C	-1.931121000	1.219011000	0.678482000
C	-3.235578000	0.406255000	0.439621000
C	-3.238500000	-0.128397000	-0.963970000
C	-2.161946000	-0.998602000	-1.229263000
C	-0.050452000	0.962389000	-1.061692000
C	-0.177557000	2.480480000	-1.124355000
O	-1.528035000	2.748383000	-1.225519000
C	-1.992214000	2.648472000	0.130909000
C	-3.113677000	-0.761106000	1.383237000
C	-1.968573000	-1.542400000	1.144336000
O	0.231017000	3.136102000	0.128011000
C	-0.984856000	3.556533000	0.813239000
C	-4.197618000	0.139977000	-1.944375000
C	-4.085181000	-0.470501000	-3.200880000
C	-3.022902000	-1.344429000	-3.466863000
C	-2.050865000	-1.603263000	-2.488750000
C	-1.662980000	-2.614473000	1.991624000
C	-2.524965000	-2.909216000	3.057448000
C	-3.671504000	-2.136056000	3.285673000
C	-3.964803000	-1.046629000	2.453932000
O	1.273230000	0.437671000	-1.364420000
C	2.350338000	0.685707000	-0.662457000
C	3.584428000	0.056001000	-1.120948000
C	3.655289000	-0.708285000	-2.229140000
Al	2.017909000	3.201067000	0.911334000
C	1.728826000	3.176134000	2.835834000
O	2.351367000	1.449342000	0.324389000
C	3.082877000	4.375898000	-0.220052000
H	2.938577000	-1.220011000	2.083007000
H	1.741614000	-3.619630000	-1.302479000
H	4.087593000	-4.333108000	-1.629705000
H	5.890749000	-3.510940000	-0.114374000
H	5.311445000	-1.975805000	1.774905000
H	0.411421000	-1.779620000	-1.380406000
H	-0.351720000	-3.065040000	-0.407836000
H	0.051315000	0.339369000	0.998747000
H	-1.844277000	1.319415000	1.772946000
H	-4.121905000	1.022925000	0.657900000
H	-0.615657000	0.635608000	-1.946990000
H	0.379296000	2.936245000	-1.956988000
H	-3.013760000	3.050928000	0.157850000
H	-0.856239000	3.379973000	1.885841000
H	-1.164341000	4.618967000	0.599908000
H	-5.033719000	0.810532000	-1.725959000
H	-4.834967000	-0.275762000	-3.971014000
H	-2.949681000	-1.829568000	-4.442999000
H	-1.235572000	-2.294163000	-2.716673000
H	-0.762581000	-3.212319000	1.839179000
H	-2.298969000	-3.750779000	3.716361000
H	-4.336116000	-2.381039000	4.117288000
H	-4.853518000	-0.433997000	2.631078000
H	4.462004000	0.280584000	-0.514725000
H	4.610265000	-1.123774000	-2.552688000

H	2.770028000	-0.921164000	-2.830586000
H	1.281674000	4.107228000	3.218102000
H	2.685043000	3.054867000	3.368930000
H	1.083498000	2.341154000	3.152374000
H	4.152843000	4.314710000	0.033350000
H	2.790674000	5.430977000	-0.100354000
H	2.994554000	4.137205000	-1.291883000

M05-2X/def2-SVP calculations :

6-s-cis, E = -1533.136779

C	-2.148434000	-0.531760000	-1.343662000
C	-0.699427000	-0.351385000	-0.781475000
C	-0.030944000	-1.633639000	-0.251127000
C	-2.544567000	-1.997207000	-1.537355000
O	-2.070634000	-2.804462000	-0.467723000
C	-0.703115000	-2.907362000	-0.749726000
C	-1.813957000	-2.636535000	-2.723012000
O	-0.582688000	-3.039374000	-2.147617000
C	-0.724217000	0.748217000	0.348011000
C	-1.632657000	0.193978000	1.439831000
C	-2.928156000	-0.096475000	0.987935000
C	-3.149893000	0.267113000	-0.458735000
C	-2.745866000	1.713175000	-0.633066000
C	-1.427324000	1.969116000	-0.231675000
C	-0.894146000	3.246744000	-0.378731000
C	-1.688635000	4.266197000	-0.911441000
C	-3.000258000	4.009897000	-1.303962000
C	-3.532693000	2.724848000	-1.170912000
C	-3.868349000	-0.654015000	1.845179000
C	-3.518661000	-0.919122000	3.171207000
C	-2.234771000	-0.629598000	3.625219000
C	-1.285036000	-0.076415000	2.761071000
O	1.333267000	-1.646261000	-0.684540000
C	2.305761000	-1.870477000	0.211596000
O	2.111613000	-2.018828000	1.393156000
C	3.635067000	-1.887289000	-0.448697000
C	4.738236000	-2.007598000	0.288205000
C	0.669821000	1.039659000	0.873421000
O	1.501697000	1.390154000	-0.214395000
C	2.846150000	1.385018000	-0.036437000
C	3.467461000	1.265009000	1.209461000
C	4.862163000	1.258713000	1.279284000
C	5.639371000	1.380416000	0.131229000
C	5.007793000	1.511863000	-1.108444000
C	3.622163000	1.512589000	-1.196095000
H	-2.186789000	-0.059967000	-2.333580000
H	-0.053247000	0.021700000	-1.582059000
H	-0.060657000	-1.673213000	0.843086000
H	-3.633118000	-2.107245000	-1.594381000
H	-0.287614000	-3.793004000	-0.254786000
H	-1.632687000	-1.935030000	-3.545891000
H	-2.358752000	-3.512947000	-3.101533000
H	-4.182862000	0.088261000	-0.779394000
H	0.137022000	3.451803000	-0.099022000
H	-1.274514000	5.267443000	-1.022528000
H	-3.611707000	4.811197000	-1.716837000
H	-4.557074000	2.515864000	-1.479982000
H	-4.871193000	-0.880080000	1.482798000
H	-4.251101000	-1.353557000	3.850131000
H	-1.963358000	-0.837746000	4.659176000
H	-0.283502000	0.130305000	3.134772000
H	3.647332000	-1.775943000	-1.531423000
H	5.728359000	-2.006597000	-0.164378000
H	4.654297000	-2.100118000	1.371436000
H	1.072770000	0.151793000	1.379006000
H	0.625468000	1.862687000	1.605675000
H	2.884301000	1.165838000	2.121211000

H	5.340664000	1.159885000	2.253088000
H	6.725996000	1.378651000	0.199021000
H	5.601417000	1.611560000	-2.016613000
H	3.107240000	1.606582000	-2.150617000

6-s-trans, E = -1533.135974

C	-2.020478000	-0.550341000	-1.391280000
C	-0.614700000	-0.351126000	-0.735316000
C	0.010757000	-1.621245000	-0.129473000
C	-2.373359000	-2.019331000	-1.629884000
O	-1.978459000	-2.829167000	-0.530705000
C	-0.589799000	-2.902540000	-0.692336000
C	-1.530076000	-2.632323000	-2.753304000
O	-0.344574000	-3.016717000	-2.076869000
C	-0.722650000	0.770032000	0.367508000
C	-1.678906000	0.214481000	1.416965000
C	-2.938187000	-0.117006000	0.895847000
C	-3.088691000	0.225529000	-0.565659000
C	-2.709496000	1.679678000	-0.731108000
C	-1.418995000	1.968721000	-0.265183000
C	-0.908726000	3.257647000	-0.394577000
C	-1.697862000	4.254596000	-0.975634000
C	-2.981240000	3.965034000	-1.433097000
C	-3.490362000	2.668834000	-1.317022000
C	-3.910871000	-0.687466000	1.707318000
C	-3.630654000	-0.923300000	3.055247000
C	-2.383050000	-0.592316000	3.577406000
C	-1.399785000	-0.027093000	2.759801000
O	1.415090000	-1.622618000	-0.410388000
C	2.277504000	-1.894124000	0.582807000
O	1.947815000	-2.038932000	1.734010000
C	3.682940000	-1.977149000	0.117141000
C	4.034841000	-1.873349000	-1.163939000
C	0.640932000	1.091220000	0.952509000
O	1.502136000	1.467445000	-0.103078000
C	2.844021000	1.422780000	0.084785000
C	3.453922000	1.192457000	1.320645000
C	4.848753000	1.140977000	1.396023000
C	5.636010000	1.324873000	0.264633000
C	5.015225000	1.569887000	-0.963834000
C	3.630889000	1.619949000	-1.056870000
H	-2.002529000	-0.067955000	-2.376753000
H	0.084868000	0.008333000	-1.496753000
H	-0.135422000	-1.656303000	0.955198000
H	-3.450636000	-2.147347000	-1.781982000
H	-0.201222000	-3.785154000	-0.170679000
H	-1.292769000	-1.918887000	-3.551385000
H	-2.021745000	-3.515438000	-3.184975000
H	-4.098534000	0.019375000	-0.939143000
H	0.101356000	3.488410000	-0.063136000
H	-1.301779000	5.264548000	-1.072899000
H	-3.588868000	4.748981000	-1.883279000
H	-4.492481000	2.433932000	-1.676314000
H	-4.885151000	-0.945923000	1.292405000
H	-4.389237000	-1.367525000	3.698181000
H	-2.165992000	-0.778509000	4.628224000
H	-0.425464000	0.208475000	3.184837000
H	4.405604000	-2.127538000	0.917539000
H	5.080260000	-1.934575000	-1.463688000
H	3.279292000	-1.721242000	-1.933737000
H	1.036238000	0.207271000	1.470226000
H	0.555078000	1.909101000	1.686615000
H	2.864119000	1.045753000	2.221940000
H	5.317102000	0.956184000	2.362198000
H	6.721528000	1.284573000	0.335964000
H	5.617253000	1.722142000	-1.859228000
H	3.125636000	1.801318000	-2.003854000

TS 6-s-cis→6-s-trans, E = -1533.125429

C	3.570338000	1.761149000	-1.129056000
C	2.789474000	1.576749000	0.019675000
C	3.404898000	1.446807000	1.268432000
C	4.799341000	1.489035000	1.351657000
C	5.581047000	1.665312000	0.214214000
C	4.954494000	1.804663000	-1.028380000
O	1.449511000	1.531277000	-0.172743000
C	0.613934000	1.147961000	0.900830000
C	-0.748224000	0.777789000	0.343284000
C	-0.630188000	-0.350910000	-0.751193000
C	-2.046019000	-0.607473000	-1.365206000
C	-3.116894000	0.155748000	-0.531594000
C	-2.927054000	-0.162157000	0.930523000
C	-1.665308000	0.206893000	1.419227000
C	0.059433000	-1.589780000	-0.151511000
C	-0.529400000	-2.903416000	-0.652527000
O	-1.912920000	-2.857907000	-0.442761000
C	-2.365152000	-2.091956000	-1.551400000
C	-2.781270000	1.616333000	-0.726645000
C	-1.490948000	1.948184000	-0.290020000
O	-0.331663000	-3.060879000	-2.038293000
C	-1.545222000	-2.716920000	-2.685599000
C	-3.866979000	-0.747270000	1.769500000
C	-3.551199000	-0.961471000	3.113082000
C	-2.300819000	-0.594231000	3.603369000
C	-1.350925000	-0.012716000	2.758140000
C	-1.020237000	3.248855000	-0.448837000
C	-1.847634000	4.214053000	-1.030231000
C	-3.130804000	3.881700000	-1.458499000
C	-3.600644000	2.573914000	-1.312255000
O	1.449866000	-1.560966000	-0.507713000
C	2.366197000	-1.790578000	0.442674000
C	3.750102000	-1.835764000	-0.127271000
C	4.314347000	-2.972853000	-0.521731000
O	2.105443000	-1.924344000	1.609546000
H	-2.067697000	-0.152094000	-2.363341000
H	0.034444000	0.023665000	-1.536128000
H	-0.030752000	-1.603866000	0.939635000
H	-3.443171000	-2.252041000	-1.662353000
H	-0.100872000	-3.758075000	-0.115418000
H	-1.348029000	-2.019551000	-3.508416000
H	-2.031725000	-3.620276000	-3.079506000
H	-4.127907000	-0.083326000	-0.881527000
H	-0.011510000	3.513855000	-0.139877000
H	-1.481789000	5.232848000	-1.150674000
H	-3.768578000	4.640987000	-1.909208000
H	-4.602231000	2.304918000	-1.648308000
H	-4.843360000	-1.034561000	1.379332000
H	-4.283842000	-1.417358000	3.777570000
H	-2.055892000	-0.763149000	4.650968000
H	-0.374792000	0.254600000	3.159860000
H	4.278691000	-0.881090000	-0.175968000
H	5.332479000	-2.985563000	-0.908764000
H	3.781042000	-3.922770000	-0.472371000
H	1.047688000	0.286305000	1.426308000
H	0.512531000	1.975110000	1.622481000
H	2.819545000	1.303702000	2.172932000
H	5.272210000	1.378982000	2.326650000
H	6.666352000	1.696240000	0.291150000
H	5.551762000	1.943588000	-1.928793000
H	3.061415000	1.855580000	-2.086442000

6-Al-s-cis+, E = -1855.047740

C	3.086166000	-2.296407000	1.146080000
C	2.133777000	-2.460337000	0.134119000
C	2.446994000	-3.177387000	-1.022192000
C	3.738621000	-3.692384000	-1.173675000

C	4.703072000	-3.504240000	-0.189434000
C	4.364957000	-2.810560000	0.978429000
O	0.934405000	-1.850983000	0.349220000
C	-0.084530000	-1.951950000	-0.622935000
C	-1.230367000	-1.059414000	-0.173680000
C	-0.715518000	0.388169000	0.191359000
C	-1.900516000	1.192450000	0.833361000
C	-3.231619000	0.421288000	0.587552000
C	-3.325542000	-0.005853000	-0.857471000
C	-2.284143000	-0.859003000	-1.255416000
C	-0.148566000	1.089969000	-1.050179000
C	-0.246153000	2.609044000	-0.966110000
O	-1.585670000	2.911974000	-0.909429000
C	-1.941067000	2.676660000	0.457723000
C	-3.071837000	-0.830137000	1.424172000
C	-1.958761000	-1.597163000	1.055824000
O	0.292370000	3.137340000	0.293855000
C	-0.837203000	3.463309000	1.154447000
C	-4.337665000	0.335241000	-1.746503000
C	-4.319573000	-0.187613000	-3.042236000
C	-3.296708000	-1.046534000	-3.435619000
C	-2.271203000	-1.382977000	-2.545727000
C	-1.633344000	-2.740688000	1.779341000
C	-2.439732000	-3.122498000	2.855434000
C	-3.552531000	-2.364085000	3.210807000
C	-3.869309000	-1.204425000	2.498369000
O	1.147392000	0.591567000	-1.474132000
C	2.265339000	0.701777000	-0.815546000
C	3.394695000	0.021018000	-1.439049000
C	4.599288000	0.034781000	-0.856980000
Al	2.149757000	3.119699000	0.838094000
C	2.127749000	3.159128000	2.780126000
O	2.356453000	1.363091000	0.236703000
C	3.114021000	4.230265000	-0.438017000
H	-1.752846000	1.168625000	1.919938000
H	0.082839000	0.275836000	0.932401000
H	-0.770194000	0.852256000	-1.920082000
H	-2.932232000	3.108447000	0.622742000
H	0.245825000	3.125509000	-1.797798000
H	-0.605748000	3.131771000	2.169086000
H	-1.002753000	4.544568000	1.114756000
H	-4.094328000	1.018697000	0.902952000
H	-0.756834000	-3.333662000	1.525204000
H	-2.193882000	-4.021485000	3.418247000
H	-4.177045000	-2.674044000	4.047136000
H	-4.735760000	-0.605173000	2.777507000
H	-5.146535000	0.993909000	-1.430798000
H	-5.113744000	0.068620000	-3.741641000
H	-3.295602000	-1.464570000	-4.441006000
H	-1.484718000	-2.060849000	-2.874015000
H	3.194501000	-0.492220000	-2.376580000
H	5.446787000	-0.469090000	-1.318233000
H	4.755774000	0.539430000	0.096116000
H	0.295591000	-1.624654000	-1.600708000
H	-0.433160000	-2.991741000	-0.719654000
H	1.707891000	-3.346956000	-1.801486000
H	3.982122000	-4.254853000	-2.074137000
H	5.703092000	-3.915561000	-0.314661000
H	5.103535000	-2.682129000	1.768935000
H	2.800031000	-1.752858000	2.045243000
H	4.200649000	4.108622000	-0.323237000
H	2.897733000	5.297277000	-0.287858000
H	2.874594000	3.993110000	-1.485447000
H	1.697577000	4.089240000	3.178275000
H	3.153889000	3.102472000	3.170338000
H	1.573786000	2.314793000	3.215272000

6-Al-s-trans+, E = -1855.046734

C	3.687551000	-1.552558000	1.160407000
C	2.781360000	-1.900932000	0.154256000
C	3.186098000	-2.702401000	-0.914339000
C	4.513851000	-3.140875000	-0.971410000
C	5.426007000	-2.788094000	0.017009000
C	5.002736000	-1.993834000	1.087182000
O	1.528138000	-1.369794000	0.271291000
C	0.535833000	-1.766294000	-0.651037000
C	-0.807588000	-1.245278000	-0.167784000
C	-0.748187000	0.287800000	0.198019000
C	-2.122051000	0.706608000	0.836338000
C	-3.150869000	-0.444093000	0.634447000
C	-3.139989000	-0.888344000	-0.807574000
C	-1.893989000	-1.377396000	-1.229054000
C	-0.393877000	1.121375000	-1.040187000
C	-0.974195000	2.530474000	-0.994204000
O	-2.341475000	2.381544000	-0.964409000
C	-2.632947000	2.086148000	0.406449000
C	-2.594898000	-1.575276000	1.472304000
C	-1.310822000	-1.972026000	1.077004000
O	-0.664187000	3.231148000	0.256360000
C	-1.861974000	3.209859000	1.085618000
C	-4.226358000	-0.880214000	-1.674147000
C	-4.074654000	-1.375134000	-2.971931000
C	-2.844771000	-1.876966000	-3.389043000
C	-1.747703000	-1.876896000	-2.521242000
C	-0.634628000	-2.953655000	1.795915000
C	-1.258900000	-3.547917000	2.896360000
C	-2.540202000	-3.158579000	3.279764000
C	-3.213430000	-2.160810000	2.570244000
O	1.009284000	1.043313000	-1.402157000
C	2.001417000	1.441928000	-0.656457000
C	3.341242000	1.046265000	-1.072980000
C	3.562607000	0.300195000	-2.160990000
Al	1.090164000	3.807317000	0.829591000
C	0.984573000	3.959723000	2.762976000
O	1.830348000	2.160403000	0.346346000
C	1.714008000	5.078181000	-0.506452000
H	3.336731000	-0.935008000	1.985961000
H	2.494678000	-2.993013000	-1.701529000
H	4.827816000	-3.771013000	-1.802606000
H	6.455466000	-3.137140000	-0.035423000
H	5.704016000	-1.722279000	1.875180000
H	0.773439000	-1.365217000	-1.647724000
H	0.488312000	-2.862798000	-0.726645000
H	0.041182000	0.414317000	0.946577000
H	-1.967481000	0.768994000	1.920301000
H	-4.148204000	-0.138258000	0.969681000
H	-0.877811000	0.688658000	-1.922669000
H	-0.657820000	3.160685000	-1.832598000
H	-3.714465000	2.177137000	0.542466000
H	-1.565151000	3.007862000	2.117072000
H	-2.363454000	4.178631000	0.996204000
H	-5.192698000	-0.503559000	-1.339216000
H	-4.923470000	-1.379236000	-3.653779000
H	-2.734898000	-2.278108000	-4.395308000
H	-0.798646000	-2.282558000	-2.868188000
H	0.372697000	-3.259806000	1.520036000
H	-0.736871000	-4.322214000	3.456226000
H	-3.018720000	-3.631992000	4.135547000
H	-4.214149000	-1.850310000	2.870201000
H	4.143021000	1.391203000	-0.423330000
H	4.575234000	0.010510000	-2.438133000
H	2.742222000	-0.034416000	-2.794883000
H	0.265362000	4.726130000	3.085744000
H	1.960865000	4.262260000	3.167551000
H	0.716220000	3.013071000	3.253567000

H	2.779888000	5.305240000	-0.361973000
H	1.175038000	6.033441000	-0.436307000
H	1.601142000	4.714874000	-1.538907000

TS 6-Al-s-cis+→6-Al-s-trans+, E = -1855.033689

C	3.466802000	-2.089230000	1.131449000
C	2.613466000	-2.173043000	0.026483000
C	2.985243000	-2.906980000	-1.101604000
C	4.221131000	-3.559542000	-1.110714000
C	5.079039000	-3.479491000	-0.018160000
C	4.695241000	-2.739896000	1.103287000
O	1.444844000	-1.465382000	0.113880000
C	0.409643000	-1.752857000	-0.807066000
C	-0.890214000	-1.189466000	-0.255270000
C	-0.728616000	0.309833000	0.207126000
C	-2.056378000	0.770068000	0.909134000
C	-3.158336000	-0.301778000	0.664776000
C	-3.210787000	-0.649275000	-0.802923000
C	-2.008689000	-1.183974000	-1.291150000
C	-0.355827000	1.194358000	-0.987807000
C	-0.844034000	2.630684000	-0.845052000
O	-2.216023000	2.563095000	-0.780734000
C	-2.487925000	2.203074000	0.578559000
C	-2.651649000	-1.516382000	1.412416000
C	-1.405913000	-1.964556000	0.954291000
O	-0.455804000	3.236630000	0.433267000
C	-1.627752000	3.232769000	1.299796000
C	-4.314775000	-0.514679000	-1.636191000
C	-4.224922000	-0.927747000	-2.967833000
C	-3.039408000	-1.474032000	-3.452146000
C	-1.924166000	-1.601185000	-2.617632000
C	-0.775886000	-3.032327000	1.587486000
C	-1.408167000	-3.657694000	2.665850000
C	-2.651325000	-3.215439000	3.112233000
C	-3.277203000	-2.132818000	2.489163000
O	1.036273000	1.045409000	-1.387328000
C	2.061394000	1.343017000	-0.652380000
C	3.372520000	0.885775000	-1.172822000
C	4.085051000	1.645178000	-2.000167000
Al	1.346864000	3.679492000	0.970235000
C	1.314730000	3.764473000	2.908353000
O	1.963507000	2.002484000	0.392440000
C	2.017218000	4.933758000	-0.359903000
H	3.143708000	-1.515483000	1.998741000
H	2.337073000	-2.973071000	-1.972228000
H	4.509850000	-4.134659000	-1.989320000
H	6.038704000	-3.992328000	-0.035641000
H	5.355322000	-2.676225000	1.967162000
H	0.646847000	-1.309013000	-1.784493000
H	0.302744000	-2.839269000	-0.940485000
H	0.085400000	0.340638000	0.939378000
H	-1.872323000	0.754570000	1.990201000
H	-4.126373000	0.040177000	1.047597000
H	-0.881775000	0.843741000	-1.882362000
H	-0.513038000	3.289052000	-1.655707000
H	-3.557143000	2.353428000	0.753249000
H	-1.313326000	2.946834000	2.305974000
H	-2.070692000	4.233622000	1.288018000
H	-5.247171000	-0.103119000	-1.250064000
H	-5.088037000	-0.833192000	-3.624792000
H	-2.978487000	-1.810219000	-4.486000000
H	-1.010111000	-2.036916000	-3.017944000
H	0.201175000	-3.384369000	1.261341000
H	-0.923275000	-4.499187000	3.157908000
H	-3.136953000	-3.713774000	3.949679000
H	-4.248199000	-1.781621000	2.837880000
H	3.713267000	-0.089742000	-0.816797000
H	5.054471000	1.304379000	-2.360544000

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H        3.734262000      2.619445000     -2.343405000
H        0.639351000      4.546653000      3.283544000
H        2.315919000      4.009106000      3.290039000
H        1.021262000      2.811016000      3.370488000
H        3.105131000      5.058519000     -0.259943000
H        1.571506000      5.931145000     -0.240775000
H        1.822268000      4.615007000     -1.395445000
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B3LYP/def2-SVP calculations :

6-s-cis, E = -1533.332187

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C       -2.136642000     -0.439468000     -1.352102000
C       -0.680240000     -0.356911000     -0.767026000
C       -0.129566000     -1.694015000     -0.216249000
C       -2.609631000     -1.878007000     -1.604327000
O       -2.247731000     -2.736214000     -0.522548000
C       -0.874471000     -2.931826000     -0.745700000
C       -1.861469000     -2.549622000     -2.770862000
O       -0.706631000     -3.090946000     -2.142212000
C       -0.639611000      0.783087000      0.345534000
C       -1.583387000      0.304871000      1.456019000
C       -2.895639000      0.065158000      1.002663000
C       -3.099620000      0.410482000     -0.456507000
C       -2.630236000      1.839120000     -0.645597000
C       -1.293566000      2.037932000     -0.251425000
C       -0.714976000      3.300872000     -0.401966000
C       -1.471288000      4.355323000     -0.932019000
C       -2.797319000      4.152328000     -1.319913000
C       -3.379414000      2.885865000     -1.180905000
C       -3.870938000     -0.407750000      1.878652000
C       -3.546183000     -0.639774000      3.221022000
C       -2.248914000     -0.398577000      3.676635000
C       -1.264024000      0.069994000      2.795824000
O        1.264249000     -1.764792000     -0.566025000
C        2.066446000     -2.550023000      0.184747000
O        1.679753000     -3.185901000      1.139871000
C        3.464537000     -2.511533000     -0.320465000
C        4.423813000     -3.235205000      0.265662000
C        0.779735000      1.021315000      0.858462000
O        1.618176000      1.366795000     -0.227544000
C        2.955098000      1.522467000     -0.030092000
C        3.588661000      1.428091000      1.218313000
C        4.974848000      1.612475000      1.304404000
C        5.734549000      1.890821000      0.168280000
C        5.094125000      1.985818000     -1.075019000
C        3.717516000      1.804005000     -1.177968000
H       -2.133292000      0.058859000     -2.333633000
H        0.002481000     -0.049142000     -1.568873000
H       -0.217586000     -1.744241000      0.878503000
H       -3.702546000     -1.918566000     -1.721029000
H       -0.539967000     -3.840266000     -0.224747000
H       -1.569152000     -1.842403000     -3.563673000
H       -2.462876000     -3.359788000     -3.220553000
H       -4.144454000      0.275529000     -0.772602000
H        0.324581000      3.474502000     -0.123251000
H       -1.014887000      5.342329000     -1.042763000
H       -3.381486000      4.979559000     -1.731226000
H       -4.417011000      2.718578000     -1.484104000
H       -4.886502000     -0.592925000      1.517727000
H       -4.309346000     -1.008143000      3.911143000
H       -1.994853000     -0.576854000      4.724496000
H       -0.255322000      0.244813000      3.175567000
H        3.658443000     -1.866982000     -1.180930000
H        5.455504000     -3.214669000     -0.093734000
H        4.186825000     -3.866600000      1.126953000
H        1.162065000      0.115014000      1.357010000
H        0.772344000      1.831920000      1.610467000
H        3.020182000      1.215086000      2.123524000
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H	5.459415000	1.536240000	2.281442000
H	6.814647000	2.033840000	0.246488000
H	5.675087000	2.204277000	-1.975031000
H	3.202017000	1.874615000	-2.137949000

6-s-trans, E = -1533.331361

C	-2.145556000	-0.442864000	-1.311035000
C	-0.696900000	-0.460609000	-0.694183000
C	-0.306491000	-1.788795000	0.007668000
C	-2.800491000	-1.829541000	-1.381667000
O	-2.552942000	-2.574511000	-0.188503000
C	-1.218219000	-2.970853000	-0.361099000
C	-2.149964000	-2.743918000	-2.435131000
O	-1.075012000	-3.340551000	-1.720553000
C	-0.546568000	0.785200000	0.289021000
C	-1.572203000	0.552335000	1.405977000
C	-2.892891000	0.431416000	0.931222000
C	-3.012760000	0.625480000	-0.564437000
C	-2.362403000	1.951583000	-0.898911000
C	-1.022951000	2.029675000	-0.474859000
C	-0.284367000	3.184368000	-0.747078000
C	-0.886494000	4.252937000	-1.425349000
C	-2.217433000	4.170578000	-1.840474000
C	-2.959185000	3.011340000	-1.580445000
C	-3.943601000	0.190798000	1.814608000
C	-3.684684000	0.072786000	3.185805000
C	-2.377801000	0.193010000	3.661866000
C	-1.318270000	0.428422000	2.774493000
O	1.032343000	-2.152059000	-0.367267000
C	1.955803000	-2.399918000	0.583591000
O	1.777594000	-2.214754000	1.768495000
C	3.226612000	-2.921499000	0.019990000
C	3.389657000	-3.283488000	-1.257532000
C	0.872975000	0.921679000	0.838075000
O	1.787003000	1.005543000	-0.243519000
C	3.117575000	1.153921000	0.006029000
C	3.687509000	1.147584000	1.288182000
C	5.071578000	1.311846000	1.427961000
C	5.891686000	1.482455000	0.312288000
C	5.314784000	1.485478000	-0.964934000
C	3.940628000	1.323326000	-1.121338000
H	-2.065208000	-0.085317000	-2.349082000
H	0.028673000	-0.317447000	-1.504542000
H	-0.349152000	-1.685569000	1.100126000
H	-3.889442000	-1.743649000	-1.508806000
H	-1.006295000	-3.842439000	0.278153000
H	-1.768302000	-2.194035000	-3.310392000
H	-2.852673000	-3.522399000	-2.782197000
H	-4.057651000	0.582435000	-0.905466000
H	0.760994000	3.260918000	-0.447223000
H	-0.305588000	5.155879000	-1.630328000
H	-2.680729000	5.008856000	-2.367178000
H	-4.001711000	2.938149000	-1.903396000
H	-4.965747000	0.098591000	1.436682000
H	-4.506458000	-0.112301000	3.882184000
H	-2.174733000	0.102256000	4.731882000
H	-0.304177000	0.509639000	3.169795000
H	4.028389000	-3.011734000	0.757149000
H	4.344449000	-3.678896000	-1.614419000
H	2.568487000	-3.198131000	-1.973408000
H	1.122528000	0.061327000	1.478546000
H	0.939078000	1.832396000	1.461478000
H	3.071683000	1.006140000	2.176007000
H	5.506732000	1.303913000	2.430890000
H	6.969747000	1.611149000	0.432757000
H	5.943457000	1.617653000	-1.849583000
H	3.474309000	1.324863000	-2.108683000

TS 6-s-cis→6-s-trans, E = -1533.322170

C	-2.085063000	-0.561506000	-1.338636000
C	-0.647845000	-0.404419000	-0.722038000
C	-0.079929000	-1.685196000	-0.067607000
C	-2.531059000	-2.025066000	-1.474324000
O	-2.178237000	-2.781515000	-0.315457000
C	-0.798978000	-2.974631000	-0.497349000
C	-1.751783000	-2.783874000	-2.564817000
O	-0.605508000	-3.258941000	-1.869642000
C	-0.661970000	0.808776000	0.311053000
C	-1.639850000	0.397385000	1.418837000
C	-2.933294000	0.111891000	0.939082000
C	-3.086858000	0.345248000	-0.547830000
C	-2.624666000	1.761048000	-0.828035000
C	-1.306441000	2.007418000	-0.400214000
C	-0.735055000	3.262571000	-0.625008000
C	-1.481286000	4.263545000	-1.262108000
C	-2.789414000	4.014023000	-1.682490000
C	-3.363505000	2.754345000	-1.469111000
C	-3.935519000	-0.306160000	1.812531000
C	-3.656390000	-0.438388000	3.178437000
C	-2.377439000	-0.153274000	3.659871000
C	-1.365827000	0.261325000	2.782257000
O	1.316970000	-1.769743000	-0.415099000
C	2.153267000	-2.376100000	0.449405000
O	1.807122000	-2.841419000	1.508628000
C	3.566033000	-2.359226000	-0.052755000
C	4.100308000	-3.338453000	-0.783444000
C	0.733346000	1.101189000	0.859685000
O	1.613658000	1.376238000	-0.213402000
C	2.944878000	1.522728000	0.023859000
C	3.528625000	1.506852000	1.300248000
C	4.915276000	1.666984000	1.427318000
C	5.723333000	1.844788000	0.304202000
C	5.131789000	1.863622000	-0.966818000
C	3.756309000	1.704162000	-1.110386000
H	-2.060337000	-0.151605000	-2.359925000
H	0.049970000	-0.134670000	-1.524538000
H	-0.167753000	-1.648955000	1.027142000
H	-3.620830000	-2.093645000	-1.605710000
H	-0.461481000	-3.828753000	0.108574000
H	-1.448688000	-2.142443000	-3.407977000
H	-2.335552000	-3.635546000	-2.957144000
H	-4.118005000	0.174768000	-0.890611000
H	0.291584000	3.469623000	-0.322128000
H	-1.031267000	5.245122000	-1.431502000
H	-3.365895000	4.799760000	-2.177505000
H	-4.387036000	2.550966000	-1.797085000
H	-4.936473000	-0.526614000	1.431132000
H	-4.440646000	-0.763410000	3.866680000
H	-2.158840000	-0.253806000	4.725895000
H	-0.372648000	0.472965000	3.183400000
H	4.155932000	-1.485082000	0.246597000
H	5.145851000	-3.299301000	-1.100600000
H	3.517650000	-4.211338000	-1.093071000
H	1.102473000	0.238539000	1.439440000
H	0.688233000	1.963722000	1.550040000
H	2.921146000	1.376350000	2.195905000
H	5.360686000	1.653590000	2.425606000
H	6.802891000	1.969820000	0.413845000
H	5.751172000	2.002222000	-1.856893000
H	3.279854000	1.711128000	-2.092671000

cyclopentadiene, E = -193.871517

C	-1.180915000	-0.284454000	0.000000000
C	-0.735340000	0.992912000	-0.000001000
C	0.734470000	0.993554000	-0.000001000
C	1.181162000	-0.283420000	0.000000000

C	0.000532000	-1.216164000	0.000001000
H	-2.220830000	-0.613847000	0.000001000
H	-1.355071000	1.891752000	-0.000002000
H	1.353413000	1.892938000	-0.000002000
H	2.221365000	-0.611900000	0.000000000
H	0.000831000	-1.886754000	-0.881317000
H	0.000831000	-1.886752000	0.881320000

TS 6-s-cis→S-adduct, E = -1727.176826

C	-2.014740000	-1.458614000	-1.308247000
C	-0.984014000	-0.485641000	-0.635741000
C	0.151777000	-1.185771000	0.152219000
C	-1.512303000	-2.905103000	-1.391990000
O	-0.904150000	-3.306989000	-0.166908000
C	0.344216000	-2.665979000	-0.228318000
C	-0.334744000	-3.069308000	-2.375093000
O	0.805459000	-2.813947000	-1.563570000
C	-1.776710000	0.542966000	0.286376000
C	-2.410232000	-0.309319000	1.392358000
C	-3.249107000	-1.326501000	0.894663000
C	-3.407057000	-1.293815000	-0.610576000
C	-3.845707000	0.109464000	-0.978149000
C	-2.950543000	1.101229000	-0.533519000
C	-3.209914000	2.441394000	-0.832279000
C	-4.358574000	2.784298000	-1.558934000
C	-5.243553000	1.796137000	-1.995246000
C	-4.983602000	0.450058000	-1.707763000
C	-3.875606000	-2.214658000	1.766862000
C	-3.676413000	-2.090611000	3.147514000
C	-2.851695000	-1.080443000	3.645865000
C	-2.213265000	-0.190763000	2.770369000
O	1.345989000	-0.430130000	-0.083755000
C	2.417682000	-0.659520000	0.725550000
O	2.385298000	-1.456967000	1.645980000
C	3.577510000	0.136853000	0.336865000
C	4.747077000	0.067406000	1.101633000
C	-0.853197000	1.625339000	0.843023000
O	-0.246289000	2.316933000	-0.232352000
C	0.708088000	3.252837000	0.014854000
C	1.110254000	3.656920000	1.297063000
C	2.100032000	4.638949000	1.432946000
C	2.691357000	5.223358000	0.312883000
C	2.283022000	4.816323000	-0.964776000
C	1.301228000	3.840729000	-1.116976000
C	5.993784000	-1.241087000	0.129941000
C	5.636695000	-0.758362000	-1.264036000
C	5.341759000	-2.482334000	0.288447000
C	4.300093000	-2.577272000	-0.653181000
C	4.314536000	-1.443469000	-1.457670000
H	-2.166080000	-1.125163000	-2.346637000
H	-0.491715000	0.101146000	-1.421303000
H	-0.057166000	-1.194359000	1.232766000
H	-2.340502000	-3.596821000	-1.605905000
H	1.045286000	-3.152554000	0.461016000
H	-0.375411000	-2.359990000	-3.217879000
H	-0.286903000	-4.096597000	-2.777792000
H	-4.116123000	-2.054191000	-0.969676000
H	-2.521298000	3.225184000	-0.516409000
H	-4.558452000	3.834854000	-1.785202000
H	-6.138145000	2.071064000	-2.560009000
H	-5.671115000	-0.330020000	-2.047455000
H	-4.522331000	-3.003438000	1.372498000
H	-4.168755000	-2.783937000	3.834073000
H	-2.698253000	-0.980960000	4.723352000
H	-1.566750000	0.586674000	3.182668000
H	3.425599000	0.901557000	-0.424601000
H	5.445494000	0.906754000	1.058757000
H	4.683485000	-0.434513000	2.068864000

H	-0.078236000	1.173777000	1.483892000
H	-1.435591000	2.326961000	1.468737000
H	0.663861000	3.219522000	2.190017000
H	2.406710000	4.946250000	2.436362000
H	3.461448000	5.989225000	0.429916000
H	2.735251000	5.265368000	-1.853190000
H	0.970777000	3.511925000	-2.104397000
H	6.962752000	-1.024916000	0.588432000
H	5.647483000	0.328379000	-1.420767000
H	6.364687000	-1.203808000	-1.972870000
H	5.522895000	-3.189037000	1.100071000
H	3.535871000	-3.354223000	-0.686793000
H	3.621967000	-1.249442000	-2.277301000

TS 6-s-cis→R-adduct, E = -1727.176826

C	-2.676527000	-0.905352000	-1.293248000
C	-1.258728000	-0.416211000	-0.823339000
C	-0.290596000	-1.553887000	-0.401620000
C	-2.726942000	-2.400435000	-1.626855000
O	-2.048238000	-3.163337000	-0.632356000
C	-0.698867000	-2.935497000	-0.953924000
C	-1.910584000	-2.756650000	-2.883437000
O	-0.606574000	-2.980667000	-2.367618000
C	-1.458810000	0.648491000	0.345673000
C	-2.080928000	-0.138971000	1.504986000
C	-3.291834000	-0.769497000	1.156324000
C	-3.752600000	-0.451481000	-0.250219000
C	-3.780897000	1.057222000	-0.373871000
C	-2.536573000	1.653836000	-0.096847000
C	-2.407870000	3.041775000	-0.200119000
C	-3.513064000	3.820536000	-0.570065000
C	-4.743774000	3.221145000	-0.845040000
C	-4.878071000	1.830281000	-0.750218000
C	-3.970921000	-1.556325000	2.084647000
C	-3.450203000	-1.715103000	3.374992000
C	-2.254525000	-1.086507000	3.727438000
C	-1.564916000	-0.301069000	2.793055000
O	1.022667000	-1.196104000	-0.862392000
C	2.072829000	-1.934983000	-0.406853000
O	1.950482000	-2.787208000	0.455094000
C	4.391000000	-2.507030000	-1.018688000
C	3.325513000	-1.600829000	-1.083264000
C	-0.148182000	1.325609000	0.740007000
O	0.400323000	1.972207000	-0.394117000
C	1.493537000	2.766923000	-0.263254000
C	2.116859000	3.066471000	0.958675000
C	3.233451000	3.913482000	0.976847000
C	3.738849000	4.460693000	-0.202257000
C	3.112881000	4.155282000	-1.419154000
C	2.001511000	3.317723000	-1.454306000
H	-2.925248000	-0.372602000	-2.224105000
H	-0.773332000	0.104550000	-1.658341000
H	-0.262740000	-1.672264000	0.691802000
H	-3.766833000	-2.755060000	-1.681896000
H	-0.076930000	-3.726342000	-0.516590000
H	-1.895821000	-1.948022000	-3.632614000
H	-2.291798000	-3.676359000	-3.362643000
H	-4.729940000	-0.901798000	-0.477873000
H	-1.454350000	3.531799000	-0.004385000
H	-3.405269000	4.905752000	-0.643851000
H	-5.601564000	3.834879000	-1.131973000
H	-5.838305000	1.351673000	-0.963201000
H	-4.908629000	-2.044503000	1.805067000
H	-3.981665000	-2.329672000	4.105924000
H	-1.849449000	-1.207178000	4.735332000
H	-0.628156000	0.175661000	3.089565000
H	5.123007000	-2.500914000	-1.830074000
H	4.189950000	-3.488020000	-0.584708000

H	3.293291000	-0.802858000	-1.825239000
H	0.572749000	0.587796000	1.131236000
H	-0.349417000	2.058148000	1.541970000
H	1.746247000	2.650121000	1.895268000
H	3.710078000	4.140760000	1.934124000
H	4.610092000	5.119056000	-0.178056000
H	3.496313000	4.576203000	-2.352470000
H	1.501620000	3.070738000	-2.393014000
C	4.249154000	-0.015634000	0.634625000
C	5.559555000	-0.345149000	-0.019979000
C	4.078743000	-0.884745000	1.705739000
C	4.992272000	-1.948838000	1.583999000
C	5.714666000	-1.797878000	0.383970000
H	3.706655000	0.916772000	0.478150000
H	5.630128000	-0.126711000	-1.093698000
H	6.354164000	0.238208000	0.488871000
H	3.294008000	-0.819791000	2.460449000
H	5.030051000	-2.822232000	2.237057000
H	6.619385000	-2.371307000	0.164508000

TS 6-s-trans→R-adduct, E = -1727.174901

C	-2.063009000	-1.305453000	-1.294205000
C	-0.898783000	-0.540340000	-0.565097000
C	-0.031352000	-1.426276000	0.363982000
C	-1.912383000	-2.832154000	-1.250532000
O	-1.509767000	-3.272884000	0.044815000
C	-0.147630000	-2.930453000	0.065509000
C	-0.738927000	-3.337987000	-2.110204000
O	0.365927000	-3.264497000	-1.217971000
C	-1.522124000	0.692068000	0.232664000
C	-2.429425000	0.065774000	1.299504000
C	-3.431175000	-0.763515000	0.757347000
C	-3.438267000	-0.786899000	-0.755874000
C	-3.511172000	0.652266000	-1.221113000
C	-2.461753000	1.446860000	-0.722414000
C	-2.391550000	2.793958000	-1.088864000
C	-3.363214000	3.337658000	-1.940306000
C	-4.399604000	2.542572000	-2.433823000
C	-4.472422000	1.190735000	-2.075291000
C	-4.322891000	-1.433569000	1.592720000
C	-4.225866000	-1.277662000	2.981031000
C	-3.236558000	-0.455398000	3.523202000
C	-2.334060000	0.214524000	2.685350000
O	1.328826000	-0.987525000	0.251174000
C	2.159683000	-1.248594000	1.305817000
O	1.778787000	-1.844176000	2.295303000
C	3.877535000	0.167206000	0.093731000
C	3.512005000	-0.724229000	1.110512000
C	-0.444330000	1.584140000	0.846207000
O	0.385639000	2.096369000	-0.180774000
C	1.362483000	2.992365000	0.125650000
C	1.700113000	3.382421000	1.430458000
C	2.729532000	4.311571000	1.628415000
C	3.424474000	4.855888000	0.548110000
C	3.080517000	4.462613000	-0.752503000
C	2.059233000	3.540419000	-0.966336000
C	4.488082000	-2.746965000	0.074836000
C	5.619011000	-1.816825000	-0.261705000
C	3.632021000	-2.794325000	-1.021658000
C	3.934457000	-1.718281000	-1.876687000
C	4.943960000	-0.929766000	-1.289471000
H	-2.038062000	-1.024448000	-2.358481000
H	-0.222204000	-0.126605000	-1.323711000
H	-0.342731000	-1.323199000	1.413312000
H	-2.862470000	-3.327255000	-1.499600000
H	0.371521000	-3.517175000	0.835606000
H	-0.555213000	-2.715831000	-3.001139000
H	-0.896236000	-4.382908000	-2.431648000

H	-4.265367000	-1.390780000	-1.157118000
H	-1.582917000	3.428991000	-0.727827000
H	-3.304447000	4.393081000	-2.218532000
H	-5.154541000	2.973514000	-3.096532000
H	-5.282125000	0.561244000	-2.455706000
H	-5.097050000	-2.075798000	1.163524000
H	-4.925275000	-1.799669000	3.638875000
H	-3.159905000	-0.332687000	4.606431000
H	-1.564291000	0.845559000	3.133890000
H	4.702594000	0.856497000	0.290178000
H	3.094430000	0.573280000	-0.546192000
H	4.147605000	-0.866295000	1.985489000
H	0.160014000	1.015574000	1.572396000
H	-0.924508000	2.416375000	1.392941000
H	1.179397000	2.968044000	2.293454000
H	2.986196000	4.607814000	2.649033000
H	4.224874000	5.580561000	0.713719000
H	3.612848000	4.882245000	-1.610348000
H	1.775321000	3.226223000	-1.972930000
H	4.507169000	-3.466418000	0.895048000
H	6.095705000	-1.306250000	0.585301000
H	6.404764000	-2.400995000	-0.783165000
H	2.781964000	-3.465041000	-1.147497000
H	3.369081000	-1.453163000	-2.771851000
H	5.488880000	-0.158858000	-1.841054000

TS 6-s-trans→S-adduct, E = -1727.171646

C	-2.287437000	-1.061839000	-1.262134000
C	-0.988926000	-0.578301000	-0.508848000
C	-0.390429000	-1.618155000	0.484889000
C	-2.578517000	-2.558161000	-1.089573000
O	-2.379020000	-2.956420000	0.266324000
C	-0.981912000	-3.035405000	0.342981000
C	-1.569014000	-3.464811000	-1.821013000
O	-0.552040000	-3.668188000	-0.849990000
C	-1.312059000	0.812638000	0.209764000
C	-2.405627000	0.486496000	1.237647000
C	-3.566195000	-0.064738000	0.661131000
C	-3.497932000	-0.161128000	-0.847303000
C	-3.162261000	1.217806000	-1.369902000
C	-1.971071000	1.735488000	-0.829158000
C	-1.534500000	3.001128000	-1.233027000
C	-2.282768000	3.734740000	-2.163662000
C	-3.461086000	3.211104000	-2.699913000
C	-3.902741000	1.943290000	-2.302424000
C	-4.646607000	-0.435867000	1.459176000
C	-4.578568000	-0.257741000	2.846317000
C	-3.429130000	0.284815000	3.423957000
C	-2.338961000	0.654150000	2.623580000
O	1.019700000	-1.766613000	0.284214000
C	1.889578000	-1.555094000	1.312183000
O	1.588937000	-0.926670000	2.311417000
C	3.188324000	-2.187475000	1.079763000
C	3.364894000	-3.271476000	0.207621000
C	-0.087956000	1.434310000	0.879664000
O	0.911505000	1.718194000	-0.096215000
C	2.012050000	2.429633000	0.282944000
C	2.477018000	2.507581000	1.604975000
C	3.631919000	3.247085000	1.886177000
C	4.328462000	3.907832000	0.871765000
C	3.859042000	3.824239000	-0.445017000
C	2.708192000	3.095116000	-0.740690000
H	-2.140177000	-0.890122000	-2.339762000
H	-0.209063000	-0.383635000	-1.255888000
H	-0.568487000	-1.301559000	1.521575000
H	-3.619965000	-2.784865000	-1.360716000
H	-0.693839000	-3.660394000	1.202448000
H	-1.152090000	-2.997035000	-2.728394000

H	-2.021459000	-4.433278000	-2.098703000
H	-4.432252000	-0.548305000	-1.279944000
H	-0.612088000	3.425074000	-0.837971000
H	-1.936914000	4.725615000	-2.469401000
H	-4.039789000	3.789740000	-3.424561000
H	-4.827028000	1.525993000	-2.712477000
H	-5.543609000	-0.862551000	1.001555000
H	-5.425117000	-0.544071000	3.475585000
H	-3.374199000	0.423389000	4.506693000
H	-1.448357000	1.068207000	3.099449000
H	3.911729000	-1.981955000	1.869934000
H	4.137557000	-4.004410000	0.454432000
H	2.483882000	-3.681426000	-0.289006000
H	0.314353000	0.753895000	1.643855000
H	-0.384461000	2.375590000	1.377086000
H	1.968962000	1.970806000	2.405636000
H	3.989541000	3.298485000	2.918082000
H	5.227605000	4.483696000	1.102783000
H	4.390999000	4.337695000	-1.250422000
H	2.325978000	3.028110000	-1.761533000
C	4.398448000	-2.559108000	-1.431164000
C	5.250228000	-1.589091000	-0.637069000
C	3.414730000	-1.779414000	-2.069195000
C	3.304638000	-0.544174000	-1.404582000
C	4.257176000	-0.489083000	-0.392592000
H	4.809409000	-3.470896000	-1.872781000
H	5.754814000	-1.994543000	0.249814000
H	6.036442000	-1.197104000	-1.314421000
H	2.742860000	-2.135151000	-2.852249000
H	2.527832000	0.199982000	-1.575161000
H	4.428283000	0.364263000	0.264850000

R-adduct, E = -1727.227884

C	-2.380311000	-1.206176000	-1.332923000
C	-1.138443000	-0.464512000	-0.715791000
C	-0.096677000	-1.391827000	-0.041117000
C	-2.192711000	-2.726688000	-1.435336000
O	-1.580764000	-3.248131000	-0.254928000
C	-0.239215000	-2.872971000	-0.428705000
C	-1.159161000	-3.131738000	-2.503603000
O	0.071216000	-3.098274000	-1.791077000
C	-1.658160000	0.649337000	0.298061000
C	-2.391600000	-0.114002000	1.408391000
C	-3.452388000	-0.907509000	0.929228000
C	-3.673396000	-0.777004000	-0.561853000
C	-3.828779000	0.699410000	-0.863618000
C	-2.731306000	1.468963000	-0.434076000
C	-2.722235000	2.845191000	-0.675885000
C	-3.806723000	3.444807000	-1.330779000
C	-4.893792000	2.676290000	-1.752811000
C	-4.903393000	1.294678000	-1.522706000
C	-4.206605000	-1.685002000	1.805996000
C	-3.910401000	-1.674282000	3.174633000
C	-2.860498000	-0.889411000	3.654896000
C	-2.096343000	-0.111168000	2.774107000
O	1.220935000	-0.957654000	-0.417467000
C	2.176938000	-0.835797000	0.527447000
O	1.971681000	-0.987246000	1.710379000
C	3.897310000	-1.127817000	-1.422830000
C	3.501740000	-0.429902000	-0.080555000
C	-0.514001000	1.499731000	0.849077000
O	0.191296000	2.090445000	-0.229722000
C	1.301617000	2.837720000	0.013668000
C	1.824847000	3.087348000	1.291770000
C	2.980413000	3.868523000	1.423568000
C	3.617702000	4.404288000	0.304090000
C	3.087685000	4.152606000	-0.968907000
C	1.940453000	3.377068000	-1.117616000

C	4.731305000	-0.715711000	0.848080000
C	5.874230000	-0.581690000	-0.183328000
C	4.755400000	-2.219953000	1.089160000
C	5.105715000	-2.804774000	-0.068125000
C	5.316713000	-1.700645000	-1.094589000
H	-2.515422000	-0.840250000	-2.362383000
H	-0.607855000	0.057941000	-1.521580000
H	-0.179620000	-1.352172000	1.053037000
H	-3.159815000	-3.233194000	-1.568189000
H	0.406473000	-3.504676000	0.201077000
H	-1.125393000	-2.438473000	-3.359558000
H	-1.348746000	-4.152545000	-2.880434000
H	-4.540639000	-1.359826000	-0.905497000
H	-1.873861000	3.458479000	-0.371596000
H	-3.796634000	4.522563000	-1.512663000
H	-5.736591000	3.150928000	-2.261901000
H	-5.750286000	0.685635000	-1.851904000
H	-5.028472000	-2.297758000	1.425089000
H	-4.501929000	-2.280100000	3.865677000
H	-2.628513000	-0.879683000	4.722816000
H	-1.275915000	0.488025000	3.173445000
H	3.947317000	-0.397833000	-2.245016000
H	3.182445000	-1.907324000	-1.718399000
H	3.416176000	0.658858000	-0.243637000
H	0.168307000	0.880218000	1.453576000
H	-0.922629000	2.284919000	1.511618000
H	1.349839000	2.679156000	2.183535000
H	3.381061000	4.056070000	2.423282000
H	4.517404000	5.013054000	0.418216000
H	3.573986000	4.566501000	-1.856272000
H	1.514054000	3.170817000	-2.101444000
H	4.767363000	-0.078506000	1.740285000
H	5.914734000	0.405953000	-0.671975000
H	6.859516000	-0.824234000	0.241578000
H	4.429586000	-2.705926000	2.009653000
H	5.126970000	-3.874546000	-0.287925000
H	5.906596000	-1.969479000	-1.982090000

S-adduct, E = -1727.229511

C	-2.204256000	-1.289099000	-1.299924000
C	-1.050865000	-0.459601000	-0.628993000
C	-0.035035000	-1.298037000	0.182883000
C	-1.934153000	-2.800451000	-1.316353000
O	-1.395072000	-3.240578000	-0.069673000
C	-0.064626000	-2.799921000	-0.148364000
C	-0.797220000	-3.191113000	-2.280057000
O	0.367846000	-3.055892000	-1.474888000
C	-1.697305000	0.685214000	0.270193000
C	-2.481127000	-0.046489000	1.366904000
C	-3.461251000	-0.921023000	0.857287000
C	-3.571401000	-0.886521000	-0.651637000
C	-3.770886000	0.562144000	-1.050029000
C	-2.745599000	1.408411000	-0.587273000
C	-2.781302000	2.768201000	-0.906541000
C	-3.839165000	3.276106000	-1.673068000
C	-4.854625000	2.432171000	-2.127930000
C	-4.818562000	1.066341000	-1.819221000
C	-4.245301000	-1.684458000	1.720242000
C	-4.060472000	-1.578455000	3.104334000
C	-3.092084000	-0.711989000	3.614547000
C	-2.298115000	0.052764000	2.748482000
O	1.274708000	-0.765925000	-0.081679000
C	2.244965000	-0.962787000	0.839885000
O	2.045676000	-1.506138000	1.900478000
C	3.566877000	-0.398809000	0.359971000
C	4.799830000	-0.890825000	1.169993000
C	-0.632052000	1.615413000	0.847455000
O	0.116849000	2.185556000	-0.209739000

C	1.229922000	2.916413000	0.066799000
C	1.658079000	3.248821000	1.361386000
C	2.824052000	4.007655000	1.529668000
C	3.564255000	4.440575000	0.429368000
C	3.127108000	4.109335000	-0.860831000
C	1.971483000	3.354581000	-1.045124000
C	5.705482000	-1.527347000	0.061464000
C	5.451610000	-0.543218000	-1.103730000
C	4.964383000	-2.753639000	-0.452803000
C	3.906365000	-2.324188000	-1.161253000
C	3.929892000	-0.801628000	-1.121825000
H	-2.275746000	-0.978110000	-2.353484000
H	-0.474980000	0.040106000	-1.417743000
H	-0.230604000	-1.230575000	1.262454000
H	-2.860095000	-3.363390000	-1.504367000
H	0.557833000	-3.367637000	0.557765000
H	-0.730845000	-2.534624000	-3.162593000
H	-0.900486000	-4.236491000	-2.621004000
H	-4.382242000	-1.530237000	-1.023250000
H	-1.987491000	3.438614000	-0.576277000
H	-3.864923000	4.341490000	-1.916019000
H	-5.677433000	2.835594000	-2.723718000
H	-5.609838000	0.399038000	-2.172844000
H	-5.004023000	-2.360292000	1.315944000
H	-4.675396000	-2.173492000	3.784181000
H	-2.948061000	-0.627343000	4.694562000
H	-1.544683000	0.719522000	3.172579000
H	3.466507000	0.698934000	0.412650000
H	5.316431000	-0.048986000	1.656104000
H	4.512689000	-1.606755000	1.951504000
H	0.035617000	1.054917000	1.522805000
H	-1.114682000	2.409622000	1.446629000
H	1.096152000	2.929969000	2.239222000
H	3.149321000	4.261239000	2.542126000
H	4.471232000	5.032505000	0.571104000
H	3.694574000	4.443009000	-1.733642000
H	1.617655000	3.086078000	-2.042524000
H	6.748125000	-1.684596000	0.371218000
H	5.720036000	0.499730000	-0.867182000
H	5.942098000	-0.848135000	-2.040399000
H	5.200411000	-3.784881000	-0.180719000
H	3.090390000	-2.916759000	-1.579339000
H	3.328989000	-0.281550000	-1.877172000

[6-Al-*s-cis*]$^{+}$, E **=** -1855.274718

C	3.120924000	-2.657262000	1.103008000
C	2.184573000	-2.665472000	0.056832000
C	2.411345000	-3.451876000	-1.081255000
C	3.581341000	-4.220029000	-1.163871000
C	4.518608000	-4.210598000	-0.130827000
C	4.279317000	-3.425481000	1.005216000
O	1.086810000	-1.861417000	0.228043000
C	0.023175000	-1.927426000	-0.703881000
C	-1.142811000	-1.077959000	-0.195334000
C	-0.684062000	0.396510000	0.206156000
C	-1.906256000	1.135664000	0.879392000
C	-3.205499000	0.292653000	0.648837000
C	-3.319631000	-0.110609000	-0.805388000
C	-2.236888000	-0.892695000	-1.255340000
C	-0.132654000	1.170036000	-1.012862000
C	-0.347730000	2.685951000	-0.922690000
O	-1.707998000	2.892081000	-0.860179000
C	-2.037930000	2.624393000	0.516515000
C	-2.971437000	-0.970615000	1.454554000
C	-1.833313000	-1.684043000	1.038559000
O	0.161029000	3.268257000	0.338732000
C	-0.990411000	3.496047000	1.208304000
C	-4.385493000	0.179990000	-1.655609000

C	-4.382826000	-0.316746000	-2.965297000
C	-3.317530000	-1.099784000	-3.413508000
C	-2.240078000	-1.387023000	-2.562921000
C	-1.462099000	-2.845511000	1.720314000
C	-2.237213000	-3.294183000	2.798188000
C	-3.371071000	-2.585398000	3.201287000
C	-3.738789000	-1.411871000	2.531089000
O	1.202483000	0.735046000	-1.401023000
C	2.348407000	1.037498000	-0.843982000
C	3.474940000	0.262227000	-1.364401000
C	4.727361000	0.461713000	-0.926398000
Al	2.038714000	3.569324000	0.793386000
C	2.156887000	3.451987000	2.734373000
O	2.479200000	1.919294000	0.028417000
C	2.716486000	4.961402000	-0.391715000
H	-1.737302000	1.114781000	1.965979000
H	0.122412000	0.298724000	0.945498000
H	-0.712225000	0.897832000	-1.905605000
H	-3.058967000	2.990915000	0.683695000
H	0.097048000	3.240475000	-1.762179000
H	-0.724753000	3.184753000	2.225044000
H	-1.248410000	4.564203000	1.180610000
H	-4.089138000	0.845067000	0.998809000
H	-0.574371000	-3.408507000	1.431077000
H	-1.949544000	-4.207552000	3.324016000
H	-3.972540000	-2.945708000	4.039072000
H	-4.624246000	-0.852156000	2.844543000
H	-5.226263000	0.780544000	-1.298015000
H	-5.220066000	-0.098977000	-3.632301000
H	-3.322644000	-1.497989000	-4.430795000
H	-1.423443000	-2.008070000	-2.936342000
H	3.234303000	-0.494291000	-2.112495000
H	5.556773000	-0.132771000	-1.316247000
H	4.953483000	1.213334000	-0.165526000
H	0.364416000	-1.570297000	-1.689695000
H	-0.316813000	-2.969560000	-0.832510000
H	1.692532000	-3.483950000	-1.900319000
H	3.750201000	-4.836174000	-2.050546000
H	5.423989000	-4.816892000	-0.202044000
H	4.998863000	-3.419545000	1.827797000
H	2.915205000	-2.049094000	1.986434000
H	3.812872000	5.055621000	-0.304231000
H	2.298623000	5.948268000	-0.126265000
H	2.496014000	4.794077000	-1.460043000
H	1.688017000	4.314698000	3.238892000
H	3.215219000	3.456207000	3.049319000
H	1.707443000	2.535791000	3.154360000

[6-Al-*s*-*trans*]$^{+}$, E = -1855.273160

C	3.712593000	-1.702793000	1.213298000
C	2.826947000	-1.981606000	0.160381000
C	3.254034000	-2.751779000	-0.930202000
C	4.569756000	-3.237410000	-0.955652000
C	5.455273000	-2.960211000	0.085488000
C	5.017343000	-2.190028000	1.171518000
O	1.570746000	-1.443715000	0.275445000
C	0.571853000	-1.794685000	-0.664185000
C	-0.783607000	-1.278881000	-0.178796000
C	-0.738554000	0.267543000	0.208589000
C	-2.125275000	0.661324000	0.858562000
C	-3.147720000	-0.501491000	0.627578000
C	-3.131309000	-0.934266000	-0.822570000
C	-1.873431000	-1.402927000	-1.252230000
C	-0.395621000	1.151328000	-1.011047000
C	-1.005947000	2.557283000	-0.935448000
O	-2.373123000	2.392728000	-0.901220000
C	-2.647849000	2.056097000	0.472450000
C	-2.594278000	-1.647641000	1.452081000

C	-1.301880000	-2.035171000	1.056258000
O	-0.696784000	3.259771000	0.329450000
C	-1.888804000	3.181946000	1.171394000
C	-4.225329000	-0.947508000	-1.686522000
C	-4.074145000	-1.439419000	-2.989272000
C	-2.833194000	-1.914688000	-3.417098000
C	-1.728798000	-1.894573000	-2.552839000
C	-0.641994000	-3.047544000	1.757507000
C	-1.282121000	-3.674440000	2.835066000
C	-2.569009000	-3.290357000	3.218172000
C	-3.229212000	-2.266195000	2.527805000
O	1.010914000	1.095471000	-1.391176000
C	2.022749000	1.640236000	-0.761592000
C	3.358139000	1.270091000	-1.224990000
C	3.588393000	0.462152000	-2.272062000
Al	1.045654000	3.987350000	0.856407000
C	1.080739000	3.951201000	2.802478000
O	1.882322000	2.458944000	0.170142000
C	1.447197000	5.456222000	-0.361440000
H	3.353905000	-1.111403000	2.058441000
H	2.580849000	-2.991463000	-1.753746000
H	4.895062000	-3.845459000	-1.803560000
H	6.476316000	-3.346322000	0.059153000
H	5.697960000	-1.973870000	1.998779000
H	0.818610000	-1.368047000	-1.651098000
H	0.516991000	-2.890028000	-0.784513000
H	0.051577000	0.392968000	0.960836000
H	-1.971160000	0.699127000	1.946745000
H	-4.151501000	-0.202602000	0.961642000
H	-0.873331000	0.731425000	-1.906538000
H	-0.706560000	3.206429000	-1.771563000
H	-3.733255000	2.134579000	0.616545000
H	-1.576357000	2.962353000	2.198664000
H	-2.420344000	4.142781000	1.120704000
H	-5.200136000	-0.589021000	-1.344864000
H	-4.930821000	-1.460074000	-3.666792000
H	-2.719472000	-2.311088000	-4.428780000
H	-0.771921000	-2.279955000	-2.910628000
H	0.367128000	-3.358120000	1.484841000
H	-0.767254000	-4.471341000	3.376739000
H	-3.062333000	-3.788722000	4.055916000
H	-4.236270000	-1.960711000	2.824742000
H	4.171666000	1.715147000	-0.648751000
H	4.609793000	0.222693000	-2.576636000
H	2.773045000	0.028183000	-2.854749000
H	0.390288000	4.685020000	3.253403000
H	2.088492000	4.219171000	3.165320000
H	0.844470000	2.962465000	3.231994000
H	2.487633000	5.801454000	-0.231431000
H	0.802011000	6.329639000	-0.162249000
H	1.327189000	5.202789000	-1.429039000

TS [6-Al-*s*-*cis*]$^{+}$→ [6-Al-*s*-*trans*]$^{+}$, E **=** -1855.262108

C	-2.963999000	-2.799177000	-1.221604000
C	-2.053588000	-2.784503000	-0.151664000
C	-2.270705000	-3.603275000	0.965158000
C	-3.401507000	-4.430514000	1.000418000
C	-4.312124000	-4.446348000	-0.056473000
C	-4.085739000	-3.625538000	-1.169172000
O	-0.993829000	-1.923801000	-0.280599000
C	0.030257000	-1.923179000	0.697698000
C	1.173606000	-1.026903000	0.218748000
C	0.661225000	0.415862000	-0.229994000
C	1.870548000	1.197906000	-0.877914000
C	3.199524000	0.425097000	-0.578901000
C	3.277037000	0.056450000	0.887166000
C	2.216147000	-0.767704000	1.314028000
C	0.036532000	1.189215000	0.951061000

C	0.172642000	2.712094000	0.826605000
O	1.521595000	2.987495000	0.803943000
C	1.912735000	2.700572000	-0.553142000
C	3.056157000	-0.863706000	-1.365339000
C	1.938322000	-1.622650000	-0.975918000
O	-0.321836000	3.233905000	-0.465181000
C	0.844503000	3.494933000	-1.305169000
C	4.295939000	0.413218000	1.769266000
C	4.267841000	-0.058517000	3.087940000
C	3.223938000	-0.881964000	3.513686000
C	2.192891000	-1.235543000	2.631051000
C	1.648896000	-2.813972000	-1.646047000
C	2.483344000	-3.244787000	-2.686207000
C	3.595915000	-2.489668000	-3.063506000
C	3.882760000	-1.287666000	-2.404468000
O	-1.292454000	0.687594000	1.309734000
C	-2.435392000	0.956969000	0.746050000
C	-3.578048000	0.141206000	1.235215000
C	-4.346690000	0.510493000	2.260971000
Al	-2.202417000	3.459938000	-0.970671000
C	-2.274274000	3.248011000	-2.903852000
O	-2.585490000	1.823921000	-0.128477000
C	-2.948901000	4.861555000	0.157801000
H	-2.766052000	-2.165076000	-2.088638000
H	-1.577218000	-3.609872000	1.806117000
H	-3.563460000	-5.070045000	1.871632000
H	-5.188533000	-5.096600000	-0.019833000
H	-4.785392000	-3.635212000	-2.008588000
H	-0.372891000	-1.567721000	1.660443000
H	0.416297000	-2.944286000	0.858760000
H	-0.114338000	0.265825000	-0.993527000
H	1.743020000	1.141111000	-1.968832000
H	4.068245000	1.013342000	-0.907448000
H	0.597101000	0.967421000	1.869265000
H	-0.328012000	3.263672000	1.636169000
H	2.918288000	3.116451000	-0.697222000
H	0.628653000	3.137580000	-2.318800000
H	1.045806000	4.575605000	-1.305071000
H	5.120284000	1.046343000	1.430051000
H	5.068992000	0.210748000	3.780036000
H	3.209872000	-1.260012000	4.538581000
H	1.391918000	-1.886271000	2.987481000
H	0.780167000	-3.415940000	-1.377677000
H	2.259016000	-4.180902000	-3.202829000
H	4.244027000	-2.835963000	-3.871934000
H	4.751593000	-0.691861000	-2.697318000
H	-3.751581000	-0.786490000	0.676050000
H	-5.187334000	-0.112892000	2.574861000
H	-4.174184000	1.433007000	2.823294000
H	-1.820435000	4.100311000	-3.438884000
H	-3.325293000	3.203160000	-3.238940000
H	-1.786740000	2.327723000	-3.268688000
H	-4.049269000	4.886455000	0.073378000
H	-2.589981000	5.859132000	-0.150000000
H	-2.713765000	4.751357000	1.230517000

TS [6-Al-*s-cis*]$^{+}$→ [Al-R-aAdduct]$^{+}$, E = -2049.135396

C	1.240175000	3.622005000	-1.589793000
C	0.604661000	3.282694000	-0.383653000
C	0.833194000	4.052023000	0.766488000
C	1.700549000	5.151469000	0.699213000
C	2.339016000	5.488735000	-0.494512000
C	2.100435000	4.716839000	-1.640178000
O	-0.207240000	2.183355000	-0.422545000
C	-1.010165000	1.868656000	0.700372000
C	-1.972158000	0.739342000	0.330024000
C	-1.218007000	-0.534473000	-0.269999000
C	-2.308229000	-1.563423000	-0.772506000

C	-3.717000000	-1.119508000	-0.254685000
C	-3.655538000	-0.813540000	1.225954000
C	-2.751710000	0.219573000	1.545211000
C	-0.240295000	-1.155602000	0.758231000
C	-0.082238000	-2.672193000	0.595965000
O	-1.328703000	-3.236113000	0.771563000
C	-1.978569000	-3.040748000	-0.497547000
C	-3.987111000	0.184087000	-0.978549000
C	-3.025496000	1.172430000	-0.704973000
O	0.298276000	-3.077038000	-0.775472000
C	-0.899043000	-3.586824000	-1.430754000
C	-4.423969000	-1.415835000	2.220928000
C	-4.301530000	-0.984817000	3.548042000
C	-3.413567000	0.043403000	3.869270000
C	-2.633457000	0.645535000	2.871332000
C	-3.123002000	2.416825000	-1.333508000
C	-4.180773000	2.667092000	-2.217945000
C	-5.134144000	1.681508000	-2.482521000
C	-5.035675000	0.429088000	-1.863725000
O	0.973899000	-0.397479000	0.932225000
C	2.038713000	-0.343614000	0.129887000
C	2.886973000	0.770775000	0.328507000
Al	2.068147000	-2.858704000	-1.570407000
C	1.771339000	-2.626572000	-3.486342000
O	2.267412000	-1.242319000	-0.733922000
C	3.221362000	-4.209885000	-0.748800000
C	4.007075000	1.009518000	-0.484902000
H	1.036470000	3.017085000	-2.475764000
H	0.343462000	3.815132000	1.711288000
H	1.867606000	5.751444000	1.597467000
H	3.006970000	6.351565000	-0.539015000
H	2.582102000	4.977992000	-2.586001000
H	-0.370433000	1.573868000	1.548270000
H	-1.595980000	2.749709000	1.015821000
H	-0.632182000	-0.188344000	-1.132786000
H	-2.360107000	-1.472906000	-1.867492000
H	-4.471201000	-1.883646000	-0.491158000
H	-0.689277000	-1.080441000	1.758859000
H	0.647449000	-3.106538000	1.294798000
H	-2.883278000	-3.662601000	-0.500240000
H	-0.931482000	-3.195061000	-2.454151000
H	-0.863262000	-4.685787000	-1.433826000
H	-5.129270000	-2.211261000	1.965004000
H	-4.908616000	-1.447659000	4.329519000
H	-3.327669000	0.387859000	4.902557000
H	-1.951377000	1.451875000	3.148194000
H	-2.385472000	3.198588000	-1.151894000
H	-4.257232000	3.643699000	-2.701779000
H	-5.958067000	1.886647000	-3.170079000
H	-5.779123000	-0.346713000	-2.066818000
H	2.562838000	1.501309000	1.067369000
H	1.404709000	-3.547068000	-3.973626000
H	2.719420000	-2.374691000	-3.993793000
H	1.061653000	-1.816528000	-3.727927000
H	4.287468000	-4.027782000	-0.971216000
H	2.993934000	-5.214438000	-1.147130000
H	3.126947000	-4.275650000	0.349145000
H	4.347918000	2.044299000	-0.564287000
H	4.103236000	0.435172000	-1.407737000
C	4.528403000	-0.453303000	2.316404000
C	5.687929000	0.422280000	0.485902000
C	5.600607000	-0.977207000	0.380192000
C	4.838254000	-1.489265000	1.460984000
C	5.291416000	0.765568000	1.908978000
H	3.939744000	-0.532444000	3.231973000
H	6.435370000	0.999462000	-0.063709000
H	5.989447000	-1.569515000	-0.450487000
H	4.525146000	-2.527757000	1.569898000

H	6.222018000	0.798479000	2.512851000
H	4.784516000	1.726724000	2.066458000

TS [6-Al-*s-cis*]$^{+}$→ [Al-S-aAdduct]$^{+}$, E = -2049.134238

C	1.387915000	3.670216000	-1.364936000
C	0.738942000	3.238872000	-0.193831000
C	1.106235000	3.784113000	1.046075000
C	2.122594000	4.748416000	1.102117000
C	2.772223000	5.175852000	-0.056749000
C	2.394167000	4.631978000	-1.292625000
O	-0.231729000	2.299057000	-0.363703000
C	-1.030075000	1.901409000	0.734024000
C	-2.029719000	0.845459000	0.263324000
C	-1.293078000	-0.413866000	-0.382436000
C	-2.382039000	-1.371759000	-0.992267000
C	-3.799463000	-0.919478000	-0.502784000
C	-3.787738000	-0.707019000	0.996541000
C	-2.867825000	0.275531000	1.414724000
C	-0.343826000	-1.089621000	0.640169000
C	-0.326675000	-2.619429000	0.549794000
O	-1.613073000	-3.102218000	0.567682000
C	-2.095880000	-2.859338000	-0.763090000
C	-4.005934000	0.435854000	-1.149096000
C	-3.031788000	1.378271000	-0.773867000
O	0.210788000	-3.050834000	-0.752246000
C	-0.921763000	-3.399670000	-1.595422000
C	-4.610549000	-1.345230000	1.923021000
C	-4.525244000	-1.003000000	3.278702000
C	-3.619591000	-0.026578000	3.697664000
C	-2.786032000	0.612925000	2.768677000
C	-3.080468000	2.666310000	-1.313870000
C	-4.100582000	3.004148000	-2.213276000
C	-5.064633000	2.063151000	-2.581325000
C	-5.016133000	0.768350000	-2.050215000
O	0.951345000	-0.448198000	0.530611000
C	2.141814000	-0.985384000	0.831180000
Al	2.135640000	-3.315317000	-1.014609000
C	2.504542000	-2.594529000	-2.797386000
O	2.485314000	-2.116898000	0.353398000
C	2.582601000	-5.110862000	-0.396550000
C	4.230435000	-0.695852000	2.094395000
C	2.978221000	-0.226217000	1.675819000
H	1.071417000	3.247479000	-2.320857000
H	0.602866000	3.484324000	1.965522000
H	2.393971000	5.177221000	2.070369000
H	3.552564000	5.938026000	-0.003920000
H	2.880849000	4.969923000	-2.211206000
H	-0.393263000	1.497340000	1.538822000
H	-1.574839000	2.769086000	1.147553000
H	-0.655777000	-0.035977000	-1.192398000
H	-2.383408000	-1.225994000	-2.082914000
H	-4.565014000	-1.644642000	-0.814328000
H	-0.698067000	-0.890576000	1.665171000
H	0.263944000	-3.097284000	1.342962000
H	-3.001005000	-3.465959000	-0.898738000
H	-0.796119000	-2.915560000	-2.572193000
H	-0.956959000	-4.493056000	-1.705585000
H	-5.327993000	-2.101074000	1.592041000
H	-5.174624000	-1.495030000	4.006517000
H	-3.562297000	0.248221000	4.753576000
H	-2.092390000	1.379618000	3.120284000
H	-2.331742000	3.413596000	-1.051514000
H	-4.139165000	4.014542000	-2.627281000
H	-5.858513000	2.336552000	-3.280366000
H	-5.769437000	0.027473000	-2.331944000
H	2.035376000	-3.212047000	-3.584383000
H	3.585584000	-2.601365000	-3.022062000
H	2.144979000	-1.560857000	-2.939105000

H	3.676285000	-5.263392000	-0.376568000
H	2.177314000	-5.889536000	-1.066334000
H	2.213486000	-5.332124000	0.619621000
H	4.662925000	-0.257209000	2.995968000
H	4.469040000	-1.748661000	1.937499000
H	2.575324000	0.720202000	2.035528000
C	5.738828000	0.155115000	0.919911000
C	4.296308000	1.299300000	-0.531106000
C	4.638329000	0.100368000	-1.110345000
C	5.566396000	-0.571517000	-0.263885000
C	5.142757000	1.525567000	0.678220000
H	6.578341000	-0.013493000	1.597922000
H	3.589468000	2.032308000	-0.924029000
H	4.249168000	-0.290439000	-2.050319000
H	6.028319000	-1.537383000	-0.479419000
H	5.971307000	2.206105000	0.391609000
H	4.633958000	2.010359000	1.522688000

[Al-R-adduct]$^{+}$, E = -2049.171641

C	1.578055000	3.357400000	-1.655686000
C	0.890349000	3.127321000	-0.452548000
C	1.173085000	3.909462000	0.676589000
C	2.147328000	4.914218000	0.590812000
C	2.836888000	5.144031000	-0.600003000
C	2.544106000	4.359788000	-1.724060000
O	-0.026528000	2.109442000	-0.471076000
C	-0.871517000	1.909856000	0.647428000
C	-1.914243000	0.845448000	0.302645000
C	-1.252059000	-0.489932000	-0.268893000
C	-2.407773000	-1.449380000	-0.758896000
C	-3.782339000	-0.901594000	-0.246265000
C	-3.697872000	-0.570796000	1.228278000
C	-2.727651000	0.406878000	1.527440000
C	-0.334608000	-1.164307000	0.776175000
C	-0.256546000	-2.688203000	0.621179000
O	-1.535355000	-3.170513000	0.798664000
C	-2.172377000	-2.942522000	-0.473035000
C	-3.961906000	0.402802000	-0.997399000
C	-2.932721000	1.326860000	-0.745231000
O	0.100009000	-3.115889000	-0.748337000
C	-1.127548000	-3.560674000	-1.400841000
C	-4.502894000	-1.101874000	2.234863000
C	-4.351274000	-0.652786000	3.552980000
C	-3.398699000	0.322498000	3.853668000
C	-2.581262000	0.852190000	2.844437000
C	-2.938507000	2.558863000	-1.404351000
C	-3.975780000	2.863468000	-2.296051000
C	-4.998394000	1.943394000	-2.537268000
C	-4.990255000	0.701642000	-1.889630000
O	0.931759000	-0.463162000	0.947977000
C	2.026305000	-0.565038000	0.234464000
C	3.098406000	0.388636000	0.639932000
C	3.893497000	-0.113326000	1.940746000
Al	1.888077000	-3.036388000	-1.545426000
C	1.616240000	-2.704950000	-3.446273000
O	2.173958000	-1.420663000	-0.654524000
C	2.963425000	-4.421514000	-0.695018000
C	4.241606000	0.627135000	-0.384903000
C	5.532058000	0.327379000	0.454494000
C	5.539384000	-1.169324000	0.716093000
C	4.560304000	-1.433959000	1.597979000
C	5.097802000	0.848625000	1.843277000
H	1.330003000	2.747103000	-2.526695000
H	0.644020000	3.757731000	1.617732000
H	2.358196000	5.525451000	1.471915000
H	3.589116000	5.933390000	-0.658394000
H	3.067253000	4.537714000	-2.666978000
H	-0.272631000	1.602609000	1.520675000

H	-1.388259000	2.847537000	0.916015000
H	-0.635693000	-0.204726000	-1.132564000
H	-2.453668000	-1.365830000	-1.854556000
H	-4.587297000	-1.616948000	-0.467312000
H	-0.778910000	-1.047831000	1.774290000
H	0.443598000	-3.163351000	1.324099000
H	-3.114026000	-3.506596000	-0.471805000
H	-1.135018000	-3.176383000	-2.427529000
H	-1.155331000	-4.659672000	-1.393232000
H	-5.258346000	-1.854935000	1.994647000
H	-4.986199000	-1.059276000	4.343555000
H	-3.290356000	0.681984000	4.879637000
H	-1.848818000	1.618623000	3.105806000
H	-2.145143000	3.288612000	-1.241227000
H	-3.981557000	3.830724000	-2.803932000
H	-5.805833000	2.191346000	-3.230171000
H	-5.787565000	-0.023030000	-2.076306000
H	2.597202000	1.327230000	0.912487000
H	3.280562000	-0.080981000	2.850635000
H	1.206935000	-3.584763000	-3.972855000
H	2.580845000	-2.482053000	-3.935241000
H	0.950260000	-1.850869000	-3.658081000
H	4.033166000	-4.292768000	-0.934039000
H	2.680198000	-5.424755000	-1.058849000
H	2.883235000	-4.442204000	0.405222000
H	4.223774000	1.670760000	-0.730058000
H	4.161760000	-0.020573000	-1.267902000
H	6.447865000	0.748716000	0.020650000
H	6.176522000	-1.892218000	0.202616000
H	4.238394000	-2.414642000	1.953388000
H	5.842413000	0.654052000	2.628068000
H	4.817882000	1.913861000	1.852408000

[Al-S-adduct]$^{+}$, E = -2049.171101

C	1.720957000	3.165586000	-1.842395000
C	1.028485000	3.042036000	-0.625829000
C	1.326463000	3.903383000	0.440076000
C	2.317440000	4.881415000	0.277004000
C	3.011298000	5.005916000	-0.927068000
C	2.705583000	4.141941000	-1.986970000
O	0.091122000	2.044290000	-0.569144000
C	-0.722222000	1.913248000	0.583207000
C	-1.822071000	0.886940000	0.306557000
C	-1.245411000	-0.486888000	-0.265764000
C	-2.463776000	-1.401399000	-0.687768000
C	-3.788498000	-0.784531000	-0.125029000
C	-3.623799000	-0.430774000	1.337288000
C	-2.599544000	0.507977000	1.574189000
C	-0.320158000	-1.188313000	0.752867000
C	-0.309152000	-2.715362000	0.611082000
O	-1.596754000	-3.143105000	0.852475000
C	-2.281932000	-2.900397000	-0.391344000
C	-3.943650000	0.512556000	-0.894137000
C	-2.864021000	1.393457000	-0.706541000
O	-0.034400000	-3.169813000	-0.769636000
C	-1.308602000	-3.573984000	-1.356936000
C	-4.406985000	-0.905687000	2.388245000
C	-4.178230000	-0.439146000	3.689041000
C	-3.171005000	0.497508000	3.928318000
C	-2.376101000	0.970871000	2.874223000
C	-2.843589000	2.610822000	-1.391958000
C	-3.904193000	2.944581000	-2.244947000
C	-4.976469000	2.067454000	-2.421868000
C	-4.995505000	0.839914000	-1.747985000
O	0.984816000	-0.546572000	0.877590000
C	2.031465000	-0.682585000	0.108014000
Al	1.700057000	-3.123807000	-1.681131000
C	1.319657000	-2.787584000	-3.562176000

O	2.085773000	-1.516593000	-0.813541000
C	2.800779000	-4.526674000	-0.893601000
C	3.345007000	0.734423000	1.861669000
C	4.858356000	0.426203000	2.112858000
C	3.158088000	0.262470000	0.382916000
C	4.579572000	-0.283816000	-0.010051000
C	4.830525000	-1.515877000	0.853556000
C	4.994773000	-1.089267000	2.116828000
C	5.454541000	0.756708000	0.724839000
H	1.460722000	2.495644000	-2.664837000
H	0.798355000	3.831539000	1.391048000
H	2.540455000	5.554374000	1.108721000
H	3.778153000	5.774230000	-1.045071000
H	3.233132000	4.235555000	-2.939439000
H	-0.104175000	1.608158000	1.443722000
H	-1.191301000	2.878325000	0.840177000
H	-0.654613000	-0.248411000	-1.160798000
H	-2.554342000	-1.330985000	-1.781482000
H	-4.633268000	-1.466935000	-0.295976000
H	-0.722516000	-1.044354000	1.764781000
H	0.403992000	-3.211092000	1.286194000
H	-3.246347000	-3.422043000	-0.339897000
H	-1.349590000	-3.204765000	-2.388295000
H	-1.379533000	-4.670676000	-1.329606000
H	-5.204949000	-1.628042000	2.196149000
H	-4.795333000	-0.801675000	4.514343000
H	-3.001881000	0.870798000	4.941045000
H	-1.599891000	1.708245000	3.088510000
H	-2.012348000	3.307146000	-1.279397000
H	-3.888793000	3.900607000	-2.773444000
H	-5.801481000	2.337955000	-3.084992000
H	-5.831615000	0.148596000	-1.884540000
H	0.874898000	-3.662222000	-4.068079000
H	2.258395000	-2.571416000	-4.102089000
H	0.651071000	-1.926950000	-3.735995000
H	3.834385000	-4.485635000	-1.279033000
H	2.414160000	-5.528095000	-1.152316000
H	2.865612000	-4.479557000	0.206893000
H	3.138011000	1.810244000	1.951844000
H	2.689007000	0.205749000	2.565913000
H	5.276093000	0.953566000	2.980294000
H	2.916387000	1.135560000	-0.254024000
H	4.727563000	-0.397684000	-1.091168000
H	4.809956000	-2.547299000	0.498385000
H	5.124498000	-1.703429000	3.010308000
H	6.526147000	0.525079000	0.651246000
H	5.277352000	1.794982000	0.401207000