Supplementary Information

An experimental estimate of the relative aromaticity of the cyclooctatetraene dianion by fusion to dimethyldihydropyrene

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CONTENTS

General information: Both proton (500.1 MHz for ^{1}H) and carbon (125.8 MHz for ^{13}C) NMR spectra were recorded on a Bruker AVANCE 500 NMR spectrometer unless otherwise stated. For air-sensitive compounds, the NMR spectra were measured in J-Young NMR tubes and the samples were loaded in a glovebox.

In NMR assignments, H-1,2 stands for H-1 ***and*** H-2; and H-1/2 stands for H-1 ***or*** H-2.

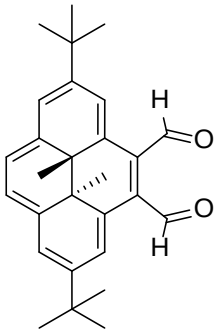
Infrared spectra were recorded on a Bruker IFS25 FT-IR spectrometer and only the major peaks are reported. All samples were prepared as potassium bromide pellets unless otherwise specified. UV-vis spectra were recorded on a Cary 5 UV-VIS-NIR spectrometer in suitable solvents. Melting points were determined on a Reichert 7905 melting point apparatus with an Omega Engineering Model 199 Chromel alumel thermocouple. Mass spectrometry was carried out at the University of British Columbia, Vancouver, B.C., Canada.

Silica gel (Merck silica gel, 60-200 mesh) used for chromatography was deactivated with 5% (w/w) of water.

All chemicals were purchased from Sigma-Aldrich Company unless otherwise stated. Acetonitrile was distilled from calcium hydride. Ether, benzene and THF-d_8 were dried over sodium and benzophenone. *tert*-Butanol was used without any purification.

All evaporations were carried out under vacuum.

2,7-Di-*tert*-butyl-4,5-diformyl-*trans*-10b,10c-dimethyl-10b,10c-dihydropyrene 8

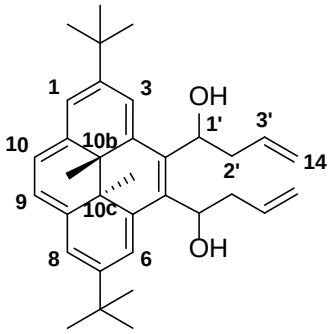


A solution of freshly made[1] dimethyldioxirane in acetone was added to a solution of 2,7-di-t-butyl-trans-11b,11c-dimethyl-11b,11cdihydropyrenyl[4,5-c]furan[2] (160 mg, 0.416 mmol) in acetone (20 mL) at room temperature until the disappearance of the purple color of the furan. The reaction mixture was then diluted with hexanes and subsequently washed with water three times. The organic layer was dried over $MgSO_4$. And the acetone was evaporated to afford crude **8**. The yield dropped to 60% when the crude product was chromatographed on a 30 cm column of silica gel, eluting with DCM. Noted that the concentration of the dimethyldioxirane in acetone varies from batch to batch. The dialdehyde **8** could be further purified by recrystalization from cyclohexane as green crystals, mp 205-207^{o}C. ^{1}H NMR (500 MHz, C_6D_6) δ 11.31 (s, 2H, H-17,18), 9.56 (s, 2H, H-3,6), 8.351 (s, 1H, H-1 or 8), 8.349 (s, 1H, H-8 or 1), 8.17 (s, 2H, H-9,10), 1.51 (s, 18H, H-11,16), -3.43 (s, 6H, H-13,14). ^{13}C NMR (125.8 MHz, C_6D_6) δ 190.83 (C-17 or 18), 190.80 (C-18 or 17), 152.18 (C-2,7), 140.84 (C-10a,10d), 139.66 (C-3a,5a), 127.47 (C-4,5), 126.99 (C-9,10), 124.07 (C-1,8), 118.58 (C-3,6), 36.92 (C-12,15), 32.13 (C-10b,10c), 31.77 (C-11,16), 16.13 (C-13,14). IR (NaCl, thin film) ν 2964, 2921, 2901, 2866, 1677, 1649, 1265, 886, 737 cm^{-1}. EI MS, *m/z*, 400 (M^+), HRMS calc'd for $C_{28}H_{32}O_2$ 400.2402, found 400.2391.

1 Murray, R. W. and Jeyaraman, R. *J. Org. Chem.* **1985**, *50*, 2847-2853

2 Mitchell, R. H.; Ward, T. R. *Tetrahedron*, **2001**, *57*, 3689-3695.

4,5-*Bis*-(1'-hydoxy-3'-butenyl)-2,7-di-*tert*-butyl-10b,10c-dimethyl-*trans*-10b,10c-dihydropyrene 9

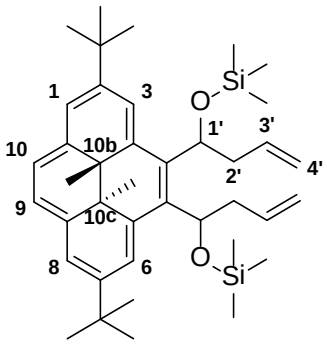


Allyl magnesium bromide was generated from allyl bromide (0.50 mL, 5.8 mmol) and magnesium (0.14 g, 5.8 mmol) in ether (12 mL). The reaction was refluxed for 30 min and then cooled to room temperature. A solution of DHP aldehyde **8** (230 mg, 0.574 mmol) in THF (13 mL) was then added dropwise with stirring. The reaction was then stirred for three hours before it was quenched by addition of ice water. The organic layer was separated and washed with water and brine. Solvents were removed to afford a green oil **9** (320 mg, quantitative). The NMR spectra were consistent with the presence of two diastereomers in a *ca.* 3:2 ratio, which were used directly in the next step to prepare **10**.

9: ^{1}H NMR (500 MHz, $CDCl_3$) δ (four singlets with total integral 2H) 9.32, 9.17, 9.13, 9.06, (five peaks with total integral of 4H between 8.40 and 8.24 ppm) 8.39 (s), 8.36 (d, J = 1.2 Hz), 8.32 (s), 8.32 (s), 8.25 (s), 6.54-6.38 (m, 2H, H-1'), 6.10-5.93 (m, 2H, H-3'), 5.29-4.89 (m, 4H, H-4'), 3.43-2.75 (m, 4H, H-2'), (four singlets with total integral 18H) 1.66, 1.66, 1.65, 1.65, (four singlets with total integral 6H for the internal methyl protons) -3.74, -3.79, -3.81, -3.82; ^{13}C NMR (125 MHz $CDCl_3$) δ 145.62, 145.36, 145.25, 138.23, 137.96, 136.27, 136.23, 136.10, 135.95, 133.47, 132.97, 132.57, 123.91, 123.77, 123.09, 121.12, 121.02, 120.92, 120.09, 118.02, 117.86, 117.80, 117.73, 72.20, 71.80, 71.72, 70.47, 44.34, 44.30, 43.49, 42.96, 36.38, 32.10, 32.07, 32.03, 29.93, 15.28, 14.95, 14.49; IR (KBr) v 3377, 3074, 3.43, 3005, 2963, 2923, 2865, 1640, 1593, 1479, 1462, 1442, 1391, 1375, 1361, 1343, 1268, 1235, 1198, 1127, 1027, 992, 939, 913, 882, 859, 795, 681, 651 cm^{-1}; EI MS *m/z* 484 (M^+); HRMS calcd for $C_{34}H_{44}O_2$: 484.3341, found 484.3338.

4,5-*Bis*-(1'-trimethylsilyloxy-3'-butenyl)-2,7-di-*tert*-butyl-10b,10c-dimethyl-*trans*-10b,10c-dihydropyrene 10

This procedure was adapted from Corey.[1] Mixed isomers of diol **9** (0.61 g, 1.3 mmol) were dissolved in DMF (40 mL). Imidazole (1.6 g, 32 mmol) and then TMSCl (1.5 mL, 12 mmol) were added. The reaction was stirred for 5 hours at room temperature. Then water was added and the mixture was extracted with ethyl acetate three times. The organic layer was washed with aqueous sodium bicarbonate solution. The solution was then dried and evaporated to afford mixed isomers of **10** as a green solid (quantitative), used directly in the next step.

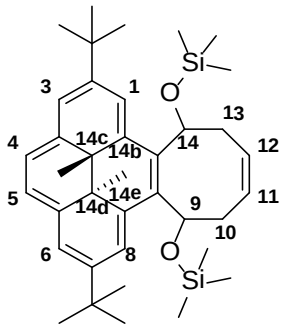


10: ^{1}H NMR (500 MHz, $CDCl_3$) δ (18 singlets with integral of 6H in the aromatic proton region)10.03, 10.02, 9.91, 9.88, 9.76, 9.73 8.80, 8.73, 8.71, 8.42, 8.38, 8.37, 8.35, 8.32, 8.30, 8.28, 8.25, 8.24, 6.74-5.61 (m, 4H, H-1',3'), 5.34-4.89 (m, 4H, H-4'), 3.76-2.30 (m, 4H, H-2'), (3 peaks for the *tert*-butyl protons, integral of 18) 1.661, 1.657, 1.65, (12 peaks for the methyl protons on TMS with integral 18H) 0.19, 0.18, 0.14, 0.13, 0.11, 0.08, 0.03, 0.00, -0.01, -0.06, -0.07, -0.12, (8 peaks for internal methyl protons with integral 6H) -3.77, -3.86, -3.89, -3.90, -3.91, -3.93, -3.95, -4.00; IR (film) *v* 3076, 2962, 2866, 1640, 1594, 1479, 1463, 1444, 1391, 1361, 1344, 1250, 1126, 1077, 994, 951, 913, 882, 841, 748, 737, 684, 648 cm^{-1}; UV-vis (toluene) λ_{max} (ε_{max}, L Mol^{-1} cm^{-1}) nm 353 (87,700), 390 (49,400), 486 (8,390), 655 (1,100); EI MS *m/z* 628 (M^+); HRMS calcd for $C_{40}H_{60}O_2Si_2$: 628.4132, found 628.4122.

1 Corey, E. J. and Venkateswarlu, A. *J. Am. Chem. Soc.* **1972**, *94*, 6190-6191

2,7-Di-*tert*-butyl-9,14-*bis*-trimethylsilyloxy-*trans*-14c,14d-dimethyl-9,10,13,14,14c,14d-hexahydrocycloocta[14a:14f; e]pyrene 11

DHP dialkene **10** (100 mg, 0.16 mmol) and Grubbs first generation catalyst benzylidene-bis-(tricyclohexylphospine)dichlororuthenium[1] (19 mg, 0.023 mmol) were mixed in a Schlenk tube. Then benzene (450 mL) was added through a syringe under argon. The mixture was warmed to 55^{o}C for 15 hours. The reaction was concentrated to about 50 mL. The resulting solution was filtered through a flash column and rinsed with hexanes and DCM (1:1) to remove the catalyst. The solvents were then removed and the residual was chromatographed on a silica gel column eluting with hexanes and DCM (10:1) to afford a green solid **11** (70 mg, 73% yield).

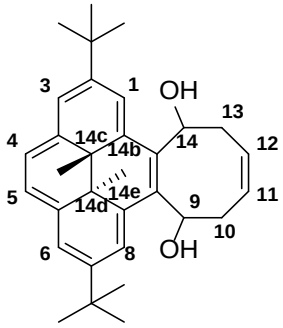


11: ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.95 (d, J = 1.2 Hz, 1H), 8.82 (s, 1H), 8.42, 8.34 (s, 1H), 8.33 (s, 1H), 7.18-6.55 (m, 2H), 5.33-5.05 (m , 2H), 3.46-2.80 (m, 4H), three singlets 1.69, 1.68, 1.67 (s, 18H), three singlets 0.24, 0.11, 0.00 (s, 18H), four singlets -3.65 (v. small), -3.95 (s, 6H), -4.01 (v. small) -4.11 (s, 6H); ^{13}C NMR (125 MHz $CDCl_3$) δ 144.91, 137.56, 132.96, 132.41, 132.20, 131.12, 127.22, 123.18, 122.93, 122.58, 120.59, 120.30, 115.50, 72.47, 68.31, 40.28, 39.79, 36.48, 36.39, 32.34, 32.27, 32.20, 30.36, 29.74, 14.35, 1.08, 0.64, 0.22; IR (KBr) ν 3027, 2958, 2901, 1591, 1477, 1462, 1441, 1390, 1361, 1261, 1249, 1072, 1039, 1025, 1002, 879, 841, 756, 717, 682, 657, 644 cm^{-1}; EI MS m/z 600 (M^{+}); HRMS calcd for $C_{38}H_{56}O_2Si_2$: 600.3819, found 600.3817.

1 S. J. Miller, S. H. Kim, Z. R. Chen, R. H. Grubbs, *J. Am. Chem. Soc.*, 1995, **117**, 2108

2,7-di-*tert*-butyl-9,14-dihydoxy-*trans*-14c,14d-dimethyl-9,10,13,14,14c,14d - hexahydrocycloocta[14a:14f; e]pyrene 12

The TMS protected diol **11** (300 mg, 0.500 mmol) was dissolved in THF and methanol (1:1 ratio, 30 mL). Anhydrous potassium carbonate (780 mg, 5.60 mmol) was added. The reaction was stirred at room temperature for 8 hours. The solvents were then removed to afford green product **12** (280 mg, quantitative).



12: ^{1}H NMR (500 MHz, $CDCl_3$)[*1] δ 8.45 (s, 2H, H-3,6), 8.35 (AB, J = 7.6 Hz, 1H, H-4), 8.34 (AB, J = 7.6 Hz, 1H, H-5), 8.30 (d, J = 1.1 Hz, 1H, H-1), 8.29 (d, J = 1.0 Hz, 1H, H-8), 6.47-6.45 (m, 2H, H-9/14), 5.22-5.14 (m, 2H, H-11,12), 3.31-3.25 (m, 2H, H-10,13), 3.20-3.15 (m, 1H, H-13), 2.95-2.90 (m, 1H, H-10), 1.66 (s, 9H, 2/7-C($C\underline{H}_3$)$_3$), 1.66 (s, 9H, 2/7-C($C\underline{H}_3$)$_3$), -3.96 (s, 3H, 14d-$C\underline{H}_3$), -3.99 (s, 3H, 14c-$C\underline{H}_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.40 (C-2/7), 145.36 (C-2/7), 136.80 (C-3a), 136.70 (C-5a), 134.64 (C-14a/14f), 134.56 (C-14a/14f), 127.87 (C-14e), 127.74 (C-14b), 125.94 (C-11,12), 123.13 (C-4), 123.01 (C-5), 120.76 (C-3/6), 120.48 (C-3/6), 118.09 (C-1), 116.95 (C-8), 81.98 (C-9/14), 81.61 (C-9/14), 40.72 (C-10), 39.32 (C-13), 36.23 (2,7-$\underline{C}(CH_3)_3$), 32.21 (2,7-C($\underline{C}H_3$)$_3$), 31.49 (C-14c), 30.10 (C-14d), 14.86 (14c/14d-$\underline{C}H_3$), 14.63 (14c/14d-$\underline{C}H_3$);

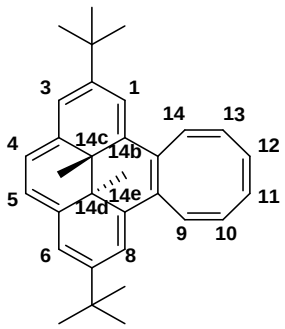
[*1] The assignments are based on the assumption that the proton with chemical shift 8.30 ppm is H-1.

(9Z,11Z,13Z)-2,7-di-*tert*-butyl-*trans*-14c,14d-dimethyl-14c,14d-dihydrocycloocta[e]pyrene 5; Cyclooctatetraene 5

Method a): The cyclized diol **12** (115 mg, 0.252 mmol) was dissolved in benzene (6 mL) and then *p*-toluenesulfonic acid (30 mg, 0.17 mmol) was added in one portion. The resulting mixture was stirring for 1 hour at room temperature under argon. It was washed with water to remove acid. The organic layer was then dried over $MgSO_4$. The solvent was removed and the residue was chromatographed on silica gel. The green COT product **5** was eluted first with hexanes (7.5 mg, 7.1% yield). The green O-bridged alkene product **13** was eluted last with hexanes and DCM (1:1) (81 mg, 73% yield).

Method b): Freshly distilled 4-toluenesulfonyl chloride (25 mg, 0.13 mmol) (or methylsulfonyl chloride with triethylamine in DCM) was added to a solution of the alcohol **12** (30 mg, 0.066 mmol) in dry pyridine (2 mL). The reaction mixture was heated to 110°C for one and half hours. The solvents and excess reactant were removed and the residue was chromatographed to afford the green cyclic ether **13** (20 mg, 70% yield) with no observed formation of the COT **5**.

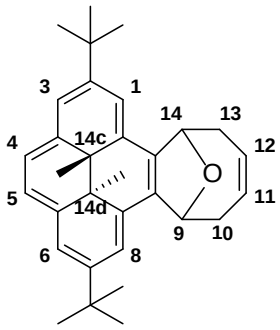
Method c): Potassium *tert*-butoxide (95%, 26 mg, 0.23 mmol) was added to a solution of the diol **12** (30 mg, 0.066 mmol) in THF (3mL) at 0°C. Intense color appeared right away. The mixture was kept at 0°C for 2 hours and the NMR showed only the cyclic ether **13**.



COT 5: m.p 155-156°C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (s, 2H, H-1,8), 8.34 (s, 2H, H-3,6), 8.22 (s, 2H, H-4,5), 7.65 (s, 2H, H-9,14), 6.48 (s, 2H, H-10,13), 6.05 (s, 2H, H-11,12), 1.64 (s, 18H, 2,7-C(C$\underline{H}_3$)$_3$), -3.70 (s, 6H, 14c,14d-C$\underline{H}_3$); ^{13}C NMR (125 MHz, C_6D_6)[1] δ 145.50 (C-2,7), 137.58 (C-3a,5a), 134.47 (C-14b,14e), 133, 132, 131.04 (C-10,13), 122.56 (C-4,5), 120.79 (C-

3,6), 118.54 (C-1,8), 36.28 (2,7-C(CH$_3$)$_3$), 32.19 (2,7-C(CH$_3$)$_3$), 30.25 (C-14c,14d), 15.3 (14c,14d-CH$_3$); IR (film) *v* 2963, 1593, 1460, 1361, 1342, 1258, 1236, 909, 877, 826, 792, 734, 659 cm^{-1}; UV-vis (toluene) λ_{max} (ε_{max}, L Mol^{-1} cm^{-1}) nm 309 (10,800), 359 (24,600), 395 (26,700), 495 (8,900), 664 (1,400); EI MS *m/z* 420 (M$^+$); HRMS calcd for $C_{32}H_{36}$: 420.2817, found: 420.2819.

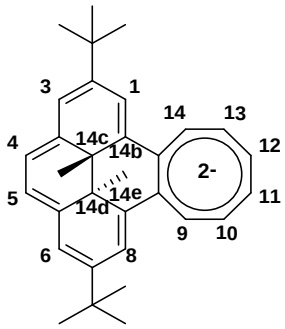
[1] Peaks at δ133, 132 and 15.3 are broad. Signals for C14a and C14f are missing in the spectrum. No short range correlations were found for the C-H on C9, C11, C12 and C14 in the HSQC spectrum.



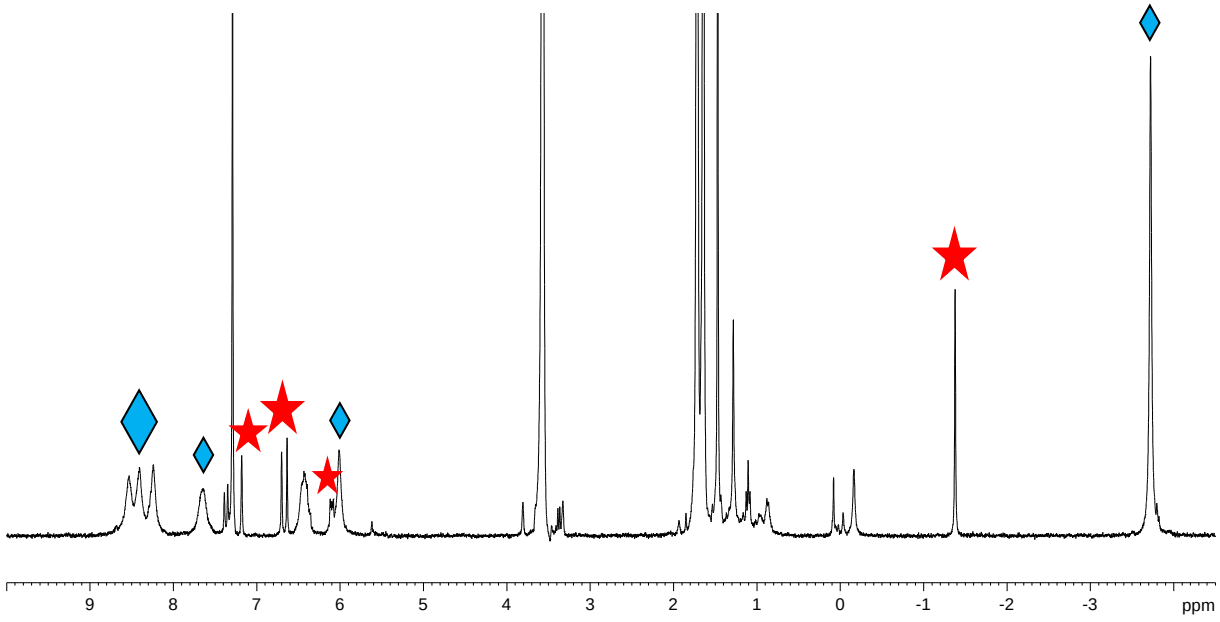
Cyclic ether 13: m.p. 160-161°C. ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 8.45 (s, 2H, H-3,6), 8.35 and 8.34 (AB, *J* = 7.6 Hz, 2H, H-4/5), 8.30 (d, *J* = 0.6 Hz, 1H, H-1/8), 8.29 (s, 1H, H-1/8), 6.46-6.45 (m, 2H, H-9,14), 5.21-5.14 (m, 2H, H-11,12), 3.30-3.26 (m, 2H, H-10/13), 3.20-3.15 (m, 1H, H-10/13), 2.94-2.90 (m, 1H, H-10/13), 1.66 (s, 9H, 2/7-C(CH$_3$)$_3$), 1.65 (s, 9H, 2/7-C(CH$_3$)$_3$), -3.96 (s, 3H, 13c/13d-CH$_3$), -3.99 (s, 3H, 13c/13d-CH$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 145.40 (C-2/7), 145.36 (C-2/7), 136.79 (C-3a/5a), 136.69 (C-3a/5a), 134.62 (C-14a/14f), 134.54 (C-14a/14f), 127.85 (C-14b/14e), 127.73 (C-14b/14e), 125.94 (C-11,12), 123.13 (C-4/5), 123.01 (C-4/5), 120.76 (C-3/6), 120.49 (C-3/6), 118.09 (C-1/8), 116.95 (C-1/8), 81.98 (C-9/14), 81.62 (C-9/14), 40.71 (C-10/13), 39.32 (C-10/13), 36.24 (2-C(CH$_3$)$_3$), 32.21 (2/7-C(CH$_3$)$_3$), 31.48 (C-14c/14d), 30.10 (C-14c/14d), 14.88 (14c/14d-CH$_3$), 14.64 (14c/14d-CH$_3$); IR (KBr) *v* 2961, 2921, 2902, 2877, 1600, 1460, 1360, 1346, 1235, 1200, 1098, 1044, 1019, 888, 868, 852, 673, 645 cm^{-1}; UV-vis (toluene) λ_{max} (ε_{max}, L Mol^{-1} cm^{-1}) nm 349 (98,200), 387 (48,000), 485 (9,280), 651 (939); EI MS *m/z* 438 (M$^+$); HRMS calcd for $C_{32}H_{38}O$: 438.2923, found: 438.2919.

DHP[e]cyclooctatetraene (COT) dianion 6

COT **5** (~5.0 mg, 0.011 mmol) in THF-d_8 (0.6 mL) was placed in a sealed NMR tube, flushed with argon. A piece of potassium (~100 mg, 2.56 mmol) was adhered to the upper part of the NMR tube. When the potassium was immersed in the THF solution by upending the tube, the green color turned immediately red, indicating the formation of the dianion **6·2K**$^+$. The ^{1}H NMR spectrum obtained is shown below. Further reaction led to the loss of NMR signals.

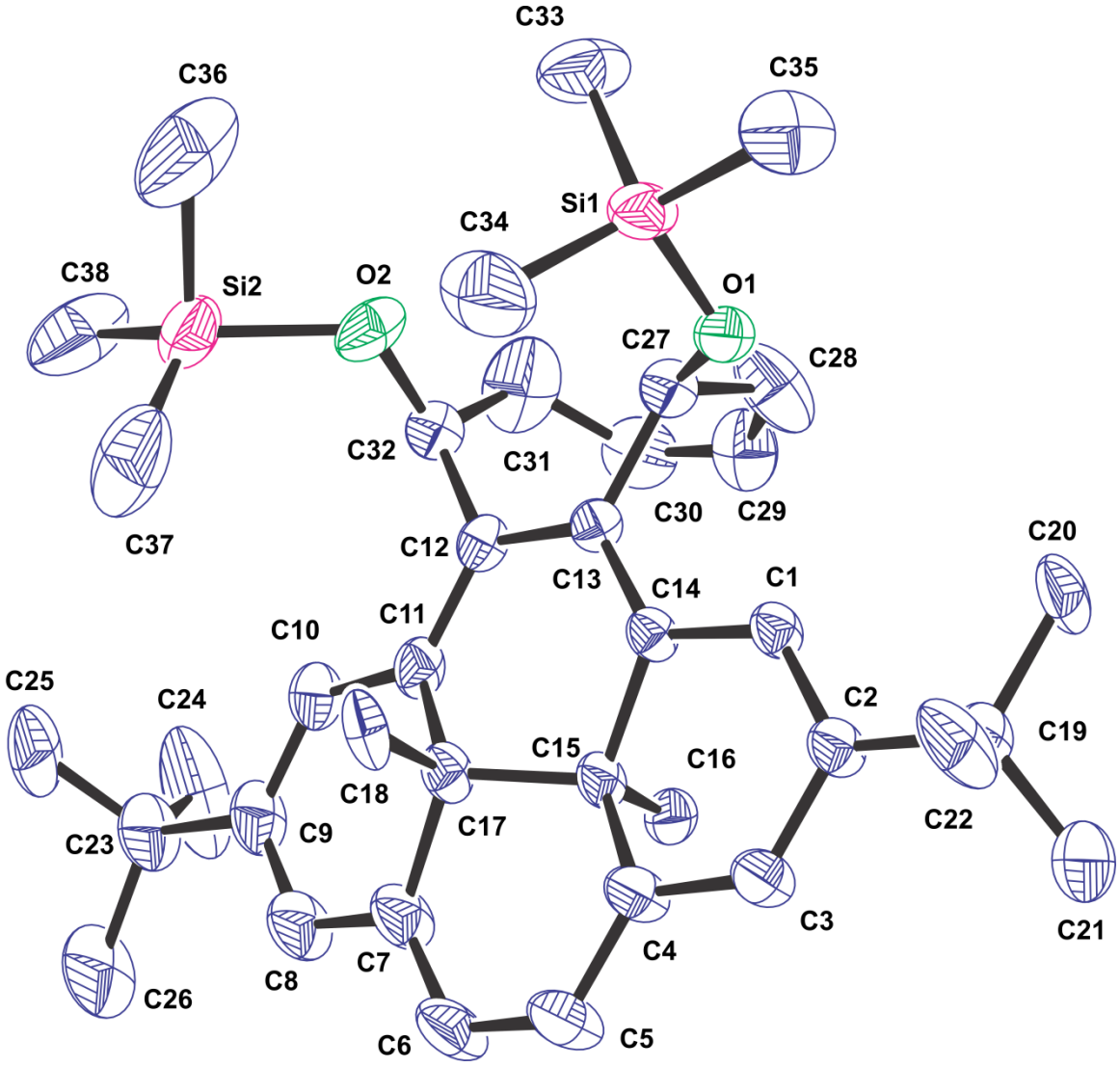


6·2K$^+$: ^{1}H NMR (500 MHz, THF-d_6) δ 7.37 (d, J = 11.9 Hz, 2H, H-9, 14), 7.18 (s, 2H, H-1,8), 6.70 (s, 2H, H-3,6), 6.64 (s, 2H, H-4,5), 6.44-6.40 (m, 2H, H-10,13), 6.11 (dd, J = 7.7, 3.1 Hz, 2H, H-11,12), 1.47 (s, 18H, 2,7-C(C$\underline{H}_3$)$_3$), -1.38 (s, 6H, 14c,14d-C$\underline{H}_3$). No other characterization data are available due to fast decomposition of the sample.



The ^{1}H NMR spectrum for the dianion 6 (★) plus unconverted 5 ◆

The crystal structure of 2,7-di-tert-butyl-9,14-*bis*-trimethylsilyloxy-trans-14c,14d-dimethyl-9,10,13,14,14c,14d-hexahydrocycloocta[14a:14f; e]pyrene 11



ORTEP3 drawing (30% probability level) of 1,2-DHP[e]fused 3,8-*bis*(trimethylsilyloxo)-cycloocta-1,5-diene 11

Experimental

Data Collection

A green plate crystal of $C_{38}H_{56}O_2Si_2$ having approximate dimensions of 0.10 x 0.22 x 0.35 mm was mounted on a glass fiber. All measurements were made on a Bruker APEX II diffractometer with graphite monochromated Mo-Kα radiation..

The data were collected at a temperature of -170.0 ± 0.1°C to a maximum 2θ value of 50.9°. Data were collected in a series of φ and ω scans in 0.50° oscillations with 10.0-second exposures. The crystal-to-detector distance was 40.00 mm.

Data Reduction

Of the 24305 reflections that were collected, 6665 were unique (R_{int} = 0.047); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 1.26 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.886 and 0.987, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions. The material crystallizes with disorder with respect to the orientation of the two methyl substituents on the central pyrene system (C15, C16, C17, and C18). Additionally, both $OSiMe_3$ substituents are disordered, each being modeled in two orientations. Finally, the methyls of both t-butyl substituents were also disordered in two orientations. Mild restraints were employed on bond lengths and angles, as well as anisotropic thermal parameters. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 6665 reflections and 554 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.161$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2)/ \Sigma w(Fo^2)^2]^{1/2} = 0.232$$

The standard deviation of an observation of unit weight[5] was 1.05. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.34 and –0.27 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXL-97[10] via the WinGX[11] interface.

References

(1) SAINT. Version 7.60A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2009).

(2) SADABS. Bruker Nonius area detector scaling and absorption correction - V2008/1, Bruker AXS Inc., Madison, Wisconsin, USA (2008).

(3) SIR97 - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. (1999) J. Appl. Cryst. 32, 115-119.

(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) SHELXTL Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA. (1997).

(11) WinGX – V1.70 – Farrugia, L.J.; J. Appl. Cryst., 32, 837 (1999).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{38}H_{56}O_2Si_2$
Formula Weight	601.01
Crystal Color, Habit	green, plate
Crystal Dimensions	0.10 X 0.22 X 0.35 mm
Crystal System	triclinic
Lattice Type	primitive
Lattice Parameters	a = 10.120(1) Å b = 10.179(2) Å c = 17.871(3) Å α = 90.724(4) ^{o} β = 94.432(9) ^{o} γ = 94.513(5) ^{o} V = 1829.5(6) Å^3
Space Group	*P* -1 (#2)
Z value	2
D_{calc}	1.091 g/cm^3
F_{000}	656.00
μ(MoKα)	1.26 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker X8 APEX II
Radiation	MoKα (λ = 0.71073 Å) graphite monochromated
Data Images	1541 exposures @ 10.0 seconds
Detector Position	40.00 mm
$2\theta_{max}$	50.9^{o}
No. of Reflections Measured	Total: 24305
Corrections	Unique: 6665 (R_{int} = 0.047) Absorption (T_{min} = 0.886, T_{max}= 0.987) Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w=1/($\sigma^2(Fo^2)$+(0.0672P) ^{2}+ 2.2159P)
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>0.00σ(I))	6665
No. Variables	554
Reflection/Parameter Ratio	12.03
Residuals (refined on F^2, all data): R1; wR2	0.161; 0.232
Goodness of Fit Indicator	1.05
No. Observations (I>2.00σ(I))	3282
Residuals (refined on F): R1; wR2	0.082; 0.193
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.34 e^-/Å^3
Minimum peak in Final Diff. Map	-0.27 e^-/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for db007.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	occ
C(1)	15066(4)	1298(3)	2571(2)	48(1)	
C(2)	15672(4)	586(4)	2040(2)	53(1)	
C(3)	15476(4)	912(4)	1287(2)	61(1)	
C(4)	14730(4)	1928(4)	1039(2)	60(1)	
C(5)	14543(5)	2282(4)	297(2)	79(2)	
C(6)	13860(5)	3348(5)	83(2)	81(2)	
C(7)	13301(5)	4126(5)	596(3)	74(1)	
C(8)	12651(5)	5228(5)	400(3)	81(2)	
C(9)	12117(5)	6005(5)	931(3)	77(1)	
C(10)	12213(4)	5646(4)	1681(3)	65(1)	
C(11)	12838(4)	4545(4)	1959(2)	56(1)	
C(12)	12963(4)	4160(3)	2715(2)	47(1)	
C(13)	13672(4)	3066(3)	2928(2)	45(1)	
C(14)	14279(4)	2328(3)	2405(2)	44(1)	
C(15)	14411(14)	2904(13)	1621(8)	50(3)	0.53(2)
C(16)	15577(9)	4021(12)	1698(5)	56(3)	0.53(2)
C(17)	13103(13)	3463(11)	1376(5)	52(3)	0.53(2)
C(18)	11911(10)	2348(11)	1314(6)	63(3)	0.53(2)
C(19)	16522(5)	-539(4)	2272(2)	61(1)	
C(20)	15756(9)	-1823(6)	2016(5)	89(3)	0.72(1)
C(21)	17850(10)	-350(11)	1904(6)	104(4)	0.72(1)
C(22)	16857(11)	-584(9)	3110(4)	77(3)	0.72(1)
C(23)	11372(5)	7206(5)	691(3)	96(2)	0.72(1)
C(24)	9923(6)	6925(7)	852(5)	105(3)	0.80(1)
C(25)	11363(9)	7407(8)	-167(4)	130(4)	0.80(1)
C(26)	11992(9)	8395(6)	1103(6)	171(6)	0.80(1)
C(27)	12378(4)	4973(4)	3305(2)	63(1)	0.67(1)
C(28)	13302(7)	5707(6)	3868(4)	126(2)	
C(29)	14752(6)	5804(5)	3802(3)	89(2)	
C(30)	15495(6)	4835(6)	3935(3)	92(2)	
C(31)	15125(7)	3465(5)	4124(3)	110(2)	
C(32)	13879(4)	2790(4)	3764(2)	59(1)	0.80(1)
C(33)	9269(14)	3568(17)	2271(9)	151(6)	0.67(1)

C(34)	8820(13)	5939(12)	3096(9)	144(6)	0.67(1)
C(35)	8811(15)	3343(14)	3937(11)	200(9)	0.67(1)
C(36)	11820(8)	1666(7)	4988(4)	111(3)	0.80(1)
C(37)	13038(9)	-893(6)	4652(4)	98(3)	0.80(1)
C(38)	11227(7)	343(9)	3440(4)	138(4)	0.80(1)
O(1)	11258(5)	4258(4)	3589(3)	79(2)	0.67(1)
O(2)	13810(3)	1464(3)	3953(2)	57(1)	0.80(1)
Si(1)	9586(5)	4399(6)	3169(3)	96(2)	0.67(1)
Si(2)	12462(3)	664(3)	4240(2)	69(1)	0.80(1)
C(15B)	13801(16)	2560(15)	1580(9)	48(3)	0.47(2)
C(16B)	12397(13)	1825(11)	1422(6)	57(3)	0.47(2)
C(17B)	13807(14)	4012(12)	1446(6)	49(3)	0.47(2)
C(18B)	15241(11)	4719(13)	1617(6)	58(3)	0.47(2)
C(27B)	12378(4)	4973(4)	3305(2)	63(1)	0.33(1)
O(1B)	11186(9)	5409(9)	3139(5)	73(4)	0.33(1)
Si(1B)	9853(8)	4660(9)	3546(5)	71(2)	0.33(1)
C(35B)	9380(30)	4240(30)	4356(15)	144(11)	0.33(1)
C(34B)	9570(20)	6377(18)	3514(14)	98(7)	0.33(1)
C(33B)	9230(40)	3740(40)	2696(16)	163(15)	0.33(1)
C(22B)	17570(20)	-50(20)	2909(17)	84(8)	0.28(1)
C(21B)	17180(30)	-1200(30)	1637(11)	93(9)	0.28(1)
C(20B)	15532(18)	-1592(17)	2637(16)	81(8)	0.28(1)
O(2B)	12550(19)	1936(13)	3919(9)	90(6)	0.20(1)
Si(2B)	12160(20)	396(18)	3996(9)	150(10)	0.20(1)
C(32B)	13879(4)	2790(4)	3764(2)	59(1)	0.20(1)
C(38B)	11960(30)	-470(20)	3080(11)	100(10)	0.20(1)
C(37B)	13360(30)	-367(18)	4658(12)	70(9)	0.20(1)
C(36B)	10720(50)	690(50)	4540(30)	193(19)	0.20(1)

C(26B)	11000(30)	7930(20)	1400(8)	130(13)	0.20(1)
C(25B)	12230(20)	8227(17)	277(13)	71(8)	0.20(1)
C(24B)	10103(18)	6840(30)	206(14)	144(15)	0.20(1)

Table 3. Bond lengths [A] and angles [deg] for db007.

C(1)-C(14)	1.387(5)
C(1)-C(2)	1.395(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.392(5)
C(2)-C(19)	1.528(5)
C(3)-C(4)	1.385(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(5)
C(4)-C(15)	1.500(14)
C(4)-C(15B)	1.567(16)
C(5)-C(6)	1.376(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.385(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(6)
C(7)-C(17B)	1.573(11)
C(7)-C(17)	1.577(11)
C(8)-C(9)	1.395(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.393(6)
C(9)-C(23)	1.535(6)
C(10)-C(11)	1.407(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.411(5)
C(11)-C(17B)	1.519(11)
C(11)-C(17)	1.559(10)
C(12)-C(13)	1.411(5)
C(12)-C(27)	1.516(5)
C(13)-C(14)	1.399(5)
C(13)-C(32)	1.526(5)
C(14)-C(15)	1.538(15)
C(14)-C(15B)	1.542(17)
C(15)-C(17)	1.518(18)
C(15)-C(16)	1.569(19)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.586(18)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(22)	1.513(9)
C(19)-C(20)	1.513(8)
C(19)-C(21B)	1.532(19)
C(19)-C(21)	1.541(10)
C(19)-C(22B)	1.54(2)
C(19)-C(20B)	1.59(2)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800

C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(26)	1.479(6)
C(23)-C(24B)	1.512(8)
C(23)-C(24)	1.522(6)
C(23)-C(25B)	1.535(8)
C(23)-C(26B)	1.544(8)
C(23)-C(25)	1.549(6)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-O(1)	1.428(6)
C(27)-C(28)	1.473(7)
C(27)-H(27)	1.0000
C(27)-H(27B)	0.972(4)
C(28)-C(29)	1.477(8)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.299(7)
C(29)-H(29)	0.9500
C(30)-C(31)	1.466(7)
C(30)-H(30)	0.9500
C(31)-C(32)	1.484(7)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-O(2)	1.394(5)
C(32)-H(32)	1.0000
C(32)-H(32B)	0.970(4)
C(33)-Si(1)	1.800(14)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-Si(1)	1.805(12)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-Si(1)	1.931(14)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-Si(2)	1.859(6)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-Si(2)	1.872(6)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-Si(2)	1.833(6)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800

C(38)-H(38C)	0.9800
O(1)-Si(1B)	1.507(9)
O(1)-H(27B)	0.804(4)
O(2)-Si(2)	1.652(5)
O(2)-H(32B)	0.907(3)
Si(1)-O(1B)	1.854(11)
C(15B)-C(17B)	1.50(2)
C(15B)-C(16B)	1.56(2)
C(16B)-H(16D)	0.9800
C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-C(18B)	1.574(19)
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
Si(1B)-C(35B)	1.61(3)
Si(1B)-C(34B)	1.794(19)
Si(1B)-C(33B)	1.82(2)
C(35B)-H(35D)	0.9800
C(35B)-H(35E)	0.9800
C(35B)-H(35F)	0.9800
C(34B)-H(34D)	0.9800
C(34B)-H(34E)	0.9800
C(34B)-H(34F)	0.9800
C(33B)-H(33D)	0.9800
C(33B)-H(33E)	0.9800
C(33B)-H(33F)	0.9800
C(22B)-H(22D)	0.9800
C(22B)-H(22E)	0.9800
C(22B)-H(22F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
O(2B)-Si(2B)	1.60(2)
Si(2B)-C(38B)	1.837(9)
Si(2B)-C(37B)	1.849(9)
Si(2B)-C(36B)	1.86(4)
C(38B)-H(38D)	0.9800
C(38B)-H(38E)	0.9800
C(38B)-H(38F)	0.9800
C(37B)-H(37D)	0.9800
C(37B)-H(37E)	0.9800
C(37B)-H(37F)	0.9800
C(36B)-H(36D)	0.9800
C(36B)-H(36E)	0.9800
C(36B)-H(36F)	0.9800
C(26B)-H(26D)	0.9800
C(26B)-H(26E)	0.9800
C(26B)-H(26F)	0.9800
C(25B)-H(25D)	0.9800
C(25B)-H(25E)	0.9800
C(25B)-H(25F)	0.9800
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800

C(24B)-H(24F)	0.9800
C(14)-C(1)-C(2)	124.5(3)
C(14)-C(1)-H(1)	117.7
C(2)-C(1)-H(1)	117.7
C(3)-C(2)-C(1)	118.6(3)
C(3)-C(2)-C(19)	120.3(3)
C(1)-C(2)-C(19)	121.1(3)
C(4)-C(3)-C(2)	123.3(4)
C(4)-C(3)-H(3)	118.3
C(2)-C(3)-H(3)	118.3
C(5)-C(4)-C(3)	124.2(4)
C(5)-C(4)-C(15)	117.0(6)
C(3)-C(4)-C(15)	116.8(6)
C(5)-C(4)-C(15B)	115.0(7)
C(3)-C(4)-C(15B)	119.7(7)
C(15)-C(4)-C(15B)	25.7(5)
C(6)-C(5)-C(4)	122.1(4)
C(6)-C(5)-H(5)	119.0
C(4)-C(5)-H(5)	119.0
C(5)-C(6)-C(7)	122.1(4)
C(5)-C(6)-H(6)	118.9
C(7)-C(6)-H(6)	118.9
C(8)-C(7)-C(6)	123.3(4)
C(8)-C(7)-C(17B)	116.9(5)
C(6)-C(7)-C(17B)	117.0(5)
C(8)-C(7)-C(17)	120.0(5)
C(6)-C(7)-C(17)	114.6(5)
C(17B)-C(7)-C(17)	32.1(4)
C(7)-C(8)-C(9)	122.1(4)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(10)-C(9)-C(8)	119.3(4)
C(10)-C(9)-C(23)	120.0(5)
C(8)-C(9)-C(23)	120.7(4)
C(9)-C(10)-C(11)	124.7(4)
C(9)-C(10)-H(10)	117.7
C(11)-C(10)-H(10)	117.7
C(10)-C(11)-C(12)	126.2(4)
C(10)-C(11)-C(17B)	114.4(5)
C(12)-C(11)-C(17B)	116.5(5)
C(10)-C(11)-C(17)	117.1(5)
C(12)-C(11)-C(17)	114.9(4)
C(17B)-C(11)-C(17)	32.8(4)
C(11)-C(12)-C(13)	120.7(3)
C(11)-C(12)-C(27)	119.1(3)
C(13)-C(12)-C(27)	120.2(3)
C(14)-C(13)-C(12)	121.9(3)
C(14)-C(13)-C(32)	120.2(3)
C(12)-C(13)-C(32)	117.6(3)
C(1)-C(14)-C(13)	125.7(3)
C(1)-C(14)-C(15)	114.6(6)
C(13)-C(14)-C(15)	117.7(5)
C(1)-C(14)-C(15B)	119.2(6)
C(13)-C(14)-C(15B)	114.2(6)
C(15)-C(14)-C(15B)	25.7(5)
C(4)-C(15)-C(17)	109.2(10)

C(4)-C(15)-C(14)	114.3(9)
C(17)-C(15)-C(14)	107.4(10)
C(4)-C(15)-C(16)	107.9(9)
C(17)-C(15)-C(16)	110.9(13)
C(14)-C(15)-C(16)	107.2(9)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-C(11)	108.4(9)
C(15)-C(17)-C(7)	106.2(10)
C(11)-C(17)-C(7)	109.0(7)
C(15)-C(17)-C(18)	111.4(12)
C(11)-C(17)-C(18)	110.1(7)
C(7)-C(17)-C(18)	111.5(7)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(19)-C(20)	108.5(5)
C(22)-C(19)-C(2)	113.2(4)
C(20)-C(19)-C(2)	108.0(4)
C(22)-C(19)-C(21B)	128.9(8)
C(20)-C(19)-C(21B)	68.8(12)
C(2)-C(19)-C(21B)	115.8(8)
C(22)-C(19)-C(21)	107.0(6)
C(20)-C(19)-C(21)	111.3(6)
C(2)-C(19)-C(21)	108.9(4)
C(21B)-C(19)-C(21)	43.2(11)
C(22)-C(19)-C(22B)	36.7(10)
C(20)-C(19)-C(22B)	137.6(11)
C(2)-C(19)-C(22B)	109.3(9)
C(21B)-C(19)-C(22B)	110.7(13)
C(21)-C(19)-C(22B)	74.4(11)
C(22)-C(19)-C(20B)	69.8(9)
C(20)-C(19)-C(20B)	44.3(8)
C(2)-C(19)-C(20B)	104.8(7)
C(21B)-C(19)-C(20B)	109.6(13)
C(21)-C(19)-C(20B)	144.0(7)
C(22B)-C(19)-C(20B)	106.0(13)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5

C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(26)-C(23)-C(24B)	136.7(12)
C(26)-C(23)-C(24)	111.7(5)
C(24B)-C(23)-C(24)	46.0(11)
C(26)-C(23)-C(9)	109.6(4)
C(24B)-C(23)-C(9)	112.8(11)
C(24)-C(23)-C(9)	107.9(4)
C(26)-C(23)-C(25B)	60.7(8)
C(24B)-C(23)-C(25B)	108.6(7)
C(24)-C(23)-C(25B)	138.6(9)
C(9)-C(23)-C(25B)	112.8(9)
C(26)-C(23)-C(26B)	48.2(9)
C(24B)-C(23)-C(26B)	107.8(7)
C(24)-C(23)-C(26B)	66.5(10)
C(9)-C(23)-C(26B)	108.8(10)
C(25B)-C(23)-C(26B)	105.6(6)
C(26)-C(23)-C(25)	110.5(4)
C(24B)-C(23)-C(25)	61.2(10)
C(24)-C(23)-C(25)	105.8(4)
C(9)-C(23)-C(25)	111.3(5)
C(25B)-C(23)-C(25)	52.4(8)
C(26B)-C(23)-C(25)	139.4(10)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(1)-C(27)-C(28)	115.8(5)
O(1)-C(27)-C(12)	110.6(4)
C(28)-C(27)-C(12)	118.0(4)
O(1)-C(27)-H(27)	103.4
C(28)-C(27)-H(27)	103.4
C(12)-C(27)-H(27)	103.4
O(1)-C(27)-H(27B)	32.6(2)
C(28)-C(27)-H(27B)	99.0(5)
C(12)-C(27)-H(27B)	98.8(4)
H(27)-C(27)-H(27B)	135.9
C(27)-C(28)-C(29)	121.3(5)
C(27)-C(28)-H(28A)	107.0
C(29)-C(28)-H(28A)	107.0

C(27)-C(28)-H(28B)	107.0
C(29)-C(28)-H(28B)	107.0
H(28A)-C(28)-H(28B)	106.8
C(30)-C(29)-C(28)	123.7(6)
C(30)-C(29)-H(29)	118.2
C(28)-C(29)-H(29)	118.2
C(29)-C(30)-C(31)	129.9(6)
C(29)-C(30)-H(30)	115.0
C(31)-C(30)-H(30)	115.0
C(30)-C(31)-C(32)	119.2(4)
C(30)-C(31)-H(31A)	107.5
C(32)-C(31)-H(31A)	107.5
C(30)-C(31)-H(31B)	107.5
C(32)-C(31)-H(31B)	107.5
H(31A)-C(31)-H(31B)	107.0
O(2)-C(32)-C(31)	109.2(4)
O(2)-C(32)-C(13)	115.7(3)
C(31)-C(32)-C(13)	113.0(4)
O(2)-C(32)-H(32)	106.1
C(31)-C(32)-H(32)	106.1
C(13)-C(32)-H(32)	106.1
O(2)-C(32)-H(32B)	40.3(2)
C(31)-C(32)-H(32B)	92.5(4)
C(13)-C(32)-H(32B)	91.5(3)
H(32)-C(32)-H(32B)	146.3
Si(1)-C(33)-H(33A)	109.5
Si(1)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
Si(1)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(1)-C(34)-H(34A)	109.5
Si(1)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(1)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Si(1)-C(35)-H(35A)	109.5
Si(1)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
Si(1)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
Si(2)-C(36)-H(36A)	109.5
Si(2)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
Si(2)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
Si(2)-C(37)-H(37A)	109.5
Si(2)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
Si(2)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
Si(2)-C(38)-H(38A)	109.5
Si(2)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
Si(2)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(27)-O(1)-Si(1B)	126.4(5)
C(27)-O(1)-H(27B)	40.7(3)
Si(1B)-O(1)-H(27B)	164.1(6)
C(32)-O(2)-Si(2)	123.4(3)
C(32)-O(2)-H(32B)	43.8(2)
Si(2)-O(2)-H(32B)	157.9(3)
C(33)-Si(1)-C(34)	107.0(8)
C(33)-Si(1)-O(1B)	106.5(6)
C(34)-Si(1)-O(1B)	85.9(5)
C(33)-Si(1)-C(35)	110.1(8)
C(34)-Si(1)-C(35)	109.8(6)
O(1B)-Si(1)-C(35)	133.0(7)
O(2)-Si(2)-C(38)	109.5(3)
O(2)-Si(2)-C(36)	108.7(3)
C(38)-Si(2)-C(36)	111.8(3)
O(2)-Si(2)-C(37)	105.2(3)
C(38)-Si(2)-C(37)	112.1(4)
C(36)-Si(2)-C(37)	109.2(3)
C(17B)-C(15B)-C(14)	109.6(11)
C(17B)-C(15B)-C(16B)	112.8(15)
C(14)-C(15B)-C(16B)	108.0(10)
C(17B)-C(15B)-C(4)	109.5(11)
C(14)-C(15B)-C(4)	110.3(10)
C(16B)-C(15B)-C(4)	106.6(10)
C(15B)-C(16B)-H(16D)	109.5
C(15B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(15B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
C(15B)-C(17B)-C(11)	106.7(11)
C(15B)-C(17B)-C(7)	105.1(11)
C(11)-C(17B)-C(7)	111.3(7)
C(15B)-C(17B)-C(18B)	111.2(14)
C(11)-C(17B)-C(18B)	110.8(8)
C(7)-C(17B)-C(18B)	111.6(8)
C(17B)-C(18B)-H(18D)	109.5
C(17B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
O(1)-Si(1B)-C(35B)	102.2(11)
O(1)-Si(1B)-C(34B)	119.3(9)
C(35B)-Si(1B)-C(34B)	102.9(13)
O(1)-Si(1B)-C(33B)	98.0(14)
C(35B)-Si(1B)-C(33B)	121.5(18)
C(34B)-Si(1B)-C(33B)	113.6(17)
Si(1B)-C(35B)-H(35D)	109.5
Si(1B)-C(35B)-H(35E)	109.5
H(35D)-C(35B)-H(35E)	109.5
Si(1B)-C(35B)-H(35F)	109.5
H(35D)-C(35B)-H(35F)	109.5

H(35E)-C(35B)-H(35F)	109.5
Si(1B)-C(34B)-H(34D)	109.5
Si(1B)-C(34B)-H(34E)	109.5
H(34D)-C(34B)-H(34E)	109.5
Si(1B)-C(34B)-H(34F)	109.5
H(34D)-C(34B)-H(34F)	109.5
H(34E)-C(34B)-H(34F)	109.5
Si(1B)-C(33B)-H(33D)	109.5
Si(1B)-C(33B)-H(33E)	109.5
H(33D)-C(33B)-H(33E)	109.5
Si(1B)-C(33B)-H(33F)	109.5
H(33D)-C(33B)-H(33F)	109.5
H(33E)-C(33B)-H(33F)	109.5
C(19)-C(22B)-H(22D)	109.5
C(19)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
C(19)-C(22B)-H(22F)	109.5
H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
C(19)-C(21B)-H(21D)	109.5
C(19)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5
C(19)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(19)-C(20B)-H(20D)	109.5
C(19)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(19)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
O(2B)-Si(2B)-C(38B)	112.1(11)
O(2B)-Si(2B)-C(37B)	111.3(10)
C(38B)-Si(2B)-C(37B)	111.9(7)
O(2B)-Si(2B)-C(36B)	92.5(18)
C(38B)-Si(2B)-C(36B)	122(2)
C(37B)-Si(2B)-C(36B)	105(2)
Si(2B)-C(38B)-H(38D)	109.5
Si(2B)-C(38B)-H(38E)	109.5
H(38D)-C(38B)-H(38E)	109.5
Si(2B)-C(38B)-H(38F)	109.5
H(38D)-C(38B)-H(38F)	109.5
H(38E)-C(38B)-H(38F)	109.5
Si(2B)-C(37B)-H(37D)	109.5
Si(2B)-C(37B)-H(37E)	109.5
H(37D)-C(37B)-H(37E)	109.5
Si(2B)-C(37B)-H(37F)	109.5
H(37D)-C(37B)-H(37F)	109.5
H(37E)-C(37B)-H(37F)	109.5
Si(2B)-C(36B)-H(36D)	109.5
Si(2B)-C(36B)-H(36E)	109.5
H(36D)-C(36B)-H(36E)	109.5
Si(2B)-C(36B)-H(36F)	109.5
H(36D)-C(36B)-H(36F)	109.5
H(36E)-C(36B)-H(36F)	109.5
C(23)-C(26B)-H(26D)	109.5
C(23)-C(26B)-H(26E)	109.5

H(26D)-C(26B)-H(26E)	109.5
C(23)-C(26B)-H(26F)	109.5
H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5
C(23)-C(25B)-H(25D)	109.5
C(23)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
C(23)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(23)-C(24B)-H(24D)	109.5
C(23)-C(24B)-H(24E)	109.5
H(24D)-C(24B)-H(24E)	109.5
C(23)-C(24B)-H(24F)	109.5
H(24D)-C(24B)-H(24F)	109.5
H(24E)-C(24B)-H(24F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for db007.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	60(2)	41(2)	44(2)	3(2)	0(2)	18(2)
C(2)	72(3)	41(2)	47(2)	1(2)	1(2)	22(2)
C(3)	90(3)	51(2)	44(2)	-3(2)	4(2)	33(2)
C(4)	90(3)	49(2)	42(2)	0(2)	2(2)	24(2)
C(5)	130(4)	69(3)	43(3)	2(2)	3(3)	41(3)
C(6)	123(4)	75(3)	47(3)	12(2)	-6(3)	39(3)
C(7)	101(4)	66(3)	60(3)	12(2)	-5(3)	37(3)
C(8)	102(4)	67(3)	76(3)	24(3)	-3(3)	32(3)
C(9)	78(3)	57(3)	98(4)	24(3)	-6(3)	26(2)
C(10)	64(3)	50(3)	83(3)	6(2)	0(2)	20(2)
C(11)	56(3)	46(2)	68(3)	4(2)	4(2)	21(2)
C(12)	47(2)	35(2)	60(3)	-3(2)	6(2)	7(2)
C(13)	49(2)	39(2)	47(2)	-4(2)	4(2)	6(2)
C(14)	53(2)	34(2)	43(2)	1(2)	-2(2)	9(2)
C(15)	63(8)	43(7)	47(5)	4(5)	-1(6)	27(6)
C(16)	59(6)	53(6)	60(5)	9(5)	10(4)	20(5)
C(17)	61(7)	41(6)	55(5)	2(4)	-6(5)	18(5)
C(18)	62(6)	49(6)	75(6)	-2(5)	-32(5)	17(5)
C(19)	81(3)	50(2)	56(3)	1(2)	2(2)	36(2)
C(20)	157(8)	44(4)	68(6)	2(4)	-28(5)	46(4)
C(21)	114(8)	113(8)	98(8)	27(6)	13(6)	73(6)
C(22)	102(8)	70(6)	61(5)	-6(4)	-24(5)	55(6)
C(23)	108(5)	79(4)	108(4)	30(3)	-4(4)	54(3)
C(24)	95(6)	91(5)	130(7)	-5(5)	-34(5)	59(4)
C(25)	154(9)	99(7)	146(8)	48(6)	-16(6)	76(6)
C(26)	194(11)	31(4)	270(14)	6(6)	-119(10)	36(5)
C(28)	122(5)	104(5)	152(6)	-74(4)	-3(4)	27(4)
C(29)	108(5)	66(3)	90(4)	-21(3)	0(3)	-9(3)
C(30)	86(4)	79(4)	103(4)	-27(3)	-22(3)	2(3)
C(31)	161(6)	74(4)	87(4)	-5(3)	-47(4)	13(4)
C(33)	72(7)	165(12)	209(18)	-56(13)	0(11)	-17(7)
C(34)	145(12)	100(9)	202(16)	31(9)	95(11)	22(8)
C(35)	156(13)	142(12)	340(20)	128(13)	125(15)	100(11)
C(36)	153(7)	92(5)	105(6)	28(4)	68(5)	52(5)
C(37)	150(8)	38(5)	113(6)	12(4)	31(6)	21(5)
C(38)	108(7)	194(11)	99(7)	21(7)	-14(5)	-47(7)
O(1)	83(3)	53(3)	112(4)	23(3)	49(3)	34(2)
O(2)	72(3)	50(2)	56(2)	8(2)	17(2)	26(2)
Si(1)	66(3)	117(4)	114(4)	19(3)	25(3)	35(2)
Si(2)	87(2)	64(2)	61(1)	20(1)	24(1)	26(2)
C(15B)	61(9)	41(7)	46(6)	4(5)	3(7)	18(6)
C(16B)	62(8)	46(6)	60(6)	7(5)	-22(5)	15(5)
C(17B)	59(7)	41(6)	46(5)	9(4)	0(5)	7(5)
C(18B)	58(7)	48(7)	71(7)	14(5)	7(5)	12(5)
O(1B)	69(6)	63(6)	91(7)	2(5)	5(5)	38(5)
Si(1B)	43(3)	80(4)	92(6)	-13(4)	5(4)	21(2)
C(35B)	170(30)	150(20)	121(19)	10(17)	-8(16)	90(20)
C(34B)	87(14)	53(11)	170(20)	8(11)	36(13)	48(10)

C(33B)	150(20)	230(30)	90(20)	-90(20)	-20(17)	-70(20)
C(22B)	62(15)	77(16)	110(20)	-22(13)	-23(13)	34(11)
C(21B)	130(20)	94(17)	60(12)	-17(11)	-7(12)	81(16)
C(20B)	89(13)	48(10)	104(19)	8(11)	-6(12)	20(9)
O(2B)	106(13)	86(12)	85(11)	16(9)	34(10)	18(10)
Si(2B)	201(19)	121(12)	120(16)	22(10)	33(13)	-56(11)
C(38B)	120(20)	90(20)	80(20)	-22(16)	-20(18)	-7(18)
C(37B)	140(20)	31(16)	32(12)	-14(11)	17(13)	-26(16)
C(36B)	160(30)	160(40)	270(50)	-30(30)	70(30)	60(30)
C(26B)	100(20)	100(20)	190(30)	120(20)	20(20)	31(18)
C(25B)	120(20)	29(11)	64(16)	7(11)	-10(14)	10(12)
C(24B)	100(20)	130(20)	190(30)	-10(30)	-110(20)	42(19)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for db007.

	x	y	z	U(eq)
H(1)	15203	1063	3082	57
H(3)	15875	413	926	73
H(5)	14899	1772	-77	95
H(6)	13767	3558	-434	97
H(8)	12566	5466	-113	97
H(10)	11830	6184	2031	78
H(16A)	15389	4677	2074	84
H(16B)	15659	4446	1213	84
H(16C)	16410	3638	1856	84
H(18A)	11081	2740	1157	95
H(18B)	11831	1939	1803	95
H(18C)	12083	1678	942	95
H(20A)	16280	-2561	2163	134
H(20B)	15581	-1831	1469	134
H(20C)	14911	-1909	2251	134
H(21A)	18404	-1065	2052	156
H(21B)	18314	498	2070	156
H(21C)	17677	-362	1357	156
H(22A)	17399	-1323	3225	115
H(22B)	16035	-701	3366	115
H(22C)	17355	242	3284	115
H(24A)	9549	6125	576	158
H(24B)	9421	7670	692	158
H(24C)	9867	6797	1392	158
H(25A)	10920	6625	-432	195
H(25B)	12279	7543	-309	195
H(25C)	10884	8180	-304	195
H(26A)	12920	8547	985	256
H(26B)	11957	8266	1644	256
H(26C)	11508	9159	953	256
H(27)	11972	5685	3008	76
H(28A)	13148	5316	4361	152
H(28B)	13030	6619	3888	152
H(29)	15165	6620	3654	107
H(30)	16420	5048	3906	110
H(31A)	15067	3435	4674	132
H(31B)	15866	2937	4006	132
H(32)	13135	3178	4004	70
H(33A)	9694	2735	2283	227
H(33B)	9632	4128	1881	227
H(33C)	8308	3388	2159	227
H(34A)	8974	6424	3576	216
H(34B)	7861	5763	2972	216
H(34C)	9208	6466	2701	216
H(35A)	8999	3798	4425	301
H(35B)	9194	2488	3955	301
H(35C)	7847	3207	3822	301
H(36A)	12505	1817	5405	167
H(36B)	11028	1195	5169	167

H(36C)	11588	2515	4785	167
H(37A)	13685	-678	5081	148
H(37B)	13455	-1385	4271	148
H(37C)	12275	-1432	4819	148
H(38A)	11598	-191	3060	206
H(38B)	10994	1181	3223	206
H(38C)	10429	-133	3610	206
H(16D)	12447	885	1519	85
H(16E)	12081	1941	896	85
H(16F)	11778	2189	1750	85
H(18D)	15217	5663	1524	87
H(18E)	15855	4343	1290	87
H(18F)	15544	4589	2143	87
H(35D)	9507	3303	4434	216
H(35E)	8436	4380	4376	216
H(35F)	9905	4770	4749	216
H(34D)	9963	6768	3076	147
H(34E)	9986	6825	3972	147
H(34F)	8614	6475	3477	147
H(33D)	9433	2821	2745	244
H(33E)	9658	4127	2266	244
H(33F)	8266	3787	2617	244
H(22D)	18112	-772	3061	126
H(22E)	17120	249	3339	126
H(22F)	18142	683	2731	126
H(21D)	17695	-1906	1842	140
H(21E)	17776	-542	1405	140
H(21F)	16495	-1565	1259	140
H(20D)	16014	-2348	2803	121
H(20E)	14806	-1889	2264	121
H(20F)	15166	-1188	3068	121
H(38D)	11324	-32	2744	150
H(38E)	11618	-1386	3147	150
H(38F)	12816	-450	2863	150
H(37D)	13400	89	5147	105
H(37E)	14237	-294	4464	105
H(37F)	13063	-1298	4715	105
H(36D)	11032	1142	5017	290
H(36E)	10237	-154	4643	290
H(36F)	10119	1241	4251	290
H(26D)	10522	8696	1253	195
H(26E)	11811	8217	1714	195
H(26F)	10431	7328	1685	195
H(25D)	11711	8974	141	106
H(25E)	12510	7821	-179	106
H(25F)	13017	8537	605	106
H(24D)	9668	7636	69	216
H(24E)	9506	6256	484	216
H(24F)	10312	6378	-251	216
H(32B)	14309	1995	3663	100
H(27B)	12055	4261	3617	100

Table 6. Torsion angles [deg] for db007.

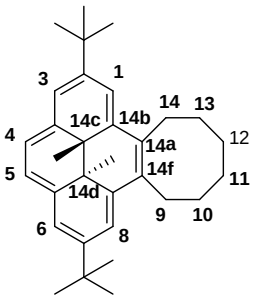
C(14)-C(1)-C(2)-C(3)	-0.4(6)
C(14)-C(1)-C(2)-C(19)	-179.8(4)
C(1)-C(2)-C(3)-C(4)	1.3(7)
C(19)-C(2)-C(3)-C(4)	-179.3(4)
C(2)-C(3)-C(4)-C(5)	178.8(5)
C(2)-C(3)-C(4)-C(15)	15.2(9)
C(2)-C(3)-C(4)-C(15B)	-13.8(9)
C(3)-C(4)-C(5)-C(6)	-176.0(5)
C(15)-C(4)-C(5)-C(6)	-12.5(10)
C(15B)-C(4)-C(5)-C(6)	16.1(10)
C(4)-C(5)-C(6)-C(7)	-0.8(9)
C(5)-C(6)-C(7)-C(8)	177.6(5)
C(5)-C(6)-C(7)-C(17B)	17.0(10)
C(5)-C(6)-C(7)-C(17)	-18.7(9)
C(6)-C(7)-C(8)-C(9)	-179.0(5)
C(17B)-C(7)-C(8)-C(9)	-18.4(10)
C(17)-C(7)-C(8)-C(9)	18.1(10)
C(7)-C(8)-C(9)-C(10)	-1.4(8)
C(7)-C(8)-C(9)-C(23)	-178.6(5)
C(8)-C(9)-C(10)-C(11)	0.9(8)
C(23)-C(9)-C(10)-C(11)	178.1(4)
C(9)-C(10)-C(11)-C(12)	179.4(4)
C(9)-C(10)-C(11)-C(17B)	19.6(9)
C(9)-C(10)-C(11)-C(17)	-16.9(9)
C(10)-C(11)-C(12)-C(13)	-176.9(4)
C(17B)-C(11)-C(12)-C(13)	-17.4(8)
C(17)-C(11)-C(12)-C(13)	19.1(8)
C(10)-C(11)-C(12)-C(27)	0.4(6)
C(17B)-C(11)-C(12)-C(27)	159.9(7)
C(17)-C(11)-C(12)-C(27)	-163.6(6)
C(11)-C(12)-C(13)-C(14)	0.3(6)
C(27)-C(12)-C(13)-C(14)	-177.0(3)
C(11)-C(12)-C(13)-C(32)	174.2(4)
C(27)-C(12)-C(13)-C(32)	-3.1(5)
C(2)-C(1)-C(14)-C(13)	-179.3(4)
C(2)-C(1)-C(14)-C(15)	-16.2(8)
C(2)-C(1)-C(14)-C(15B)	12.2(9)
C(12)-C(13)-C(14)-C(1)	175.4(4)
C(32)-C(13)-C(14)-C(1)	1.6(6)
C(12)-C(13)-C(14)-C(15)	12.7(8)
C(32)-C(13)-C(14)-C(15)	-161.1(7)
C(12)-C(13)-C(14)-C(15B)	-15.7(8)
C(32)-C(13)-C(14)-C(15B)	170.5(7)
C(5)-C(4)-C(15)-C(17)	44.2(14)
C(3)-C(4)-C(15)-C(17)	-151.0(9)
C(15B)-C(4)-C(15)-C(17)	-48(2)
C(5)-C(4)-C(15)-C(14)	164.5(7)
C(3)-C(4)-C(15)-C(14)	-30.7(12)
C(15B)-C(4)-C(15)-C(14)	73(2)
C(5)-C(4)-C(15)-C(16)	-76.4(9)
C(3)-C(4)-C(15)-C(16)	88.4(10)
C(15B)-C(4)-C(15)-C(16)	-168(3)
C(1)-C(14)-C(15)-C(4)	30.8(11)
C(13)-C(14)-C(15)-C(4)	-164.6(6)

C(15B)-C(14)-C(15)-C(4)	-76(2)
C(1)-C(14)-C(15)-C(17)	152.1(8)
C(13)-C(14)-C(15)-C(17)	-43.3(13)
C(15B)-C(14)-C(15)-C(17)	45.5(19)
C(1)-C(14)-C(15)-C(16)	-88.6(9)
C(13)-C(14)-C(15)-C(16)	76.0(8)
C(15B)-C(14)-C(15)-C(16)	165(3)
C(4)-C(15)-C(17)-C(11)	-176.1(7)
C(14)-C(15)-C(17)-C(11)	59.5(14)
C(16)-C(15)-C(17)-C(11)	-57.4(12)
C(4)-C(15)-C(17)-C(7)	-59.1(14)
C(14)-C(15)-C(17)-C(7)	176.4(6)
C(16)-C(15)-C(17)-C(7)	59.6(11)
C(4)-C(15)-C(17)-C(18)	62.5(12)
C(14)-C(15)-C(17)-C(18)	-61.9(11)
C(16)-C(15)-C(17)-C(18)	-178.8(8)
C(10)-C(11)-C(17)-C(15)	144.4(9)
C(12)-C(11)-C(17)-C(15)	-50.1(13)
C(17B)-C(11)-C(17)-C(15)	50.7(12)
C(10)-C(11)-C(17)-C(7)	29.2(10)
C(12)-C(11)-C(17)-C(7)	-165.2(5)
C(17B)-C(11)-C(17)-C(7)	-64.4(11)
C(10)-C(11)-C(17)-C(18)	-93.4(8)
C(12)-C(11)-C(17)-C(18)	72.1(7)
C(17B)-C(11)-C(17)-C(18)	172.9(14)
C(8)-C(7)-C(17)-C(15)	-147.4(8)
C(6)-C(7)-C(17)-C(15)	48.3(12)
C(17B)-C(7)-C(17)-C(15)	-53.8(12)
C(8)-C(7)-C(17)-C(11)	-30.8(11)
C(6)-C(7)-C(17)-C(11)	164.9(6)
C(17B)-C(7)-C(17)-C(11)	62.8(10)
C(8)-C(7)-C(17)-C(18)	91.0(9)
C(6)-C(7)-C(17)-C(18)	-73.3(8)
C(17B)-C(7)-C(17)-C(18)	-175.4(14)
C(3)-C(2)-C(19)-C(22)	168.4(6)
C(1)-C(2)-C(19)-C(22)	-12.1(8)
C(3)-C(2)-C(19)-C(20)	-71.4(7)
C(1)-C(2)-C(19)-C(20)	108.1(6)
C(3)-C(2)-C(19)-C(21B)	3.3(16)
C(1)-C(2)-C(19)-C(21B)	-177.3(15)
C(3)-C(2)-C(19)-C(21)	49.6(8)
C(1)-C(2)-C(19)-C(21)	-131.0(7)
C(3)-C(2)-C(19)-C(22B)	129.1(14)
C(1)-C(2)-C(19)-C(22B)	-51.4(14)
C(3)-C(2)-C(19)-C(20B)	-117.6(11)
C(1)-C(2)-C(19)-C(20B)	61.9(11)
C(10)-C(9)-C(23)-C(26)	58.7(7)
C(8)-C(9)-C(23)-C(26)	-124.2(7)
C(10)-C(9)-C(23)-C(24B)	-112.2(13)
C(8)-C(9)-C(23)-C(24B)	65.0(14)
C(10)-C(9)-C(23)-C(24)	-63.2(6)
C(8)-C(9)-C(23)-C(24)	114.0(6)
C(10)-C(9)-C(23)-C(25B)	124.2(11)
C(8)-C(9)-C(23)-C(25B)	-58.6(11)
C(10)-C(9)-C(23)-C(26B)	7.4(12)
C(8)-C(9)-C(23)-C(26B)	-175.4(12)
C(10)-C(9)-C(23)-C(25)	-178.9(5)

C(8)-C(9)-C(23)-C(25)	-1.7(7)
C(11)-C(12)-C(27)-O(1)	110.7(4)
C(13)-C(12)-C(27)-O(1)	-71.9(5)
C(11)-C(12)-C(27)-C(28)	-112.6(5)
C(13)-C(12)-C(27)-C(28)	64.7(6)
O(1)-C(27)-C(28)-C(29)	142.9(6)
C(12)-C(27)-C(28)-C(29)	8.4(9)
C(27)-C(28)-C(29)-C(30)	-73.7(9)
C(28)-C(29)-C(30)-C(31)	4.2(10)
C(29)-C(30)-C(31)-C(32)	37.1(9)
C(30)-C(31)-C(32)-O(2)	172.9(5)
C(30)-C(31)-C(32)-C(13)	42.6(7)
C(14)-C(13)-C(32)-O(2)	-43.2(5)
C(12)-C(13)-C(32)-O(2)	142.8(4)
C(14)-C(13)-C(32)-C(31)	83.7(5)
C(12)-C(13)-C(32)-C(31)	-90.3(5)
C(28)-C(27)-O(1)-Si(1B)	103.0(7)
C(12)-C(27)-O(1)-Si(1B)	-119.3(6)
C(31)-C(32)-O(2)-Si(2)	133.5(4)
C(13)-C(32)-O(2)-Si(2)	-97.7(4)
C(32)-O(2)-Si(2)-C(38)	73.9(5)
C(32)-O(2)-Si(2)-C(36)	-48.5(4)
C(32)-O(2)-Si(2)-C(37)	-165.4(4)
C(1)-C(14)-C(15B)-C(17B)	-142.6(10)
C(13)-C(14)-C(15B)-C(17B)	47.6(14)
C(15)-C(14)-C(15B)-C(17B)	-56(2)
C(1)-C(14)-C(15B)-C(16B)	94.1(11)
C(13)-C(14)-C(15B)-C(16B)	-75.6(10)
C(15)-C(14)-C(15B)-C(16B)	-179(3)
C(1)-C(14)-C(15B)-C(4)	-21.9(12)
C(13)-C(14)-C(15B)-C(4)	168.4(6)
C(15)-C(14)-C(15B)-C(4)	64(2)
C(5)-C(4)-C(15B)-C(17B)	-47.8(15)
C(3)-C(4)-C(15B)-C(17B)	143.7(10)
C(15)-C(4)-C(15B)-C(17B)	53(2)
C(5)-C(4)-C(15B)-C(14)	-168.6(7)
C(3)-C(4)-C(15B)-C(14)	22.9(12)
C(15)-C(4)-C(15B)-C(14)	-68(2)
C(5)-C(4)-C(15B)-C(16B)	74.4(10)
C(3)-C(4)-C(15B)-C(16B)	-94.1(11)
C(15)-C(4)-C(15B)-C(16B)	175(3)
C(14)-C(15B)-C(17B)-C(11)	-61.6(15)
C(16B)-C(15B)-C(17B)-C(11)	58.8(14)
C(4)-C(15B)-C(17B)-C(11)	177.3(7)
C(14)-C(15B)-C(17B)-C(7)	-179.8(7)
C(16B)-C(15B)-C(17B)-C(7)	-59.4(14)
C(4)-C(15B)-C(17B)-C(7)	59.0(15)
C(14)-C(15B)-C(17B)-C(18B)	59.3(13)
C(16B)-C(15B)-C(17B)-C(18B)	179.7(10)
C(4)-C(15B)-C(17B)-C(18B)	-61.9(13)
C(10)-C(11)-C(17B)-C(15B)	-150.1(9)
C(12)-C(11)-C(17B)-C(15B)	48.0(14)
C(17)-C(11)-C(17B)-C(15B)	-47.5(12)
C(10)-C(11)-C(17B)-C(7)	-36.0(11)
C(12)-C(11)-C(17B)-C(7)	162.1(6)
C(17)-C(11)-C(17B)-C(7)	66.6(12)
C(10)-C(11)-C(17B)-C(18B)	88.8(8)

C(12)-C(11)-C(17B)-C(18B)	-73.1(8)
C(17)-C(11)-C(17B)-C(18B)	-168.6(14)
C(8)-C(7)-C(17B)-C(15B)	151.6(9)
C(6)-C(7)-C(17B)-C(15B)	-46.5(14)
C(17)-C(7)-C(17B)-C(15B)	47.3(12)
C(8)-C(7)-C(17B)-C(11)	36.6(12)
C(6)-C(7)-C(17B)-C(11)	-161.5(6)
C(17)-C(7)-C(17B)-C(11)	-67.7(11)
C(8)-C(7)-C(17B)-C(18B)	-87.8(9)
C(6)-C(7)-C(17B)-C(18B)	74.1(8)
C(17)-C(7)-C(17B)-C(18B)	167.9(15)
C(27)-O(1)-Si(1B)-C(35B)	-140.5(12)
C(27)-O(1)-Si(1B)-C(34B)	-28.0(13)
C(27)-O(1)-Si(1B)-C(33B)	94.8(16)

Computational Results



Comparison of Selected Experimental and Calculated ^{1}H NMR Chemical Shifts

	5			**6**	
Proton	**Expt**	**Calc**		**Expt**	**C2InvS**
1	8.45	8.99		7.18	6.08
3	8.34	8.81		6.70	5.82
4	8.22	8.55		6.64	5.81
5	8.22	8.54		6.64	5.81
6	8.34	8.81		6.70	5.82
8	8.45	8.91		7.18	6.08
9	7.65	7.91		7.37	7.30
10	6.48	6.52		6.42	6.09
11	6.05	6.05		6.11	6.03
12	6.05	6.22		6.11	6.03
13	6.48	6.56		6.42	6.09
14	7.65	7.71		7.37	7.30
2-C(CH_3)$_3$	1.64	1.75		1.47	1.43
7-C(CH_3)$_3$	1.64	1.75		1.47	1.43
14c-CH_3	-3.70	-4.45		-1.38	-1.43
14d-CH_3	-3.70	-4.56		-1.38	-1.43
14cdav		-4.51			-1.43

Energies and Coordinates for 5

SCF Done: E(RB3LYP) = -1241.00328947 A.U. after 1 cycles
Zero-point correction= 0.590687 (Hartree/Particle)
Thermal correction to Energy= 0.620296
Thermal correction to Enthalpy= 0.621240
Thermal correction to Gibbs Free Energy= 0.534064
Sum of electronic and zero-point Energies= -1240.412602
Sum of electronic and thermal Energies= -1240.382994
Sum of electronic and thermal Enthalpies= -1240.382050
Sum of electronic and thermal Free Energies= -1240.469226

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.515446	-0.904124	-0.006990
2	6	0	2.808354	0.305068	0.227035
3	6	0	1.424906	0.403033	0.193320
4	6	0	0.705880	1.600704	0.479238
5	6	0	-0.701174	1.629342	0.446004
6	6	0	-1.454038	0.421093	0.304018
7	6	0	-2.833905	0.377651	0.193584
8	6	0	-3.572874	-0.824841	0.020587
9	6	0	-2.882742	-2.026309	-0.145618
10	6	0	-1.482911	-2.100357	-0.095666
11	6	0	-0.761486	-3.260823	-0.369367
12	6	0	0.645382	-3.279408	-0.358665
13	6	0	1.393841	-2.108924	-0.249085
14	6	0	2.794936	-2.084082	-0.205301
15	6	0	-0.700634	-0.896595	0.416304
16	6	0	0.638273	-0.786407	-0.334430
17	6	0	-0.502310	-1.150012	1.952279
18	6	0	0.435675	-0.519423	-1.868623
19	6	0	1.510588	2.786764	0.885966
20	6	0	-1.473980	2.878867	0.645695
21	6	0	5.054696	-0.876022	0.025184
22	6	0	5.542275	-0.392759	1.413028
23	6	0	5.568688	0.096876	-1.064152
24	6	0	-5.108645	-0.741252	-0.054069
25	6	0	-5.650869	-0.106924	1.250149
26	6	0	-5.525813	0.135211	-1.260649
27	1	0	3.381446	1.195294	0.462632
28	1	0	-3.379195	1.315332	0.181975
29	1	0	-3.424867	-2.937368	-0.379244
30	1	0	-1.304879	-4.181430	-0.574448

31	1	0	1.166684	-4.228795	-0.466905
32	1	0	3.316654	-3.032667	-0.286194
33	1	0	0.043463	-2.080650	2.129118
34	1	0	0.040112	-0.326095	2.423508
35	1	0	-1.485088	-1.230023	2.426069
36	1	0	1.417364	-0.461246	-2.347486
37	1	0	-0.130735	-1.328304	-2.337766
38	1	0	-0.085856	0.426018	-2.038595
39	1	0	6.638535	-0.364585	1.441230
40	1	0	5.178635	0.612451	1.649076
41	1	0	5.198940	-1.067755	2.205256
42	1	0	6.664982	0.137594	-1.051882
43	1	0	5.251647	-0.230675	-2.060879
44	1	0	5.194664	1.114610	-0.912953
45	1	0	-6.744880	-0.034534	1.212365
46	1	0	-5.380473	-0.713492	2.122138
47	1	0	-5.255635	0.901463	1.409568
48	1	0	-6.619058	0.205233	-1.319031
49	1	0	-5.131497	1.153764	-1.185628
50	1	0	-5.162109	-0.295697	-2.200360
51	6	0	-5.769288	-2.123257	-0.218755
52	6	0	5.678010	-2.259551	-0.242597
53	1	0	-5.475912	-2.608174	-1.156556
54	1	0	-5.517075	-2.796255	0.608589
55	1	0	-6.859225	-2.010579	-0.234567
56	1	0	5.398389	-2.990936	0.524153
57	1	0	5.381695	-2.657586	-1.219684
58	1	0	6.770895	-2.178501	-0.235563
59	6	0	-1.392490	4.036875	-0.034921
60	6	0	-0.429582	4.429034	-1.068655
61	6	0	0.910773	4.399584	-0.949539
62	6	0	1.644507	3.954956	0.239790
63	1	0	-2.287934	2.800505	1.366204
64	1	0	-2.156499	4.786778	0.181190
65	1	0	-0.853522	4.891143	-1.961396
66	1	0	1.507657	4.838456	-1.750096
67	1	0	2.385066	4.660387	0.622526
68	1	0	2.140684	2.632395	1.763029

Energies and Coordinates for 6

SCF Done: E(RB3LYP) = -1240.94207670 A.U. after 2 cycles
Zero-point correction= 0.583516 (Hartree/Particle)
Thermal correction to Energy= 0.613354
Thermal correction to Enthalpy= 0.614298
Thermal correction to Gibbs Free Energy= 0.527419
Sum of electronic and zero-point Energies= -1240.358560
Sum of electronic and thermal Energies= -1240.328723
Sum of electronic and thermal Enthalpies= -1240.327779
Sum of electronic and thermal Free Energies= -1240.414658

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007213	3.543263	-0.925880
2	6	0	0.014738	2.811755	0.297286
3	6	0	-0.137451	1.428736	0.390372
4	6	0	-0.213494	0.724146	1.649745
5	6	0	0.213494	-0.724146	1.649745
6	6	0	0.137451	-1.428736	0.390372
7	6	0	-0.014738	-2.811755	0.297286
8	6	0	-0.007213	-3.543263	-0.925880
9	6	0	0.054232	-2.861211	-2.139817
10	6	0	0.099841	-1.450323	-2.198095
11	6	0	-0.003299	-0.709422	-3.370439
12	6	0	0.003299	0.709422	-3.370439
13	6	0	-0.099841	1.450323	-2.198095
14	6	0	-0.054232	2.861211	-2.139817
15	6	0	0.399698	-0.662976	-0.912524
16	6	0	-0.399698	0.662976	-0.912524
17	6	0	1.940181	-0.386068	-0.933456
18	6	0	-1.940181	0.386068	-0.933456
19	6	0	-0.747775	1.471820	2.723488
20	6	0	0.747775	-1.471820	2.723488
21	6	0	0.145442	5.077428	-0.856897
22	6	0	1.494027	5.458735	-0.197809
23	6	0	-1.009469	5.671321	-0.013495
24	6	0	-0.145442	-5.077428	-0.856897
25	6	0	1.009469	-5.671321	-0.013495
26	6	0	-1.494027	-5.458735	-0.197809
27	1	0	0.204247	3.351918	1.220562
28	1	0	-0.204247	-3.351918	1.220562
29	1	0	-0.013184	-3.397385	-3.085372
30	1	0	-0.076816	-1.241751	-4.322571

31	1	0	0.076816	1.241751	-4.322571
32	1	0	0.013184	3.397385	-3.085372
33	1	0	2.230591	0.157859	-1.838230
34	1	0	2.237475	0.191889	-0.053240
35	1	0	2.470342	-1.345383	-0.912510
36	1	0	-2.470342	1.345383	-0.912510
37	1	0	-2.230591	-0.157859	-1.838230
38	1	0	-2.237475	-0.191889	-0.053240
39	1	0	1.604053	6.551987	-0.115350
40	1	0	1.581119	5.030634	0.805063
41	1	0	2.330210	5.073526	-0.793764
42	1	0	-0.914832	6.765141	0.080609
43	1	0	-1.976330	5.450075	-0.482066
44	1	0	-1.027645	5.239788	0.991444
45	1	0	0.914832	-6.765141	0.080609
46	1	0	1.976330	-5.450075	-0.482066
47	1	0	1.027645	-5.239788	0.991444
48	1	0	-1.604053	-6.551987	-0.115350
49	1	0	-1.581119	-5.030634	0.805063
50	1	0	-2.330210	-5.073526	-0.793764
51	6	0	-0.099841	-5.748354	-2.243631
52	6	0	0.099841	5.748354	-2.243631
53	1	0	-0.930727	-5.417899	-2.877517
54	1	0	0.833948	-5.516404	-2.768937
55	1	0	-0.169650	-6.840693	-2.138339
56	1	0	0.930727	5.417899	-2.877517
57	1	0	-0.833948	5.516404	-2.768937
58	1	0	0.169650	6.840693	-2.138339
59	6	0	0.909494	-1.372894	4.125290
60	6	0	0.423839	-0.561790	5.151795
61	6	0	-0.423839	0.561790	5.151795
62	6	0	-0.909494	1.372894	4.125290
63	1	0	1.222197	-2.382942	2.358356
64	1	0	1.542462	-2.183835	4.504485
65	1	0	0.735899	-0.883425	6.151808
66	1	0	-0.735899	0.883425	6.151808
67	1	0	-1.542462	2.183835	4.504485
68	1	0	-1.222197	2.382942	2.358356
