(Supporting Information)

Fine-Tuning of Boron Complexes with Cage-Shaped Ligand Geometry: Rational Design of Triphenolic Ligand as a Template for Structure-Control

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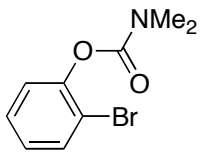
General. IR spectra were recorded as thin films or as solids in KBr pellets on a HORIBA FT-720 spectrophotometer. ^{1}H and ^{13}C NMR spectra were obtained with a 400 and 100 MHz spectrophotometer. ^{1}H, ^{13}C, and ^{29}Si NMR spectra were obtained with a 400, 100, and 78.7 MHz spectrometer, respectively, with TMS as internal standard. ^{11}B NMR spectra were obtained with a 127 MHz spectrometer with $BF_3 \cdot OEt_2$ as external standard. Mass spectra were recorded on a JEOL JMS-DS303. All reactions were carried out under nitrogen. Synthesis of boron-complexes was performed in nitrogen filled glove box.

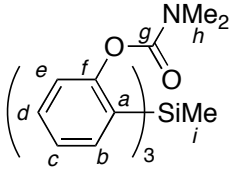
Materials. Dehydrated dichloromethane THF, and hexane were purchased and used as obtained. The compound **1**H_3 and its complexes **1**B·L (L = THF or pyridine) were prepared according to our previous report.[1] All other reagents are commercially available.

***o*-Bromopheneyl *N*,*N*-dimethylcarbamate (5)**



A 300 mL, three-necked, round-bottomed flask is equipped with a magnetic stirring bar, glass stopper, dropping funnel, and a reflux condenser under nitrogen. To a solution of NaH (300 mmol) in THF (40 mL) was slowly added *o*-bromophenol **5** (100 mmol) in THF (50 mmol) at 0 °C. After stirring for 1h, the dropping funnel was charged with *N*,*N*-dimethylcarbamoyl chloride (200 mmol) and THF (50 mL). The carbamoyl solution was slowly added to the flask and stirred for 1 h to keep at 0 °C. After stirring with warming up to rt for 12 h, H_2O (50 mL) was added to quench the reaction at 0 °C. The resultant mixture was extracted with diethyl ether (50 mL x 3). The combined organic layer was dried ($MgSO_4$) and evaporated to give the crude product, which was distilled at reduced pressure to give the pure product (93%). The spectral data of the product was in an excellent agreement with the reported data.[2] bp: 100-105 °C/ 0.1 mmHg; ^{1}H NMR: (400 MHz, $CDCl_3$) 7.57 (d, *J* = 7.9 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.21 (d, *J* = 7.9 Hz, 1H), 7.07 (t, *J* = 7.9 Hz, 1H), 3.15 (s, 3H), 3.02 (s, 3H); ^{13}C NMR: (100 MHz, $CDCl_3$) 153.6, 148.7, 132.9, 128.2, 126.6, 124.1, 116.3, 36.7, 36.4

Tris(2-*N*,*N*-dimethylcarbamoyloxyphenyl)(methyl)silane (6a)

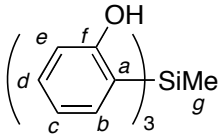


A 100 mL, three-necked, round-bottomed flask is equipped with a magnetic stirring bar, glass stopper, dropping funnel, and a reflux condenser under nitrogen. To a solution of *N*,*N*,*N'*,*N'*-tetramethylethylenediamine (2 mmol) in THF (20 mL) was slowly added Bu^{t}Li in hexane (40 mmol) at -80 °C. The color of suspension changed from yellow to pale yellow. The dropping funnel was charged with *o*-bromophneyl *N*,*N*-dimethylcarbamate **5** (20 mmol) and THF (10 mL). The carbamate solution was slowly added to the flask and stirred for 1 h to keep at -80 °C. Then $MeSiCl_3$ (7 mmol) was added to the flask. After stirring with warming up to rt for 12 h, H_2O (3 mL) was added to quench the reaction. The formed white precipitate was filtered off and the obtained solid was dissolved in dichloromethane (200 mL) and washed by water (100 mL x 3). The combined organic layer was dried ($MgSO_4$) and evaporated to give the crude product **6a**

(41%). The crude product was employed for the next step. For further purification, it was recrystallized to give the pure product. (dichloromethane/hexane = 1/6)

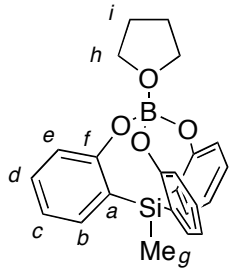
mp: 259-260 °C; ^{1}H NMR: (400 MHz, $CDCl_3$); 7.43 (ddd, *J* = 7.1 Hz, 7.1 Hz, 1.4 Hz, 3H, d-H), 7.30 (dd, *J* = 7.1 Hz, 1.4 Hz, 3H, b-H), 7.17 (dd, 7.1 Hz, 1.4 Hz, 3H, e-H), 7.13 (ddd, *J* = 7.1 Hz, 7.1 Hz, 1.4 Hz, 3H, c-H), 2.80 (s, 9H, h-H_3), 2.51 (s, 9H, h-H_3), 0.67 (s, 3H, i-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 156.3 (f), 154.2 (g), 136.8 (b), 130.9 (d), 127.1 (a), 124.5 (c), 122.3 (e), 36.5 (h), 35.9 (h), -2.34 (i); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -11.78; IR (KBr) 1724 (C=O) cm^{-1}; MS: (CI, 200 eV) *m*/*z* 537 (M^+ + 2, 35), 536 (M^+ + 1, 100), 371 ($M^+ - C_6H_4OC(O)NMe_2$, 38); HRMS: (CI, 200 eV) calculated for ($C_{28}H_{34}N_3O_6Si$) 536.2217 (M^+ + 1) found for *m*/*z* 536.2214.

Tris(2-hydroxyphenyl)(methyl)silane (3aH_3)



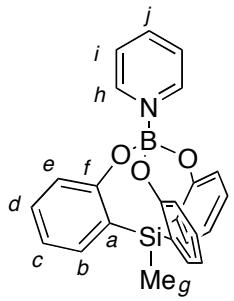
To a solution of tris(2-*N*,*N*-dimethylcarbamoyloxyphenyl)(methyl)silane **6a** (1 mmol) in dichloromethane (40 mL) and diethyl ether (40 mL) was added $LiAlH_4$ (3.5 mmol). The mixture was stirred for 6 h at rt and then quenched by H_2O (5 mL). The mixture was filtered with celite, and the filtrate was extracted with dichloromethane (10 mL x 3). The collected organic layer was dried ($MgSO_4$). The solvent was evaporated and the residue was purified by column chromatography on silicagel to give the product **3a**H_3 (84%). Rf = 0.27 (hexane/EtOAc = 2/1). mp: 80-83 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) 7.39 (dd, *J* = 7.5 Hz, 2.0 Hz, 3H, b-H), 7.34 (ddd, *J* = 7.5 Hz, 7.5 Hz, 2.0 Hz, 3H, d-H), 6.97 (dd, *J* = 7.5 Hz, 7.5 Hz, 3H, c-H), 6.79 (d, *J* = 7.5 Hz, 3H, e-H), 5.51 (brs, 3H, OH, D_2O-exchangeable), 0.95 (s, 3H, g-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 160.5 (f), 136.5 (b), 132.2 (d), 121.2 (c), 120.1 (a), 115.6 (e), -3.0 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -18.19; IR (KBr) 3348 (OH) cm^{-1}; MS: (EI, 70 eV) *m*/*z* 322 (M^+, 1.1), 228 ($M^+ - C_6H_4OH$, 80), 213 ($M^+ - CH_3$, $- C_6H_4OH$, 100); HRMS: (EI, 70 eV) calculated for ($C_{19}H_{18}O_3Si$) 322.1025 (M^+) found for *m*/*z* 322.1017.

THF Complex of 3aB (**3a**B·THF)



In a glove box, to a suspension of tris(2-hydroxyphenyl)(methyl)silane **3a**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. Evaporation of volatiles gave a viscous liquid, which was washed by hexane to give the product **3a**B·THF as a white solid (96%). ^{1}H NMR: (400 MHz, $CDCl_3$) 7.42 (dd, *J* = 7.4, 0.7 Hz, 3H, b-H), 7.25 (ddd, *J* = 8.0, 7.4, 0.7 Hz, 3H, d-H), 6.97 (dd, *J* = 7.4, 7.4 Hz, 3H, c-H), 6.87 (d, *J* = 8.0 Hz, 3H, e-H), 4.42-3.39 (m, 4H, h-H), 2.16-2.12 (m, 4H, i-H), 1.06 (s, 3H, g-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 161.9 (f), 134.2 (b), 130.9 (d), 125.9 (a), 121.4 (c), 119.3 (e), 70.2 (h), 25.3 (i), -6.7 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -21.3; ^{11}B NMR: (127 MHz, $CDCl_3$) 7.11

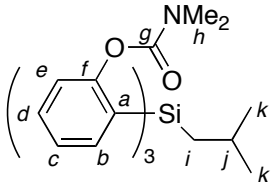
Pyridine Complex of 3aB (**3a**B·Py)



In a glove box, to a suspension of tris(2-hydroxyphenyl)(methyl)silane **3a**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. To the solution was added pyridine (0.2 mmol) at rt. After stirring for 30 min, volatiles were removed under reduced pressure. The obtained crude materials were washed with hexane and evaporated to give the pure product **3a**B·Py (94%). The product was recrystallized from dichloromethane/hexane(2/1) for X-ray analysis. ^{1}H NMR: (400 MHz,

$CDCl_3$) 9.26 (d, *J* = 7.0 Hz, 2H, h-H), 8.16 (t, *J* = 7.0 Hz, 1H, j-H), 7.75 (dd, *J* = 7.0, 7.0 Hz, 2H, i-H), 7.47 (dd, *J* = 7.5, 1.7 Hz, 3H, b-H), 7.22 (ddd, *J* = 8.2, 7.5, 1.7 Hz, 3H, d-H), 6.96 (ddd, *J* = 7.5, 7.5, 1.2 Hz, 3H, c-H), 6.83 (dd, *J* = 8.2, 1.2 Hz, 3H, e-H), 1.08 (s, 3H, g-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 162.5 (f), 143.9 (h), 141.7 (j), 134.2 (b), 130.7 (d), 126.5 (a), 125.5 (i), 121.1 (c), 119.7 (e), -6.4 (g); ^{29}Si NMR: (78.7 MHz, CD_2Cl_2) -21.1; ^{11}B NMR: (127 MHz, $CDCl_3$) 4.32

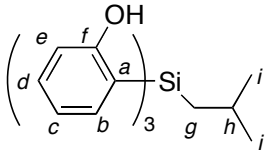
Tris(2-*N*,*N*-dimethylcarbamoyloxyphenyl)(isobutyl)silane (6b)



A 100 mL, three-necked, round-bottomed flask is equipped with a magnetic stirring bar, glass stopper, dropping funnel, and a reflux condenser under nitrogen. To a solution of *N*,*N*,*N'*,*N'*-tetramethylethylenediamine (1 mmol) in THF (20 mL) was slowly added Bu′Li in hexane (20 mmol) at -80 °C. The color of suspension changed from yellow to pale yellow. The dropping funnel was charged with *o*-bromophenyl *N*,*N*-dimethylcarbamate **5** (10 mmol) and THF (10 mL). The carbamate solution was slowly added to the flask and stirred for 1 h to keep at -80 °C. Then Bu^i$SiCl_3$ (3 mmol) was added to the flask. After stirring with warming up to rt for 12 h, H_2O (10 mL) was added to quench the reaction. The mixture was extracted with dichloromethane (20 mL x 3). The collected organic layer was dried ($MgSO_4$) and evaporated to give the crude product, which was recrystallized (dichloromethane/Et_2O/hexane = 1/3/6) to give the product **6b** (73%). mp: 158-159 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) 7.50 (dd, *J* = 7.2 Hz, 1.2 Hz, 3H, b-H), 7.39 (ddd, *J* = 7.2 Hz, 7.2 Hz, 1.2 Hz, 3H, d-H), 7.13 (dd, *J* = 7.2 Hz, 7.2 Hz, 3H, c-H), 7.10 (d, *J* = 7.2 Hz, 3H, e-H), 2.76 (s, 9H, h-H_3), 2.57 (s, 9H, h-H_3), 1.72 (tsep, *J* = 8.0 Hz, 8.0 Hz, 1H, j-H), 1.34 (d, *J* = 8.0 Hz, 2H, i-H_2), 0.83 (d, *J* = 8.0 Hz, 6H, k-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 156.4 (f), 154.1 (g), 136.7 (b), 130.6 (d), 126.5 (a), 124.0 (c), 122.4 (e), 36.4 (h), 36.0 (h), 26.2 (k), 24.9 (j), 22.6 (i); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -11.14; IR (KBr) 1716 (C=O) cm^{-1}; MS: (CI, 200 eV) *m*/*z* 579 (M^+ + 2, 40), 578 (M^+ + 1, 100), 413 ($M^+ - C_6H_4OC(O)NMe_2$, 42); HRMS: (CI, 200 eV)

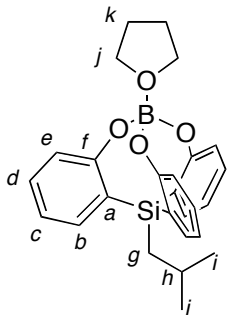
calculated for ($C_{31}H_{40}N_3O_6Si$) 578.2686 ($M^+ + 1$) found for *m*/*z* 578.2681. Analysis: calculated for $C_{31}H_{39}N_3O_6Si$: C, 64.45; H, 6.80; N, 7.27; found C, 64.19; H, 6.52; N, 7.27.

Tris(2-hydroxyphenyl)(isobutyl)silane (3bH_3)



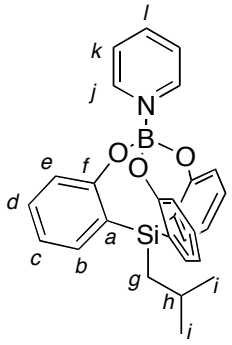
To a solution of tris(2-*N*,*N*-dimethylcarbamoyloxyphenyl)(isobutyl)silane **6b** (0.5 mmol) in dichloromethane (20 mL) and diethylether (40 mL) was added $LiAlH_4$ (2.5 mmol). The mixture was stirred for 6 h at rt and then quenched by H_2O (5 mL). The mixture was filtered with celite, and the filtrate was extracted with dichloromethane (10 mL x 3). The collected organic layer was dried ($MgSO_4$). The solvent was evaporated and the residue was purified by column chromatography on silicagel to give the product **3b**H_3 (53%). Rf = 0.31 (hexane/ether = 2/1). mp: 145-147 °C; ^{1}H NMR: (400 MHz, $CDCl_3$) 7.44 (d, *J* = 8.0 Hz, 3H, b-H), 7.26 (dd, *J* = 8.0 Hz, 8.0 Hz, 3H, d-H), 6.94 (dd, *J* = 8.0 Hz, 8.0 Hz, 3H, c-H), 6.69 (d, *J* = 8.0 Hz, 3H, e-H), 6.26 (brs, 3H, OH, D_2O-exchangeable), 1.80 (tsep, *J* = 6.8 Hz, 6.8 Hz, 1H, h-H), 1.50 (d, *J* = 6.8 Hz, 2H, g-H_2), 0.85 (d, *J* = 6.8 Hz, 6H, i-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 160.3 (f), 136.5 (b), 132.0 (d), 121.1 (c), 119.8 (a), 115.6 (e), 26.3 (i), 24.6 (h), 22.2 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -19.75; IR (KBr) 3347 (OH) cm^{-1}; MS: (EI, 70 eV) *m*/*z* 364 (M^+, 2.2), 289 (29), 271 (45), 270 (M^+ – C_6H_4OH, 56), 215 (26), 214 (99), 213 (M^+ – $CH_2CH(CH_3)_2$, – C_6H_4OH, 100); HRMS: (EI, 70 eV) calculated for ($C_{22}H_{24}O_3Si$) 364.1495 (M^+) found for *m*/*z* 364.1502. Analysis; calculated for $C_{22}H_{24}O_3Si$: C, 72.49; H, 6.64; found: C, 72.22; H, 6.37.

THF Complex of 3bB (**3b**B·THF)



In a glove box, to a suspension of tris(2-hydroxyphenyl)(isobutyl)silane **3b**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. Evaporation of volatiles gave a viscous liquid, which was washed by hexane to give the product **3b**B·THF as a white solid (95%). ^{1}H NMR: (400 MHz, $CDCl_3$) 7.57 (d, *J* = 7.5 Hz, 3H, b-H), 7.23 (dd, *J* = 8.0, 7.5 Hz, 3H, d-H), 6.96 (dd, *J* = 7.5, 7.5 Hz, 3H, c-H), 6.85 (d, *J* = 8.0 Hz, 3H, e-H), 4.02-3.99 (m, 4H, j-H), 2.65-2.55 (m, 1H, h-H), 1.99-1.96 (m, 4H, k-H), 1.73 (d, *J* = 7.2 Hz, 2H, g-H_2), 1.26 (d, *J* = 6.4 Hz, 6H, i-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 162.3 (f), 134.8 (b), 130.6 (d), 126.3 (a), 121.0 (c), 119.5 (e), 68.9 (j), 27.5 (i), 24.3 (h), 25.4 (k), 18.8 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -24.4; ^{11}B NMR: (127 MHz, $CDCl_3$) 5.87

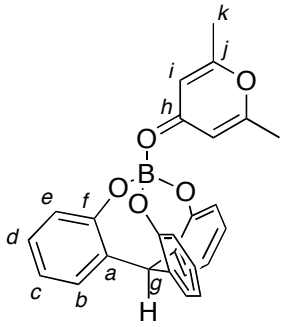
Pyridine Complex of 3bB (**3b**B·Py)



In a glove box, to a suspension of tris(2-hydroxyphenyl)(isobutyl)silane **3b**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. To the solution was added pyridine (0.2 mmol) at rt. After stirring for 30 min, volatiles were removed under reduced pressure. The obtained crude materials were washed with hexane and evaporated to give the pure product **3b**B·Py (99%). The product was

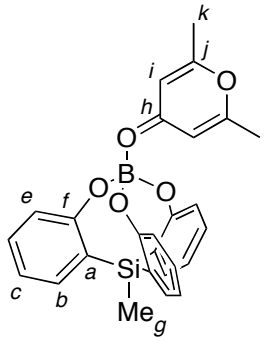
recrystallized from dichloromethane/hexane(2/1) for X-ray analysis. ^{1}H NMR: (400 MHz, $CDCl_3$) 9.23 (d, *J* = 7.5 Hz, 2H, j-H), 8.18 (t, *J* = 7.5 Hz, 1H, l-H), 7.76 (dd, *J* = 7.5, 7.5 Hz, 2H, k-H), 7.62 (dd, *J* = 7.2, 1.7 Hz, 3H, b-H), 7.21 (ddd, *J* = 8.0, 7.2, 1.7 Hz, 3H, d-H), 6.96 (ddd, *J* = 7.2, 7.2, 1.2 Hz, 3H, c-H), 6.81 (dd, *J* = 8.0, 1.2 Hz, 3H, e-H), 2.63 (tsep, *J* = 7.0, 7.0 Hz, 1H, h-H), 1.77 (d, *J* = 7.0 Hz, 2H, g-H_2), 1.29 (d, *J* = 7.0 Hz, 6H, i-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 162.7 (f), 143.9 (j), 141.7 (l), 134.8 (b), 130.5 (d), 126.9 (a), 125.5 (k), 120.8 (c), 119.9 (e), 27.6 (i), 24.9 (h), 20.8 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -24.0; ^{11}B NMR: (127 MHz, $CDCl_3$) 3.99

Pyrone Complex of 1B (**1**B·**8**)



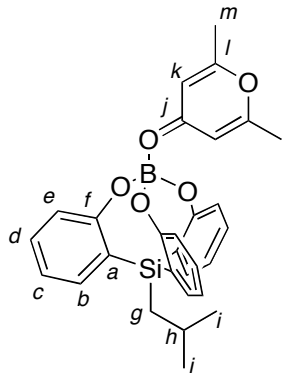
In a glove box, to a suspension of tris(2-hydroxyphenyl)methane **1**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. Volatiles were removed under reduced pressure and the residue was washed with hexane. The evaporated residue was resolved with dichloromethane (3 mL) and 2,6-dimethyl-γ-pyrone (0.1 mmol) was added to the solution. After stirring for 30 min, volatiles were removed under reduced pressure. The obtained crude materials were washed with hexane and evaporated to give the product **1**B·**8** (99%). The product was recrystallized from $CDCl_3$ for X-ray analysis. ^{1}H NMR: (400 MHz, $CDCl_3$) 7.27 (d, *J* = 7.7 Hz, 3H, b-H), 7.10 (s, 2H, i-H), 7.06 (dd, *J* = 7.7, 7.7 Hz, 3H, d-H), 6.85 (dd, *J* = 7.7, 7.7 Hz, 3H, c-H), 6.80 (d, *J* = 7.7 Hz, 3H, e-H), 5.13 (s, 1H, g-H), 2.54 (s, 6H, k-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 180.0 (h), 172.2 (j), 156.2 (f), 131.1, 131.0, 127.7, 120.7, 120.6, 113.1 (i), 58.0 (g), 20.6 (k); ^{11}B NMR: (127 MHz, $CDCl_3$) 4.57

Pyrone Complex of 3aB (**3a**B·**8**)



In a glove box, to a suspension of tris(2-hydroxyphenyl)(methyl)silane **3a**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. Volatiles were removed under reduced pressure and the residue was washed with hexane. The evaporated residue was resolved with dichloromethane (3 mL) and 2,6-dimethyl-γ-pyrone (0.1 mmol) was added to the solution. After stirring for 30 min, volatiles were removed under reduced pressure. The obtained crude materials were washed with hexane and evaporated to give the product **3a**B·**8** (98%). The product was recrystallized from $CDCl_3$ for X-ray analysis. ^{1}H NMR: (400 MHz, $CDCl_3$) 7.44 (dd, J = 7.2, 1.7 Hz, 3H, b-H), 7.20 (ddd, J = 8.0, 8.0, 1.7 Hz, 3H, d-H), 6.97 (brs, 2H, i-H), 6.93 (dd, J = 8.0, 7.2 Hz, 3H, c-H), 6.78 (d, J = 8.0 Hz, 3H, e-H), 2.44 (s, 6H, k-H_3), 1.05 (s, 3H, g-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 179.8 (j), 171.3 (j), 162.6 (f), 134.1 (b), 130.5 (d), 126.3 (a), 120.7 (c), 120.0 (e), 113.2 (i), 20.4 (k), -6.4 (g); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -21.3; ^{11}B NMR: (127 MHz, $CDCl_3$) 4.42

Pyrone Complex of 3bB (**3b**B·**8**)

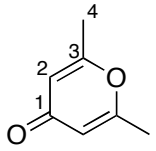


In a glove box, to a suspension of tris(2-hydroxyphenyl)(isobutyl)silane **3b**H_3 (0.1 mmol) in dichloromethane (3 mL) was added BH_3·THF in THF (0.11 mmol, 1.0 M) at rt with stirring for 1 h under release of H_2 gas. Volatiles were removed under reduced pressure and the residue was washed with hexane. The evaporated residue was resolved in dichloromethane (3 mL) and 2,6-dimethyl-γ-pyrone (0.1 mmol) was added to the solution. After stirring for 30 min, volatiles were removed under reduced pressure. The obtained crude materials were washed with hexane and evaporated to give the product **3b**B·**8** (95%). The product was recrystallized from $CDCl_3$ for X-ray analysis. ^{1}H NMR: (400 MHz, $CDCl_3$) 7.59 (dd, *J* = 8.0, 1.6 Hz, 3H, b-H), 7.19 (ddd, *J* = 8.0, 8.0, 1.6 Hz, 3H, d-H), 6.92 (dd, *J* = 8.0, 8.0 Hz, 3H, c-H), 6.77 (d, *J* = 8.0 Hz, 3H, e-H), 6.73 (brs, 2H, k-H), 2.61 (tsep, *J* = 6.8, 6.8 Hz, 1H, h-H), 2.39 (s, 6H, m-H_3), 1.73 (d, *J* = 6.8 Hz, 2H, g-H_2), 1.27 (d, *J* = 6.8 Hz, 6H, i-H_3); ^{13}C NMR: (100 MHz, $CDCl_3$) 180.0 (j), 169.9 (l), 162.9 (f), 134.7 (b), 130.3 (d), 126.7 (a), 120.4 (c), 120.1 (e), 113.3 (k), 27.6 (i), 24.9 (h), 20.9 (g), 20.3 (m); ^{29}Si NMR: (78.7 MHz, $CDCl_3$) -24.2; ^{11}B NMR: (127 MHz, $CDCl_3$) 4.55

NMR Study of Complexes of Boranes with 2,6-Dimethyl γ-Pyron 8

Equimolar amount of boron compounds (BF_3·OEt_2, **1**B·THF, **3a**B·THF, **3b**B·THF, or **2**) and 2,6-dimethyl γ-pyron **8** were mixed in $CDCl_3$. The chemical shifts of Δδ(^{13}C) in pyron moieties are shown in Table A.

Table A. NMR Study of Complexation of **8** with Boranes



8

carbon	δ(^{13}C) / ppm[a]	Δδ(^{13}C)/ ppm				
		BF_3·OEt_2	**1**B·THF	**3a**B·THF	**3b**B·THF	**2**
C1	180.181	-0.675	-0.222	-0.346	-0.231	0.477
C2	113.739	-1.926	-0.658	-0.559	-0.452	-0.527
C3	165.432	8.708	6.782	5.844	4.486	2.544
C4	19.727	0.889	0.921	0.683	0.526	0.255

[a] δ(^{13}C) of pyron **8** (boron-free).

Rate of Ligand (pyridine)-Dissociation on Cage-Shaped Borates 3aB **and 3b**B

A pyridine exchange can be descried below. B; $B(OC_6H_4)_3ER$, X; pyridine-d_5, Y; pyridine (unlabelled). Y and BY can be observed by pyridine signals by NMR.

$$BX \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B + X \qquad B + Y \underset{k_1}{\overset{k_{-1}}{\rightleftharpoons}} BY$$

The equal amount of BX and Y are mixed.

$$[BX]_0 = [Y]_0$$

No ligand-free borate B is observed.

$$[BX]_0 + [Y]_0 = [BX] + [X] + [Y] + [BY]$$
$$[X] = [BY]$$
$$[Y] = [BX]$$

$$\frac{d[B]}{dt} = k_1[BX] - k_{-1}[B][X] - k_{-1}[B][Y] + k_1[BY]$$
$$= k_1([BX] + [BY]) - k_{-1}[B]([X] + [Y]) = 0$$
$$k_1 = k_{-1}[B]$$

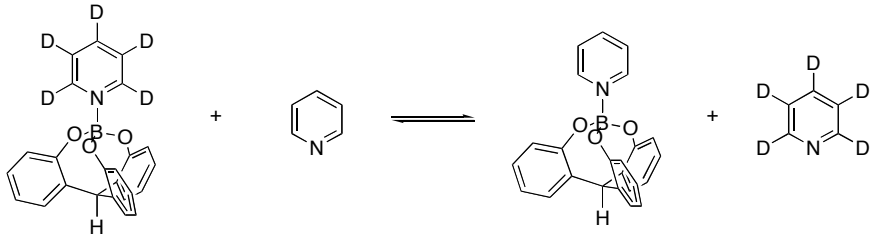
$$\frac{d[BY]}{dt} = k_{-1}[B][Y] - k_1[BY] = k_{-1}[B]([BX]_0 - [BY]) - k_1[BY]$$
$$= k_1([BX]_0 - [BY]) - k_1[BY] = k_1([BX]_0 - 2[BY])$$

$$\int \frac{d[BY]}{[BX]_0 - 2[BY]} = \int k_1 dt$$

$$\ln \frac{[BX]_0 - 2[BY]t_0}{[BX]_0 - 2[BY]} = 2k_1(t - t_0) \qquad (A)$$

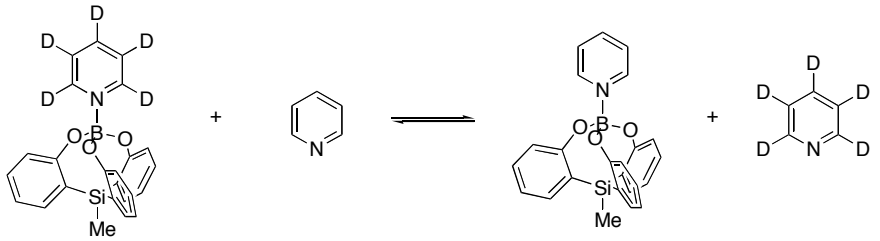
For simplification, t_0 can be voluntarily set as zero (with considering stable temperature condition experimentally). Plots based on (A) furnish a linear plot (See below).

Pyridine-Exchange on 1B.



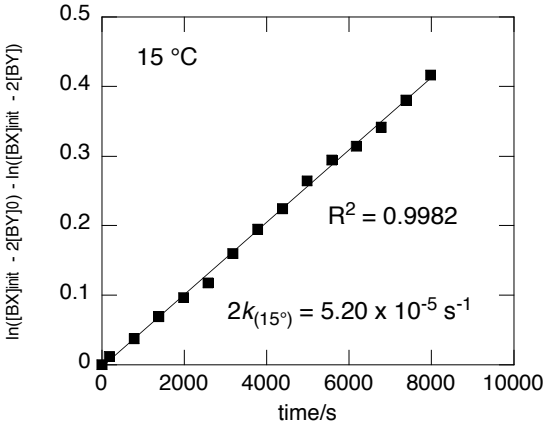
To a suspension of tris(2-hydroxyphenyl)methane (**1**H_3) (0.3 mmol) in dichloromethane (10 mL) was added BH_3·THF in THF (0.33 mmol, 1.0 M) at rt with stirring for 2 h under release of H_2 gas. To the solution was added pyridine-d_5 (3 mmol) at rt. After stirring for 1 h, volatiles were removed under reduced pressure (0.1 mmHg, 70 °C, 10 min). CD_2Cl_2 (10 mL) was added to the flask. Pyridine (unlabelled) (0.3 mol) was added to the flask. The rate constants were determined by observing the reaction at 15, 20, and 30 °C. The results are shown in Figure A.

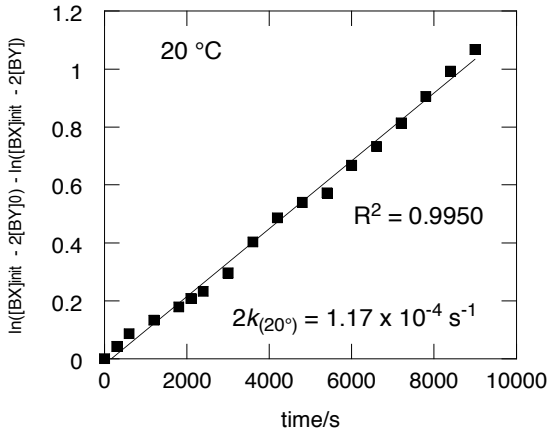
Pyridine-Exchange on 3aB.

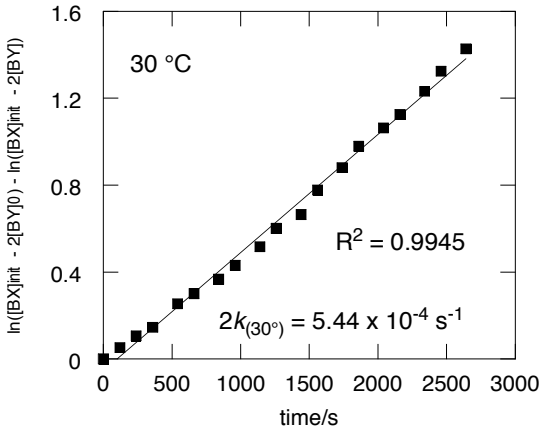


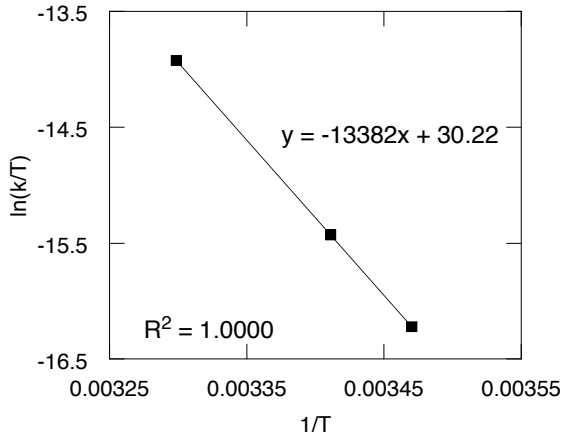
To a suspension of tris(2-hydroxyphenyl)methylsilane (**3a**H_3) (0.3 mmol) in dichloromethane (10 mL) was added BH_3·THF in THF (0.33 mmol, 1.0 M) at rt with stirring for 2 h under release of H_2 gas. To the solution was added pyridine-d_5 (3 mmol) at rt. After stirring for 1 h, volatiles were removed under reduced pressure (0.1 mmHg, 70 °C, 10 min). CD_2Cl_2 (10 mL) was added to the flask. Pyridine (unlabelled) (0.3 mol) was added to the flask. The rate constants were determined by observing the reaction at -35, -30, and -25 °C. The results are shown in Figure B.

Figure A. Kinetics plots and Arrhenius plot for Dissociation of $PyB(OC_6H_4)_3CH$ (**1**B·Py)





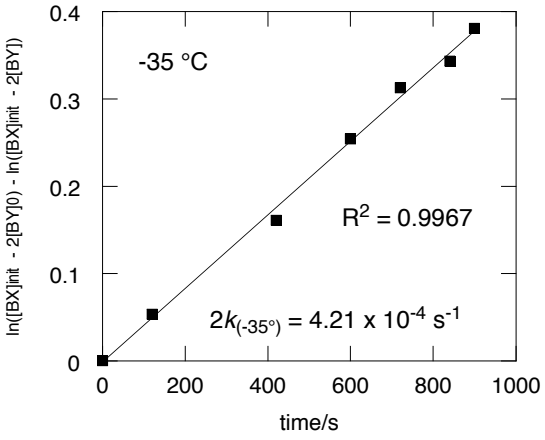


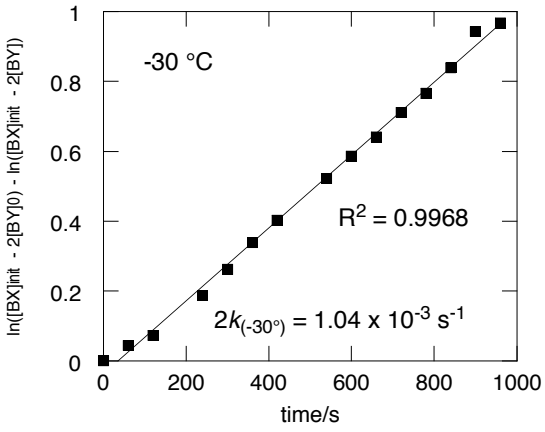


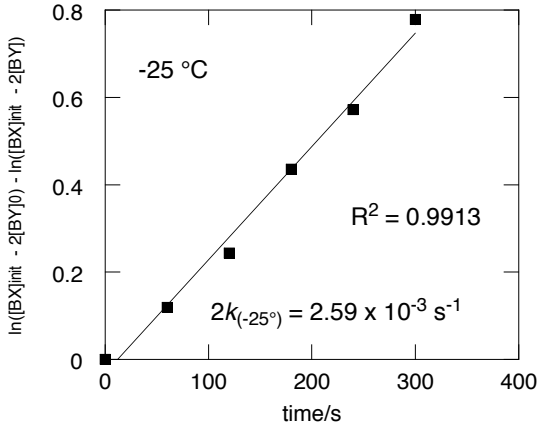
$\Delta H^{\ddagger}$ = 26.6 kcal mol^{-1}

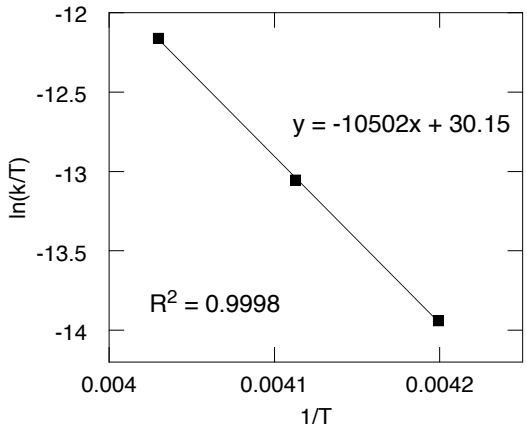
$\Delta S^{\ddagger}$ = 12.8 cal K^{-1} mol^{-1}

Figure B. Kinetics plots and Arrhenius plot for Dissociation of $PyB(OC_6H_4)_3SiMe$ (**3a**B·Py)







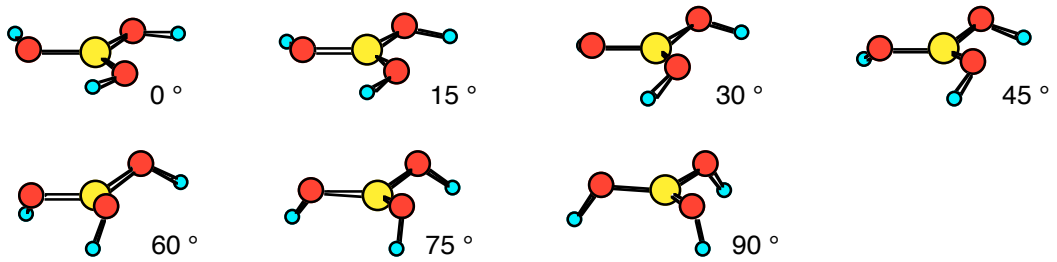


$\Delta H^{\ddagger}$ = 20.9 kcal mol^{-1}

$\Delta S^{\ddagger}$ = 12.7 cal K^{-1} mol^{-1}

Computational Method. We applied the HF/DFT hybrid method originally proposed by Becke,[3] referenced as B3PW91 three parameter hybrid functional. All calculations were performed with Gaussian 03, Revision C.02.[4] 6-31+G(d,p) were used for basis sets. All molecular geometries were fully optimized and energies were calculated including zero point energy correction by the normal mode analysis for each structure.

All species calculated in Scheme 1 in text are shown below (Scheme A).



Scheme A. The calculated species $B(OH)_3$ with varied dihedral angels in Scheme 1.

Geometries (PDB)

$B(OH)_3$ (0°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.000   0.000   0.000  1.00  0.00
ATOM      2  O   UNK     1       0.000   1.370   0.000  1.00  0.00
ATOM      3  H   UNK     1      -0.890   1.737   0.000  1.00  0.00
ATOM      4  O   UNK     1       1.187  -0.685   0.000  1.00  0.00
ATOM      5  H   UNK     1       1.949  -0.098   0.000  1.00  0.00
ATOM      6  O   UNK     1      -1.187  -0.685   0.000  1.00  0.00
ATOM      7  H   UNK     1      -1.059  -1.639   0.000  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (15°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.075   0.130   0.000  1.00  0.00
```

```
ATOM      2  O   UNK     1       0.008   0.125   1.369  1.00  0.00
ATOM      3  H   UNK     1       0.836  -0.148   1.777  1.00  0.00
ATOM      4  O   UNK     1      -0.947   0.676  -0.733  1.00  0.00
ATOM      5  H   UNK     1      -1.533   1.220  -0.197  1.00  0.00
ATOM      6  O   UNK     1       1.107  -0.510  -0.636  1.00  0.00
ATOM      7  H   UNK     1       1.132  -0.318  -1.580  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (30°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.057   0.099   0.000  1.00  0.00
ATOM      2  O   UNK     1      -0.005   0.044   1.370  1.00  0.00
ATOM      3  H   UNK     1       0.859  -0.059   1.780  1.00  0.00
ATOM      4  O   UNK     1      -0.998   0.617  -0.708  1.00  0.00
ATOM      5  H   UNK     1      -1.481   1.292  -0.221  1.00  0.00
ATOM      6  O   UNK     1       1.057  -0.569  -0.662  1.00  0.00
ATOM      7  H   UNK     1       1.189  -0.250  -1.560  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (45°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.046   0.080   0.000  1.00  0.00
ATOM      2  O   UNK     1       0.003  -0.037   1.369  1.00  0.00
ATOM      3  H   UNK     1       0.864   0.023   1.794  1.00  0.00
ATOM      4  O   UNK     1      -1.051   0.572  -0.666  1.00  0.00
ATOM      5  H   UNK     1      -1.438   1.353  -0.259  1.00  0.00
ATOM      6  O   UNK     1       1.002  -0.614  -0.703  1.00  0.00
ATOM      7  H   UNK     1       1.252  -0.201  -1.535  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (60°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.186   0.107   0.000  1.00  0.00
ATOM      2  O   UNK     1       0.025   0.072   1.368  1.00  0.00
ATOM      3  H   UNK     1       0.817  -0.106   1.881  1.00  0.00
ATOM      4  O   UNK     1      -0.530   1.033  -0.728  1.00  0.00
ATOM      5  H   UNK     1      -0.373   1.955  -0.508  1.00  0.00
ATOM      6  O   UNK     1       0.655  -1.019  -0.640  1.00  0.00
ATOM      7  H   UNK     1       1.257  -0.867  -1.374  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (75°)

```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.163   0.094   0.000  1.00  0.00
ATOM      2  O   UNK     1       0.034  -0.022   1.369  1.00  0.00
ATOM      3  H   UNK     1       0.823  -0.022   1.915  1.00  0.00
ATOM      4  O   UNK     1      -0.586   1.052  -0.654  1.00  0.00
ATOM      5  H   UNK     1      -0.329   1.974  -0.584  1.00  0.00
ATOM      6  O   UNK     1       0.600  -1.002  -0.716  1.00  0.00
ATOM      7  H   UNK     1       1.329  -0.898  -1.330  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

$B(OH)_3$ (90°)

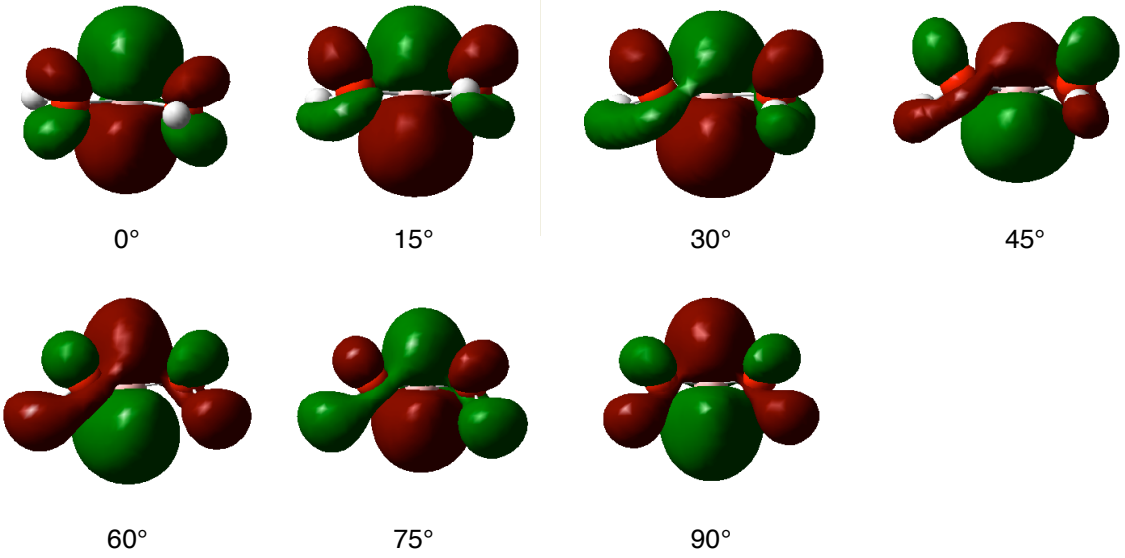
```
HEADER    PROTEIN
ATOM      1  B   UNK     1       0.000   0.000   0.004  1.00  0.00
ATOM      2  O   UNK     1       0.000   1.377   0.085  1.00  0.00
ATOM      3  H   UNK     1       0.000   1.945  -0.684  1.00  0.00
ATOM      4  O   UNK     1      -1.193  -0.689   0.085  1.00  0.00
ATOM      5  H   UNK     1      -1.684  -0.972  -0.684  1.00  0.00
ATOM      6  O   UNK     1       1.193  -0.689   0.085  1.00  0.00
ATOM      7  H   UNK     1       1.684  -0.972  -0.684  1.00  0.00
CONECT    1    2    4    6
CONECT    2    1    3
CONECT    3    2
CONECT    4    1    5
```

```
CONECT    5    4
CONECT    6    1    7
CONECT    7    6
MASTER        0    0    0    0    0    0    0    0    7    0    7    0
END
```

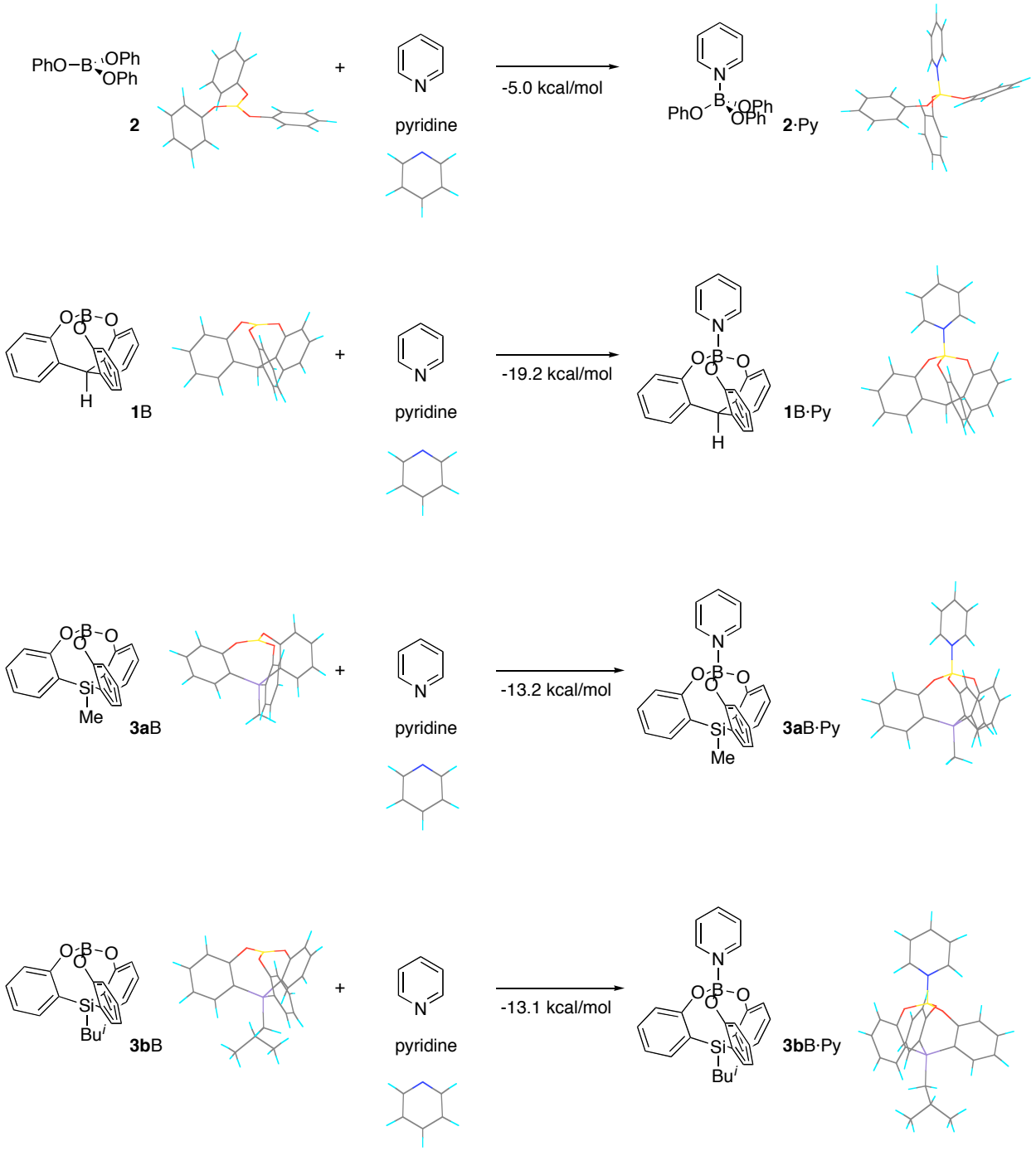
The lowest unoccupied MO which has appropriate lobe on boron for Lewis acid was picked in each structure with diheral angles (0, 15, 30, 45, 60, 75, 90 °).

Orbital	Dihedral angle/°	Hartree
21a	0	0.09505
21a	15	0.08879
21a	30	0.07450
21a	45	0.05903
20a	60	0.03687
18a	75	0.02352
18a	90	0.01809

The MO diagrams are shown below.



All species calculated in Table 1 in text are shown below (Scheme B).



Scheme B. The calculated speces in text (Table 1)

Total energies for all of the calculated species (in hartree). All energies includes zero point vibration energy correction.

2	-945.000996
2·Py	-1193.123798
1B	-981.885983
1B·Py	-1230.031378
3aB	-1272.562556
3aB·Py	-1520.698427
3bB	-1390.372649
3bB·Py	-1638.508325
pyridine	-248.11478

Geometries (PDB)

2

```
HEADER    PROTEIN
ATOM      1  B1  UNK     1       0.000   0.000   0.011  1.00  0.00
ATOM      2  O2  UNK     1       0.749  -1.145   0.023  1.00  0.00
ATOM      3  O3  UNK     1       0.617   1.220   0.023  1.00  0.00
ATOM      4  O4  UNK     1      -1.365  -0.076   0.023  1.00  0.00
ATOM      5  C5  UNK     1       0.000   2.451   0.008  1.00  0.00
ATOM      6  C6  UNK     1       0.421   3.390   0.950  1.00  0.00
ATOM      7  C7  UNK     1      -0.955   2.785  -0.953  1.00  0.00
ATOM      8  C8  UNK     1      -0.129   4.670   0.937  1.00  0.00
ATOM      9  H9  UNK     1       1.176   3.105   1.676  1.00  0.00
ATOM     10  C10 UNK     1      -1.499   4.069  -0.954  1.00  0.00
ATOM     11  H11 UNK     1      -1.272   2.048  -1.682  1.00  0.00
ATOM     12  C12 UNK     1      -1.092   5.015  -0.013  1.00  0.00
ATOM     13  H13 UNK     1       0.199   5.400   1.672  1.00  0.00
ATOM     14  H14 UNK     1      -2.245   4.329  -1.700  1.00  0.00
ATOM     15  H15 UNK     1      -1.519   6.014  -0.021  1.00  0.00
ATOM     16  C16 UNK     1      -2.123  -1.226   0.008  1.00  0.00
ATOM     17  C17 UNK     1      -3.146  -1.330   0.950  1.00  0.00
ATOM     18  C18 UNK     1      -1.935  -2.219  -0.953  1.00  0.00
ATOM     19  C19 UNK     1      -3.980  -2.447   0.937  1.00  0.00
ATOM     20  H20 UNK     1      -3.277  -0.534   1.676  1.00  0.00
ATOM     21  C21 UNK     1      -2.775  -3.333  -0.954  1.00  0.00
ATOM     22  H22 UNK     1      -1.137  -2.125  -1.682  1.00  0.00
ATOM     23  C23 UNK     1      -3.797  -3.453  -0.013  1.00  0.00
```

```
ATOM     24  H24 UNK     1      -4.776  -2.528   1.672  1.00  0.00
ATOM     25  H25 UNK     1      -2.626  -4.109  -1.700  1.00  0.00
ATOM     26  H26 UNK     1      -4.449  -4.322  -0.021  1.00  0.00
ATOM     27  C27 UNK     1       2.123  -1.226   0.008  1.00  0.00
ATOM     28  C28 UNK     1       2.889  -0.566  -0.953  1.00  0.00
ATOM     29  C29 UNK     1       2.725  -2.060   0.950  1.00  0.00
ATOM     30  C30 UNK     1       4.274  -0.737  -0.954  1.00  0.00
ATOM     31  H31 UNK     1       2.409   0.078  -1.682  1.00  0.00
ATOM     32  C32 UNK     1       4.109  -2.223   0.937  1.00  0.00
ATOM     33  H33 UNK     1       2.101  -2.571   1.676  1.00  0.00
ATOM     34  C34 UNK     1       4.889  -1.562  -0.013  1.00  0.00
ATOM     35  H35 UNK     1       4.872  -0.220  -1.700  1.00  0.00
ATOM     36  H36 UNK     1       4.577  -2.872   1.672  1.00  0.00
ATOM     37  H37 UNK     1       5.968  -1.691  -0.021  1.00  0.00
CONECT    1    2    3    4
CONECT    2    1   27
CONECT    3    1    5
CONECT    4    1   16
CONECT    5    3    6    7
CONECT    6    5    8    9
CONECT    7    5   10   11
CONECT    8    6   12   13
CONECT    9    6
CONECT   10    7   12   14
CONECT   11    7
CONECT   12    8   10   15
CONECT   13    8
CONECT   14   10
CONECT   15   12
CONECT   16    4   17   18
CONECT   17   16   19   20
CONECT   18   16   21   22
CONECT   19   17   23   24
CONECT   20   17
CONECT   21   18   23   25
CONECT   22   18
CONECT   23   19   21   26
CONECT   24   19
CONECT   25   21
CONECT   26   23
CONECT   27    2   28   29
CONECT   28   27   30   31
CONECT   29   27   32   33
CONECT   30   28   34   35
CONECT   31   28
CONECT   32   29   34   36
CONECT   33   29
CONECT   34   30   32   37
CONECT   35   30
CONECT   36   32
CONECT   37   34
MASTER        0    0    0    0    0    0    0    0   37    0   37    0
END
```

2·Py

```
HEADER    PROTEIN
ATOM      1  B1  UNK     1      -0.042  -0.244   0.212  1.00  0.00
ATOM      2  O2  UNK     1       1.054  -0.679   1.034  1.00  0.00
ATOM      3  O3  UNK     1      -0.914  -1.347  -0.093  1.00  0.00
ATOM      4  O4  UNK     1       0.271   0.549  -0.952  1.00  0.00
ATOM      5  C5  UNK     1      -2.126  -1.315  -0.700  1.00  0.00
ATOM      6  C6  UNK     1      -3.105  -2.193  -0.211  1.00  0.00
ATOM      7  C7  UNK     1      -2.429  -0.497  -1.799  1.00  0.00
ATOM      8  C8  UNK     1      -4.365  -2.244  -0.800  1.00  0.00
ATOM      9  H9  UNK     1      -2.850  -2.835   0.628  1.00  0.00
ATOM     10  C10 UNK     1      -3.699  -0.553  -2.376  1.00  0.00
ATOM     11  H11 UNK     1      -1.661   0.154  -2.200  1.00  0.00
ATOM     12  C12 UNK     1      -4.674  -1.420  -1.885  1.00  0.00
ATOM     13  H13 UNK     1      -5.110  -2.933  -0.410  1.00  0.00
ATOM     14  H14 UNK     1      -3.919   0.083  -3.231  1.00  0.00
ATOM     15  H15 UNK     1      -5.657  -1.460  -2.345  1.00  0.00
ATOM     16  C16 UNK     1       1.152   1.581  -1.030  1.00  0.00
ATOM     17  C17 UNK     1       1.292   2.187  -2.288  1.00  0.00
ATOM     18  C18 UNK     1       1.891   2.074   0.054  1.00  0.00
ATOM     19  C19 UNK     1       2.150   3.269  -2.457  1.00  0.00
ATOM     20  H20 UNK     1       0.723   1.786  -3.122  1.00  0.00
ATOM     21  C21 UNK     1       2.748   3.161  -0.130  1.00  0.00
ATOM     22  H22 UNK     1       1.817   1.594   1.023  1.00  0.00
ATOM     23  C23 UNK     1       2.884   3.767  -1.377  1.00  0.00
ATOM     24  H24 UNK     1       2.249   3.722  -3.439  1.00  0.00
ATOM     25  H25 UNK     1       3.320   3.529   0.718  1.00  0.00
ATOM     26  H26 UNK     1       3.556   4.610  -1.510  1.00  0.00
ATOM     27  C27 UNK     1       2.010  -1.567   0.654  1.00  0.00
ATOM     28  C28 UNK     1       2.055  -2.167  -0.610  1.00  0.00
ATOM     29  C29 UNK     1       2.998  -1.872   1.599  1.00  0.00
ATOM     30  C30 UNK     1       3.083  -3.061  -0.911  1.00  0.00
ATOM     31  H31 UNK     1       1.292  -1.940  -1.345  1.00  0.00
ATOM     32  C32 UNK     1       4.017  -2.767   1.285  1.00  0.00
ATOM     33  H33 UNK     1       2.953  -1.395   2.574  1.00  0.00
ATOM     34  C34 UNK     1       4.068  -3.369   0.026  1.00  0.00
ATOM     35  H35 UNK     1       3.107  -3.522  -1.896  1.00  0.00
ATOM     36  H36 UNK     1       4.777  -2.993   2.029  1.00  0.00
ATOM     37  H37 UNK     1       4.863  -4.067  -0.219  1.00  0.00
ATOM     38  H38 UNK     1      -1.444   2.031  -0.232  1.00  0.00
ATOM     39  C39 UNK     1      -1.585   1.789   0.815  1.00  0.00
ATOM     40  C40 UNK     1      -2.410   2.529   1.652  1.00  0.00
ATOM     41  C41 UNK     1      -2.525   2.154   2.987  1.00  0.00
ATOM     42  H42 UNK     1      -2.946   3.383   1.254  1.00  0.00
ATOM     43  C43 UNK     1      -1.011   0.351   2.550  1.00  0.00
ATOM     44  C44 UNK     1      -1.812   1.046   3.442  1.00  0.00
ATOM     45  H45 UNK     1      -3.162   2.716   3.664  1.00  0.00
ATOM     46  H46 UNK     1      -0.426  -0.519   2.828  1.00  0.00
ATOM     47  H47 UNK     1      -1.873   0.718   4.474  1.00  0.00
ATOM     48  N48 UNK     1      -0.900   0.726   1.264  1.00  0.00
CONECT    1    2    3    4   48
CONECT    2    1   27
CONECT    3    1    5
CONECT    4    1   16
CONECT    5    3    6    7
```

```
CONECT    6    5    8    9
CONECT    7    5   10   11
CONECT    8    6   12   13
CONECT    9    6
CONECT   10    7   12   14
CONECT   11    7
CONECT   12    8   10   15
CONECT   13    8
CONECT   14   10
CONECT   15   12
CONECT   16    4   17   18
CONECT   17   16   19   20
CONECT   18   16   21   22
CONECT   19   17   23   24
CONECT   20   17
CONECT   21   18   23   25
CONECT   22   18
CONECT   23   19   21   26
CONECT   24   19
CONECT   25   21
CONECT   26   23
CONECT   27    2   28   29
CONECT   28   27   30   31
CONECT   29   27   32   33
CONECT   30   28   34   35
CONECT   31   28
CONECT   32   29   34   36
CONECT   33   29
CONECT   34   30   32   37
CONECT   35   30
CONECT   36   32
CONECT   37   34
CONECT   38   39
CONECT   39   38   40   48
CONECT   40   39   41   42
CONECT   41   40   44   45
CONECT   42   40
CONECT   43   44   46   48
CONECT   44   41   43   47
CONECT   45   41
CONECT   46   43
CONECT   47   44
CONECT   48    1   39   43
MASTER        0    0    0    0    0    0    0    0   48    0   48    0
END
```

```
1B
HEADER    PROTEIN
ATOM      1  C1  UNK     1       0.000   0.000   0.913  1.00  0.00
ATOM      2  H2  UNK     1       0.000   0.000   2.006  1.00  0.00
ATOM      3  C3  UNK     1       0.022   1.500   0.564  1.00  0.00
ATOM      4  C4  UNK     1       0.390   2.418   1.556  1.00  0.00
ATOM      5  C5  UNK     1      -0.336   2.024  -0.691  1.00  0.00
ATOM      6  C6  UNK     1       0.384   3.791   1.325  1.00  0.00
```

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ATOM      7  H7  UNK     1       0.679   2.042   2.535  1.00  0.00
ATOM      8  C8  UNK     1      -0.359   3.394  -0.935  1.00  0.00
ATOM      9  C9  UNK     1       0.000   4.280   0.076  1.00  0.00
ATOM     10  H10 UNK     1       0.669   4.475   2.119  1.00  0.00
ATOM     11  H11 UNK     1      -0.653   3.742  -1.920  1.00  0.00
ATOM     12  H12 UNK     1      -0.017   5.350  -0.114  1.00  0.00
ATOM     13  C13 UNK     1       1.288  -0.769   0.564  1.00  0.00
ATOM     14  C14 UNK     1       1.921  -0.721  -0.691  1.00  0.00
ATOM     15  C15 UNK     1       1.899  -1.546   1.556  1.00  0.00
ATOM     16  C16 UNK     1       3.119  -1.387  -0.935  1.00  0.00
ATOM     17  C17 UNK     1       3.091  -2.228   1.325  1.00  0.00
ATOM     18  H18 UNK     1       1.429  -1.609   2.535  1.00  0.00
ATOM     19  C19 UNK     1       3.707  -2.140   0.076  1.00  0.00
ATOM     20  H20 UNK     1       3.567  -1.306  -1.920  1.00  0.00
ATOM     21  H21 UNK     1       3.541  -2.817   2.119  1.00  0.00
ATOM     22  H22 UNK     1       4.642  -2.660  -0.114  1.00  0.00
ATOM     23  C23 UNK     1      -1.310  -0.731   0.564  1.00  0.00
ATOM     24  C24 UNK     1      -2.288  -0.872   1.556  1.00  0.00
ATOM     25  C25 UNK     1      -1.585  -1.303  -0.691  1.00  0.00
ATOM     26  C26 UNK     1      -3.476  -1.563   1.325  1.00  0.00
ATOM     27  H27 UNK     1      -2.108  -0.433   2.535  1.00  0.00
ATOM     28  C28 UNK     1      -2.760  -2.008  -0.935  1.00  0.00
ATOM     29  C29 UNK     1      -3.707  -2.140   0.076  1.00  0.00
ATOM     30  H30 UNK     1      -4.210  -1.658   2.119  1.00  0.00
ATOM     31  H31 UNK     1      -2.914  -2.437  -1.920  1.00  0.00
ATOM     32  H32 UNK     1      -4.625  -2.690  -0.114  1.00  0.00
ATOM     33  O33 UNK     1      -0.721   1.168  -1.697  1.00  0.00
ATOM     34  O34 UNK     1      -0.651  -1.208  -1.697  1.00  0.00
ATOM     35  O35 UNK     1       1.372   0.040  -1.697  1.00  0.00
ATOM     36  B36 UNK     1       0.000   0.000  -1.744  1.00  0.00
CONECT    1    2    3   13   23
CONECT    2    1
CONECT    3    1    4    5
CONECT    4    3    6    7
CONECT    5    3    8   33
CONECT    6    4    9   10
CONECT    7    4
CONECT    8    5    9   11
CONECT    9    6    8   12
CONECT   10    6
CONECT   11    8
CONECT   12    9
CONECT   13    1   14   15
CONECT   14   13   16   35
CONECT   15   13   17   18
CONECT   16   14   19   20
CONECT   17   15   19   21
CONECT   18   15
CONECT   19   16   17   22
CONECT   20   16
CONECT   21   17
CONECT   22   19
CONECT   23    1   24   25
CONECT   24   23   26   27
CONECT   25   23   28   34
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CONECT   26   24   29   30
CONECT   27   24
CONECT   28   25   29   31
CONECT   29   26   28   32
CONECT   30   26
CONECT   31   28
CONECT   32   29
CONECT   33    5   36
CONECT   34   25   36
CONECT   35   14   36
CONECT   36   33   34   35
MASTER        0    0    0    0    0    0    0    0   36    0   36    0
END
```

1B·Py

```
HEADER    PROTEIN
ATOM      1  C1  UNK     1       2.004  -0.068  -0.003  1.00  0.00
ATOM      2  H2  UNK     1       3.097  -0.119  -0.009  1.00  0.00
ATOM      3  C3  UNK     1       1.707   1.303  -0.610  1.00  0.00
ATOM      4  C4  UNK     1       2.731   1.954  -1.312  1.00  0.00
ATOM      5  C5  UNK     1       0.483   1.979  -0.471  1.00  0.00
ATOM      6  C6  UNK     1       2.577   3.232  -1.840  1.00  0.00
ATOM      7  H7  UNK     1       3.682   1.438  -1.435  1.00  0.00
ATOM      8  C8  UNK     1       0.327   3.272  -0.984  1.00  0.00
ATOM      9  C9  UNK     1       1.365   3.900  -1.662  1.00  0.00
ATOM     10  H10 UNK     1       3.397   3.705  -2.373  1.00  0.00
ATOM     11  H11 UNK     1      -0.627   3.772  -0.839  1.00  0.00
ATOM     12  H12 UNK     1       1.226   4.904  -2.053  1.00  0.00
ATOM     13  C13 UNK     1       1.585  -1.254  -0.872  1.00  0.00
ATOM     14  C14 UNK     1       0.322  -1.381  -1.477  1.00  0.00
ATOM     15  C15 UNK     1       2.533  -2.254  -1.128  1.00  0.00
ATOM     16  C16 UNK     1       0.057  -2.451  -2.340  1.00  0.00
ATOM     17  C17 UNK     1       2.268  -3.333  -1.968  1.00  0.00
ATOM     18  H18 UNK     1       3.511  -2.173  -0.659  1.00  0.00
ATOM     19  C19 UNK     1       1.022  -3.422  -2.588  1.00  0.00
ATOM     20  H20 UNK     1      -0.922  -2.498  -2.808  1.00  0.00
ATOM     21  H21 UNK     1       3.030  -4.086  -2.146  1.00  0.00
ATOM     22  H22 UNK     1       0.799  -4.246  -3.262  1.00  0.00
ATOM     23  C23 UNK     1       1.647  -0.200   1.477  1.00  0.00
ATOM     24  C24 UNK     1       2.653   0.017   2.428  1.00  0.00
ATOM     25  C25 UNK     1       0.376  -0.574   1.944  1.00  0.00
ATOM     26  C26 UNK     1       2.432  -0.148   3.793  1.00  0.00
ATOM     27  H27 UNK     1       3.641   0.313   2.080  1.00  0.00
ATOM     28  C28 UNK     1       0.151  -0.757   3.313  1.00  0.00
ATOM     29  C29 UNK     1       1.171  -0.549   4.235  1.00  0.00
ATOM     30  H30 UNK     1       3.238   0.024   4.501  1.00  0.00
ATOM     31  H31 UNK     1      -0.843  -1.061   3.631  1.00  0.00
ATOM     32  H32 UNK     1       0.980  -0.695   5.295  1.00  0.00
ATOM     33  O33 UNK     1      -0.573   1.441   0.195  1.00  0.00
ATOM     34  O34 UNK     1      -0.659  -0.813   1.101  1.00  0.00
ATOM     35  O35 UNK     1      -0.670  -0.474  -1.294  1.00  0.00
ATOM     36  B36 UNK     1      -0.969   0.073   0.006  1.00  0.00
ATOM     37  H37 UNK     1      -2.707   2.157  -0.010  1.00  0.00
ATOM     38  C38 UNK     1      -3.314   1.260  -0.006  1.00  0.00
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ATOM     39  C39 UNK     1      -4.703   1.272  -0.019  1.00  0.00
ATOM     40  N40 UNK     1      -2.625   0.111   0.022  1.00  0.00
ATOM     41  C41 UNK     1      -5.388   0.060  -0.004  1.00  0.00
ATOM     42  H42 UNK     1      -5.230   2.220  -0.042  1.00  0.00
ATOM     43  C43 UNK     1      -3.275  -1.065   0.038  1.00  0.00
ATOM     44  C44 UNK     1      -4.659  -1.129   0.026  1.00  0.00
ATOM     45  H45 UNK     1      -6.474   0.040  -0.015  1.00  0.00
ATOM     46  H46 UNK     1      -2.645  -1.947   0.067  1.00  0.00
ATOM     47  H47 UNK     1      -5.151  -2.095   0.040  1.00  0.00
CONECT    1    2    3   13   23
CONECT    2    1
CONECT    3    1    4    5
CONECT    4    3    6    7
CONECT    5    3    8   33
CONECT    6    4    9   10
CONECT    7    4
CONECT    8    5    9   11
CONECT    9    6    8   12
CONECT   10    6
CONECT   11    8
CONECT   12    9
CONECT   13    1   14   15
CONECT   14   13   16   35
CONECT   15   13   17   18
CONECT   16   14   19   20
CONECT   17   15   19   21
CONECT   18   15
CONECT   19   16   17   22
CONECT   20   16
CONECT   21   17
CONECT   22   19
CONECT   23    1   24   25
CONECT   24   23   26   27
CONECT   25   23   28   34
CONECT   26   24   29   30
CONECT   27   24
CONECT   28   25   29   31
CONECT   29   26   28   32
CONECT   30   26
CONECT   31   28
CONECT   32   29
CONECT   33    5   36
CONECT   34   25   36
CONECT   35   14   36
CONECT   36   33   34   35   40
CONECT   37   38
CONECT   38   37   39   40
CONECT   39   38   41   42
CONECT   40   36   38   43
CONECT   41   39   44   45
CONECT   42   39
CONECT   43   40   44   46
CONECT   44   41   43   47
CONECT   45   41
CONECT   46   43
```

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CONECT   47   44
MASTER        0    0    0    0    0    0    0    0   47    0   47    0
END
```

3aB

```
HEADER    PROTEIN
ATOM      1 Si   UNK     1       0.000   0.000   1.090  1.00  0.00
ATOM      2  O   UNK     1       0.703   1.179  -1.731  1.00  0.00
ATOM      3  O   UNK     1      -1.372   0.019  -1.731  1.00  0.00
ATOM      4  O   UNK     1       0.669  -1.198  -1.731  1.00  0.00
ATOM      5  C   UNK     1       0.315   2.157  -0.843  1.00  0.00
ATOM      6  C   UNK     1      -0.037   1.800   0.472  1.00  0.00
ATOM      7  C   UNK     1      -0.391   2.849   1.337  1.00  0.00
ATOM      8  C   UNK     1      -0.376   4.181   0.923  1.00  0.00
ATOM      9  C   UNK     1       0.000   4.494  -0.383  1.00  0.00
ATOM     10  C   UNK     1       0.347   3.481  -1.273  1.00  0.00
ATOM     11  C   UNK     1      -2.025  -0.806  -0.843  1.00  0.00
ATOM     12  C   UNK     1      -1.540  -0.932   0.472  1.00  0.00
ATOM     13  C   UNK     1      -2.272  -1.764   1.337  1.00  0.00
ATOM     14  C   UNK     1      -3.433  -2.416   0.923  1.00  0.00
ATOM     15  C   UNK     1      -3.892  -2.247  -0.383  1.00  0.00
ATOM     16  C   UNK     1      -3.188  -1.440  -1.273  1.00  0.00
ATOM     17  C   UNK     1       1.711  -1.351  -0.843  1.00  0.00
ATOM     18  C   UNK     1       1.577  -0.868   0.472  1.00  0.00
ATOM     19  C   UNK     1       2.663  -1.086   1.337  1.00  0.00
ATOM     20  C   UNK     1       3.809  -1.765   0.923  1.00  0.00
ATOM     21  C   UNK     1       3.892  -2.247  -0.383  1.00  0.00
ATOM     22  C   UNK     1       2.841  -2.041  -1.273  1.00  0.00
ATOM     23  C   UNK     1       0.000   0.000   2.972  1.00  0.00
ATOM     24  B   UNK     1       0.000   0.000  -1.747  1.00  0.00
ATOM     25  H   UNK     1      -0.677   2.626   2.361  1.00  0.00
ATOM     26  H   UNK     1      -0.650   4.969   1.619  1.00  0.00
ATOM     27  H   UNK     1       0.021   5.529  -0.714  1.00  0.00
ATOM     28  H   UNK     1       0.638   3.697  -2.296  1.00  0.00
ATOM     29  H   UNK     1      -1.935  -1.899   2.361  1.00  0.00
ATOM     30  H   UNK     1      -3.978  -3.047   1.619  1.00  0.00
ATOM     31  H   UNK     1      -4.799  -2.746  -0.714  1.00  0.00
ATOM     32  H   UNK     1      -3.521  -1.296  -2.296  1.00  0.00
ATOM     33  H   UNK     1       2.612  -0.726   2.361  1.00  0.00
ATOM     34  H   UNK     1       4.628  -1.922   1.619  1.00  0.00
ATOM     35  H   UNK     1       4.778  -2.783  -0.714  1.00  0.00
ATOM     36  H   UNK     1       2.883  -2.401  -2.296  1.00  0.00
ATOM     37  H   UNK     1       0.799   0.637   3.364  1.00  0.00
ATOM     38  H   UNK     1      -0.951   0.373   3.364  1.00  0.00
ATOM     39  H   UNK     1       0.153  -1.010   3.364  1.00  0.00
CONECT    1    6   12   18   23
CONECT    2    5   24
CONECT    3   11   24
CONECT    4   17   24
CONECT    5    2    6   10
CONECT    6    1    5    7
CONECT    7    6    8   25
CONECT    8    7    9   26
CONECT    9    8   10   27
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CONECT   10    5    9   28
CONECT   11    3   12   16
CONECT   12    1   11   13
CONECT   13   12   14   29
CONECT   14   13   15   30
CONECT   15   14   16   31
CONECT   16   11   15   32
CONECT   17    4   18   22
CONECT   18    1   17   19
CONECT   19   18   20   33
CONECT   20   19   21   34
CONECT   21   20   22   35
CONECT   22   17   21   36
CONECT   23    1   37   38   39
CONECT   24    2    3    4
CONECT   25    7
CONECT   26    8
CONECT   27    9
CONECT   28   10
CONECT   29   13
CONECT   30   14
CONECT   31   15
CONECT   32   16
CONECT   33   19
CONECT   34   20
CONECT   35   21
CONECT   36   22
CONECT   37   23
CONECT   38   23
CONECT   39   23
MASTER        0    0    0    0    0    0    0    0   39    0   39    0
END
```

3aB·Py

```
HEADER    PROTEIN
ATOM      1 Si   UNK     1       2.082   0.009   0.122  1.00  0.00
ATOM      2  O   UNK     1      -0.682  -1.348  -0.508  1.00  0.00
ATOM      3  O   UNK     1      -0.704   1.035  -1.008  1.00  0.00
ATOM      4  O   UNK     1      -0.809   0.287   1.290  1.00  0.00
ATOM      5  N   UNK     1      -2.729  -0.038  -0.162  1.00  0.00
ATOM      6  C   UNK     1       0.285  -1.643  -1.419  1.00  0.00
ATOM      7  C   UNK     1       1.587  -1.123  -1.307  1.00  0.00
ATOM      8  C   UNK     1       2.525  -1.515  -2.277  1.00  0.00
ATOM      9  C   UNK     1       2.202  -2.396  -3.308  1.00  0.00
ATOM     10  C   UNK     1       0.908  -2.913  -3.383  1.00  0.00
ATOM     11  C   UNK     1      -0.047  -2.537  -2.443  1.00  0.00
ATOM     12  C   UNK     1       0.195   2.023  -0.757  1.00  0.00
ATOM     13  C   UNK     1       1.470   1.764  -0.219  1.00  0.00
ATOM     14  C   UNK     1       2.318   2.866  -0.013  1.00  0.00
ATOM     15  C   UNK     1       1.943   4.167  -0.342  1.00  0.00
ATOM     16  C   UNK     1       0.687   4.391  -0.908  1.00  0.00
ATOM     17  C   UNK     1      -0.182   3.324  -1.114  1.00  0.00
ATOM     18  C   UNK     1       0.036  -0.394   2.108  1.00  0.00
ATOM     19  C   UNK     1       1.375  -0.635   1.748  1.00  0.00
```

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ATOM     20  C   UNK     1       2.180  -1.321   2.673  1.00  0.00
ATOM     21  C   UNK     1       1.694  -1.738   3.911  1.00  0.00
ATOM     22  C   UNK     1       0.369  -1.463   4.252  1.00  0.00
ATOM     23  C   UNK     1      -0.458  -0.795   3.355  1.00  0.00
ATOM     24  C   UNK     1       3.965   0.037   0.246  1.00  0.00
ATOM     25  C   UNK     1      -3.420  -1.177  -0.305  1.00  0.00
ATOM     26  C   UNK     1      -4.809  -1.192  -0.281  1.00  0.00
ATOM     27  C   UNK     1      -5.493   0.008  -0.102  1.00  0.00
ATOM     28  C   UNK     1      -4.762   1.186   0.052  1.00  0.00
ATOM     29  C   UNK     1      -3.377   1.123   0.017  1.00  0.00
ATOM     30  B   UNK     1      -1.051  -0.023  -0.097  1.00  0.00
ATOM     31  H   UNK     1       3.540  -1.130  -2.222  1.00  0.00
ATOM     32  H   UNK     1       2.952  -2.680  -4.040  1.00  0.00
ATOM     33  H   UNK     1       0.639  -3.607  -4.176  1.00  0.00
ATOM     34  H   UNK     1      -1.060  -2.927  -2.492  1.00  0.00
ATOM     35  H   UNK     1       3.309   2.703   0.406  1.00  0.00
ATOM     36  H   UNK     1       2.626   4.994  -0.172  1.00  0.00
ATOM     37  H   UNK     1       0.383   5.395  -1.190  1.00  0.00
ATOM     38  H   UNK     1      -1.159   3.477  -1.564  1.00  0.00
ATOM     39  H   UNK     1       3.220  -1.526   2.426  1.00  0.00
ATOM     40  H   UNK     1       2.345  -2.263   4.605  1.00  0.00
ATOM     41  H   UNK     1      -0.023  -1.771   5.218  1.00  0.00
ATOM     42  H   UNK     1      -1.492  -0.571   3.602  1.00  0.00
ATOM     43  H   UNK     1       4.371  -0.979   0.290  1.00  0.00
ATOM     44  H   UNK     1       4.410   0.539  -0.619  1.00  0.00
ATOM     45  H   UNK     1       4.293   0.567   1.146  1.00  0.00
ATOM     46  H   UNK     1      -2.816  -2.067  -0.439  1.00  0.00
ATOM     47  H   UNK     1      -5.337  -2.131  -0.404  1.00  0.00
ATOM     48  H   UNK     1      -6.579   0.027  -0.081  1.00  0.00
ATOM     49  H   UNK     1      -5.252   2.142   0.197  1.00  0.00
ATOM     50  H   UNK     1      -2.747   1.999   0.127  1.00  0.00
CONECT    1    7   13   19   24
CONECT    2    6   30
CONECT    3   12   30
CONECT    4   18   30
CONECT    5   25   29
CONECT    6    2    7   11
CONECT    7    1    6    8
CONECT    8    7    9   31
CONECT    9    8   10   32
CONECT   10    9   11   33
CONECT   11    6   10   34
CONECT   12    3   13   17
CONECT   13    1   12   14
CONECT   14   13   15   35
CONECT   15   14   16   36
CONECT   16   15   17   37
CONECT   17   12   16   38
CONECT   18    4   19   23
CONECT   19    1   18   20
CONECT   20   19   21   39
CONECT   21   20   22   40
CONECT   22   21   23   41
CONECT   23   18   22   42
CONECT   24    1   43   44   45
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CONECT   25    5   26   46
CONECT   26   25   27   47
CONECT   27   26   28   48
CONECT   28   27   29   49
CONECT   29    5   28   50
CONECT   30    2    3    4
CONECT   31    8
CONECT   32    9
CONECT   33   10
CONECT   34   11
CONECT   35   14
CONECT   36   15
CONECT   37   16
CONECT   38   17
CONECT   39   20
CONECT   40   21
CONECT   41   22
CONECT   42   23
CONECT   43   24
CONECT   44   24
CONECT   45   24
CONECT   46   25
CONECT   47   26
CONECT   48   27
CONECT   49   28
CONECT   50   29
MASTER        0    0    0    0    0    0    0    0   50    0   50    0
END
```

3bB

```
HEADER    PROTEIN
ATOM      1 Si   UNK     1       0.322  -0.022   0.472  1.00  0.00
ATOM      2  O   UNK     1      -2.553  -0.660  -0.629  1.00  0.00
ATOM      3  O   UNK     1      -1.804   1.497  -1.281  1.00  0.00
ATOM      4  O   UNK     1      -0.950  -0.434  -2.370  1.00  0.00
ATOM      5  C   UNK     1      -2.569  -0.372   0.718  1.00  0.00
ATOM      6  C   UNK     1      -1.366  -0.048   1.374  1.00  0.00
ATOM      7  C   UNK     1      -1.460   0.212   2.752  1.00  0.00
ATOM      8  C   UNK     1      -2.670   0.132   3.440  1.00  0.00
ATOM      9  C   UNK     1      -3.834  -0.218   2.755  1.00  0.00
ATOM     10  C   UNK     1      -3.786  -0.470   1.387  1.00  0.00
ATOM     11  C   UNK     1      -0.593   2.150  -1.257  1.00  0.00
ATOM     12  C   UNK     1       0.481   1.598  -0.532  1.00  0.00
ATOM     13  C   UNK     1       1.682   2.328  -0.555  1.00  0.00
ATOM     14  C   UNK     1       1.800   3.544  -1.227  1.00  0.00
ATOM     15  C   UNK     1       0.700   4.070  -1.904  1.00  0.00
ATOM     16  C   UNK     1      -0.502   3.370  -1.922  1.00  0.00
ATOM     17  C   UNK     1      -0.217  -1.530  -1.970  1.00  0.00
ATOM     18  C   UNK     1       0.406  -1.521  -0.707  1.00  0.00
ATOM     19  C   UNK     1       1.112  -2.683  -0.354  1.00  0.00
ATOM     20  C   UNK     1       1.233  -3.769  -1.220  1.00  0.00
ATOM     21  C   UNK     1       0.638  -3.716  -2.481  1.00  0.00
ATOM     22  C   UNK     1      -0.096  -2.595  -2.858  1.00  0.00
ATOM     23  C   UNK     1       1.647  -0.137   1.831  1.00  0.00
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ATOM     24  B   UNK     1      -1.783   0.135  -1.440  1.00  0.00
ATOM     25  H   UNK     1      -0.567   0.476   3.312  1.00  0.00
ATOM     26  H   UNK     1      -2.702   0.335   4.507  1.00  0.00
ATOM     27  H   UNK     1      -4.781  -0.290   3.283  1.00  0.00
ATOM     28  H   UNK     1      -4.676  -0.736   0.826  1.00  0.00
ATOM     29  H   UNK     1       2.550   1.944  -0.032  1.00  0.00
ATOM     30  H   UNK     1       2.745   4.080  -1.216  1.00  0.00
ATOM     31  H   UNK     1       0.778   5.020  -2.425  1.00  0.00
ATOM     32  H   UNK     1      -1.373   3.746  -2.451  1.00  0.00
ATOM     33  H   UNK     1       1.580  -2.743   0.623  1.00  0.00
ATOM     34  H   UNK     1       1.792  -4.648  -0.914  1.00  0.00
ATOM     35  H   UNK     1       0.734  -4.553  -3.168  1.00  0.00
ATOM     36  H   UNK     1      -0.589  -2.535  -3.823  1.00  0.00
ATOM     37  H   UNK     1       1.370  -1.016   2.430  1.00  0.00
ATOM     38  H   UNK     1       1.445   0.719   2.490  1.00  0.00
ATOM     39  C   UNK     1       3.171  -0.175   1.510  1.00  0.00
ATOM     40  H   UNK     1       3.327  -0.117   0.424  1.00  0.00
ATOM     41  C   UNK     1       3.824  -1.476   1.992  1.00  0.00
ATOM     42  H   UNK     1       3.703  -1.590   3.076  1.00  0.00
ATOM     43  H   UNK     1       4.897  -1.477   1.774  1.00  0.00
ATOM     44  H   UNK     1       3.393  -2.360   1.512  1.00  0.00
ATOM     45  C   UNK     1       3.896   1.011   2.161  1.00  0.00
ATOM     46  H   UNK     1       4.958   1.022   1.890  1.00  0.00
ATOM     47  H   UNK     1       3.831   0.942   3.254  1.00  0.00
ATOM     48  H   UNK     1       3.464   1.974   1.870  1.00  0.00
CONECT    1    6   12   18   23
CONECT    2    5   24
CONECT    3   11   24
CONECT    4   17   24
CONECT    5    2    6   10
CONECT    6    1    5    7
CONECT    7    6    8   25
CONECT    8    7    9   26
CONECT    9    8   10   27
CONECT   10    5    9   28
CONECT   11    3   12   16
CONECT   12    1   11   13
CONECT   13   12   14   29
CONECT   14   13   15   30
CONECT   15   14   16   31
CONECT   16   11   15   32
CONECT   17    4   18   22
CONECT   18    1   17   19
CONECT   19   18   20   33
CONECT   20   19   21   34
CONECT   21   20   22   35
CONECT   22   17   21   36
CONECT   23    1   37   38   39
CONECT   24    2    3    4
CONECT   25    7
CONECT   26    8
CONECT   27    9
CONECT   28   10
CONECT   29   13
CONECT   30   14
```

```
CONECT   31   15
CONECT   32   16
CONECT   33   19
CONECT   34   20
CONECT   35   21
CONECT   36   22
CONECT   37   23
CONECT   38   23
CONECT   39   23   40   41   45
CONECT   40   39
CONECT   41   39   42   43   44
CONECT   42   41
CONECT   43   41
CONECT   44   41
CONECT   45   39   46   47   48
CONECT   46   45
CONECT   47   45
CONECT   48   45
MASTER        0    0    0    0    0    0    0    0   48    0   48    0
END
```

3bB·Py

```
HEADER    PROTEIN
ATOM      1 Si   UNK     1       1.516  -0.071  -0.310  1.00  0.00
ATOM      2  O   UNK     1      -1.277  -1.413   0.198  1.00  0.00
ATOM      3  O   UNK     1      -1.435   0.592  -1.158  1.00  0.00
ATOM      4  O   UNK     1      -1.127   0.783   1.234  1.00  0.00
ATOM      5  N   UNK     1      -3.270   0.017   0.332  1.00  0.00
ATOM      6  C   UNK     1      -0.287  -1.928   0.978  1.00  0.00
ATOM      7  C   UNK     1       1.031  -1.439   0.910  1.00  0.00
ATOM      8  C   UNK     1       1.975  -2.041   1.760  1.00  0.00
ATOM      9  C   UNK     1       1.650  -3.096   2.611  1.00  0.00
ATOM     10  C   UNK     1       0.343  -3.583   2.627  1.00  0.00
ATOM     11  C   UNK     1      -0.622  -2.997   1.815  1.00  0.00
ATOM     12  C   UNK     1      -0.697   0.055  -2.164  1.00  0.00
ATOM     13  C   UNK     1       0.641  -0.342  -1.970  1.00  0.00
ATOM     14  C   UNK     1       1.316  -0.874  -3.083  1.00  0.00
ATOM     15  C   UNK     1       0.714  -0.991  -4.334  1.00  0.00
ATOM     16  C   UNK     1      -0.602  -0.560  -4.503  1.00  0.00
ATOM     17  C   UNK     1      -1.306  -0.040  -3.421  1.00  0.00
ATOM     18  C   UNK     1      -0.211   1.779   1.106  1.00  0.00
ATOM     19  C   UNK     1       0.999   1.605   0.404  1.00  0.00
ATOM     20  C   UNK     1       1.841   2.725   0.299  1.00  0.00
ATOM     21  C   UNK     1       1.542   3.947   0.899  1.00  0.00
ATOM     22  C   UNK     1       0.368   4.070   1.643  1.00  0.00
ATOM     23  C   UNK     1      -0.506   2.992   1.741  1.00  0.00
ATOM     24  C   UNK     1       3.383  -0.105  -0.696  1.00  0.00
ATOM     25  C   UNK     1       4.475   0.122   0.390  1.00  0.00
ATOM     26  C   UNK     1       5.353   1.339   0.072  1.00  0.00
ATOM     27  C   UNK     1       5.377  -1.112   0.529  1.00  0.00
ATOM     28  C   UNK     1      -4.013  -1.094   0.234  1.00  0.00
ATOM     29  C   UNK     1      -5.399  -1.052   0.317  1.00  0.00
ATOM     30  C   UNK     1      -6.026   0.177   0.505  1.00  0.00
ATOM     31  C   UNK     1      -5.243   1.327   0.600  1.00  0.00
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ATOM     32  C   UNK     1       -3.864   1.208   0.509  1.00  0.00
ATOM     33  B   UNK     1       -1.602  -0.017   0.136  1.00  0.00
ATOM     34  H   UNK     1        2.997  -1.679   1.758  1.00  0.00
ATOM     35  H   UNK     1        2.411  -3.536   3.250  1.00  0.00
ATOM     36  H   UNK     1        0.073  -4.412   3.276  1.00  0.00
ATOM     37  H   UNK     1       -1.649  -3.352   1.824  1.00  0.00
ATOM     38  H   UNK     1        2.347  -1.201  -2.977  1.00  0.00
ATOM     39  H   UNK     1        1.270  -1.406  -5.171  1.00  0.00
ATOM     40  H   UNK     1       -1.084  -0.632  -5.475  1.00  0.00
ATOM     41  H   UNK     1       -2.333   0.298  -3.527  1.00  0.00
ATOM     42  H   UNK     1        2.763   2.638  -0.268  1.00  0.00
ATOM     43  H   UNK     1        2.222   4.787   0.797  1.00  0.00
ATOM     44  H   UNK     1        0.127   5.007   2.138  1.00  0.00
ATOM     45  H   UNK     1       -1.427   3.069   2.313  1.00  0.00
ATOM     46  H   UNK     1        3.554  -1.083  -1.167  1.00  0.00
ATOM     47  H   UNK     1        3.520   0.619  -1.512  1.00  0.00
ATOM     48  H   UNK     1        4.003   0.310   1.364  1.00  0.00
ATOM     49  H   UNK     1        5.861   1.205  -0.891  1.00  0.00
ATOM     50  H   UNK     1        6.123   1.479   0.839  1.00  0.00
ATOM     51  H   UNK     1        4.773   2.264   0.018  1.00  0.00
ATOM     52  H   UNK     1        5.931  -1.282  -0.403  1.00  0.00
ATOM     53  H   UNK     1        6.111  -0.981   1.333  1.00  0.00
ATOM     54  H   UNK     1        4.808  -2.023   0.739  1.00  0.00
ATOM     55  H   UNK     1       -3.451  -2.010   0.087  1.00  0.00
ATOM     56  H   UNK     1       -5.969  -1.972   0.236  1.00  0.00
ATOM     57  H   UNK     1       -7.108   0.240   0.576  1.00  0.00
ATOM     58  H   UNK     1       -5.688   2.305   0.745  1.00  0.00
ATOM     59  H   UNK     1       -3.196   2.058   0.578  1.00  0.00
CONECT    1    7   13   19   24
CONECT    2    6   33
CONECT    3   12   33
CONECT    4   18   33
CONECT    5   28   32
CONECT    6    2    7   11
CONECT    7    1    6    8
CONECT    8    7    9   34
CONECT    9    8   10   35
CONECT   10    9   11   36
CONECT   11    6   10   37
CONECT   12    3   13   17
CONECT   13    1   12   14
CONECT   14   13   15   38
CONECT   15   14   16   39
CONECT   16   15   17   40
CONECT   17   12   16   41
CONECT   18    4   19   23
CONECT   19    1   18   20
CONECT   20   19   21   42
CONECT   21   20   22   43
CONECT   22   21   23   44
CONECT   23   18   22   45
CONECT   24    1   25   46   47
CONECT   25   24   26   27   48
CONECT   26   25   49   50   51
CONECT   27   25   52   53   54
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CONECT   28    5   29   55
CONECT   29   28   30   56
CONECT   30   29   31   57
CONECT   31   30   32   58
CONECT   32    5   31   59
CONECT   33    2    3    4
CONECT   34    8
CONECT   35    9
CONECT   36   10
CONECT   37   11
CONECT   38   14
CONECT   39   15
CONECT   40   16
CONECT   41   17
CONECT   42   20
CONECT   43   21
CONECT   44   22
CONECT   45   23
CONECT   46   24
CONECT   47   24
CONECT   48   25
CONECT   49   26
CONECT   50   26
CONECT   51   26
CONECT   52   27
CONECT   53   27
CONECT   54   27
CONECT   55   28
CONECT   56   29
CONECT   57   30
CONECT   58   31
CONECT   59   32
MASTER        0    0    0    0    0    0    0    0   59    0   59    0
END
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Pyridine

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HEADER    PROTEIN
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ATOM      2  C2  UNK     1      -1.198  -0.672   0.000  1.00  0.00
ATOM      3  C3  UNK     1       0.000  -1.384   0.000  1.00  0.00
ATOM      4  C4  UNK     1       1.198  -0.672   0.000  1.00  0.00
ATOM      5  C5  UNK     1       1.141   0.722   0.000  1.00  0.00
ATOM      6  H6  UNK     1      -2.058   1.309   0.000  1.00  0.00
ATOM      7  H7  UNK     1      -2.157  -1.182   0.000  1.00  0.00
ATOM      8  H8  UNK     1       0.000  -2.471   0.000  1.00  0.00
ATOM      9  H9  UNK     1       2.157  -1.182   0.000  1.00  0.00
ATOM     10  H10 UNK     1       2.058   1.309   0.000  1.00  0.00
ATOM     11  N11 UNK     1       0.000   1.419   0.000  1.00  0.00
CONECT    1    2    6   11
CONECT    2    1    3    7
CONECT    3    2    4    8
CONECT    4    3    5    9
CONECT    5    4   10   11
CONECT    6    1
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CONECT     7     2
CONECT     8     3
CONECT     9     4
CONECT    10     5
CONECT    11     1     5
MASTER        0     0     0     0     0     0     0     0    11     0    11     0
END
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References

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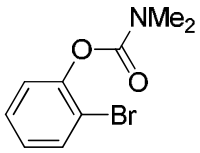
5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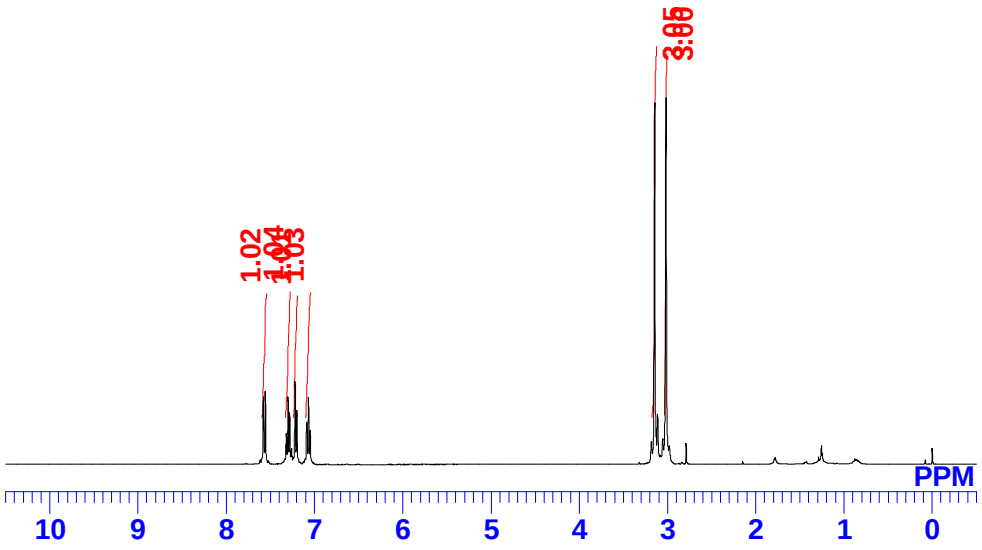
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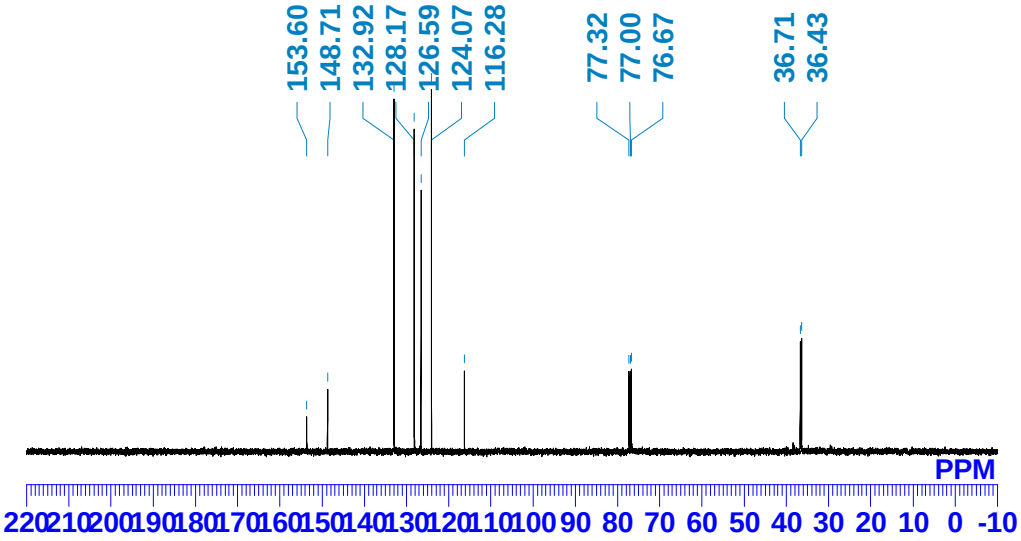
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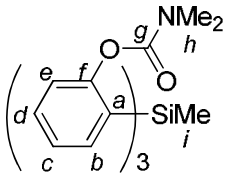
6a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O
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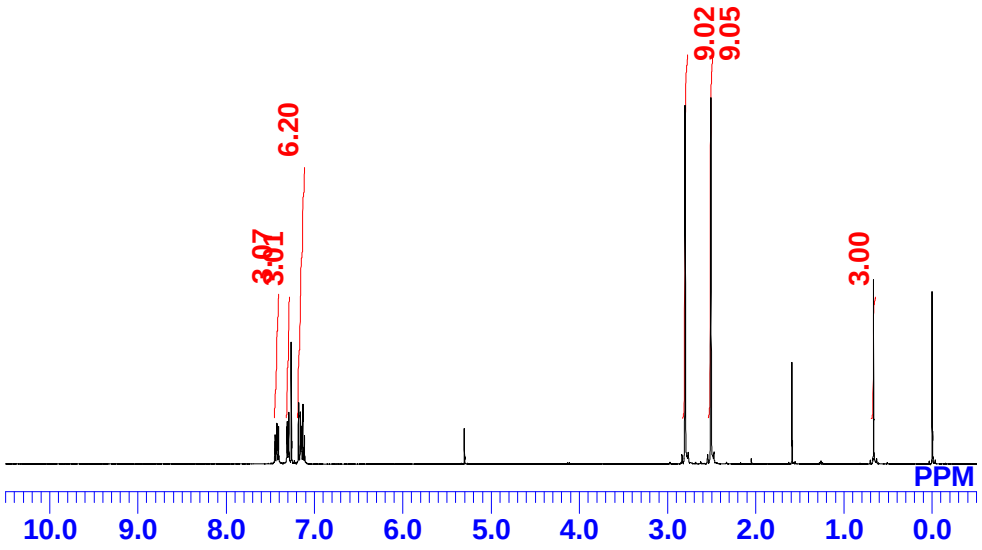
e
f
a
d
SiMe
i
c
b
3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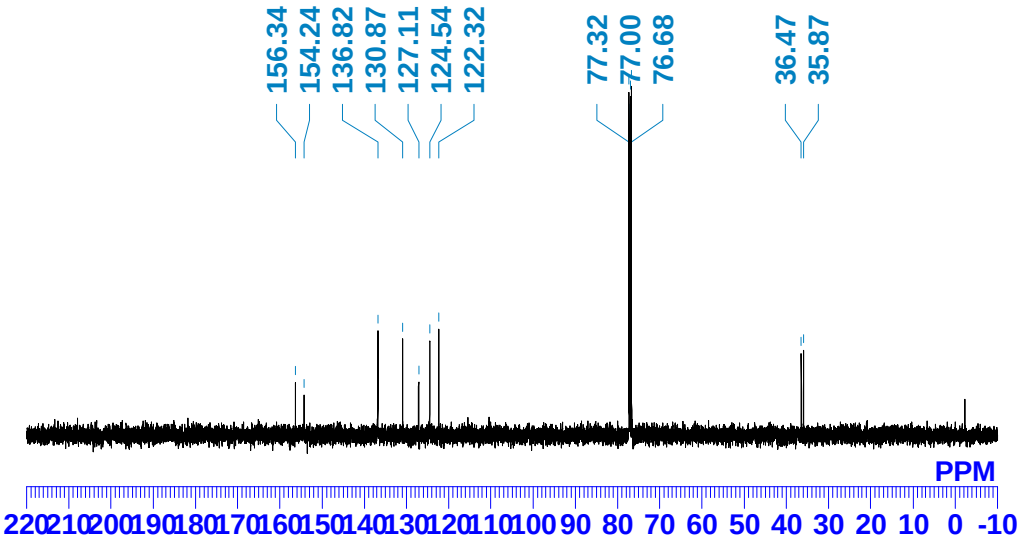
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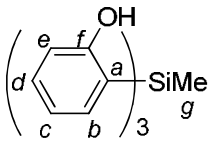
3aH_3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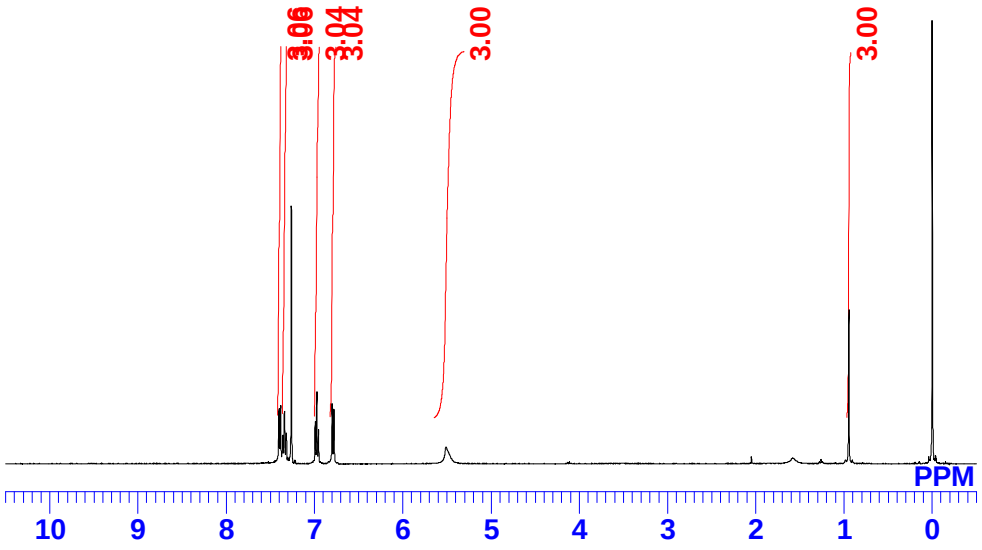
a
d
SiMe
g
c
b
3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PPM
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8
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2
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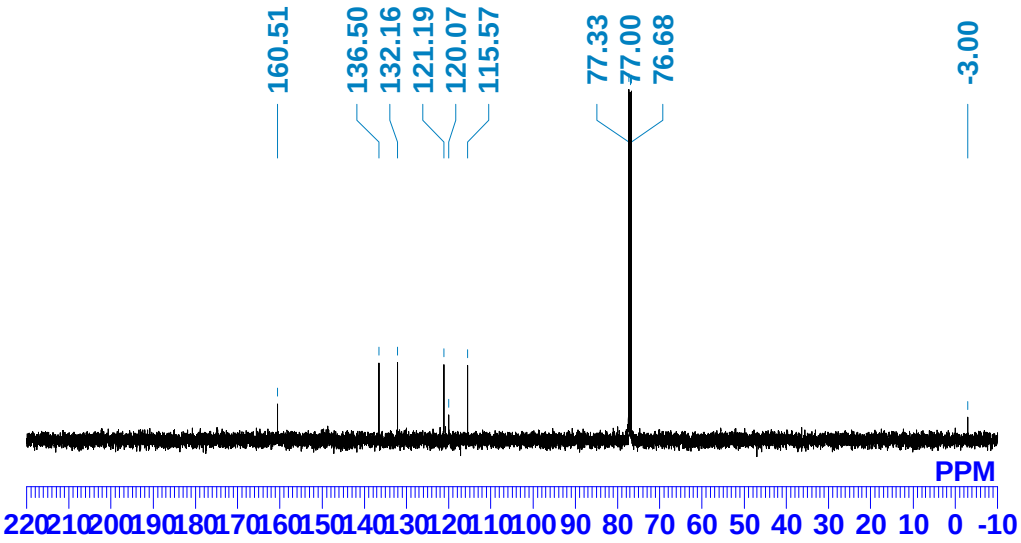
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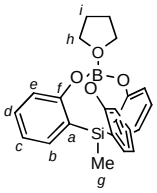
3aB·THF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B
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O
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f
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a
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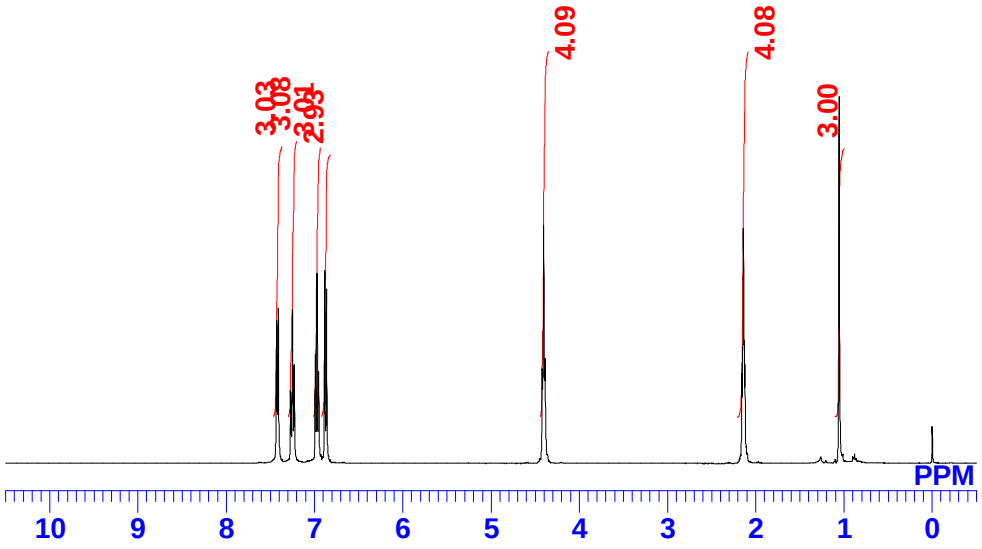
b
Si
Me
g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PPM
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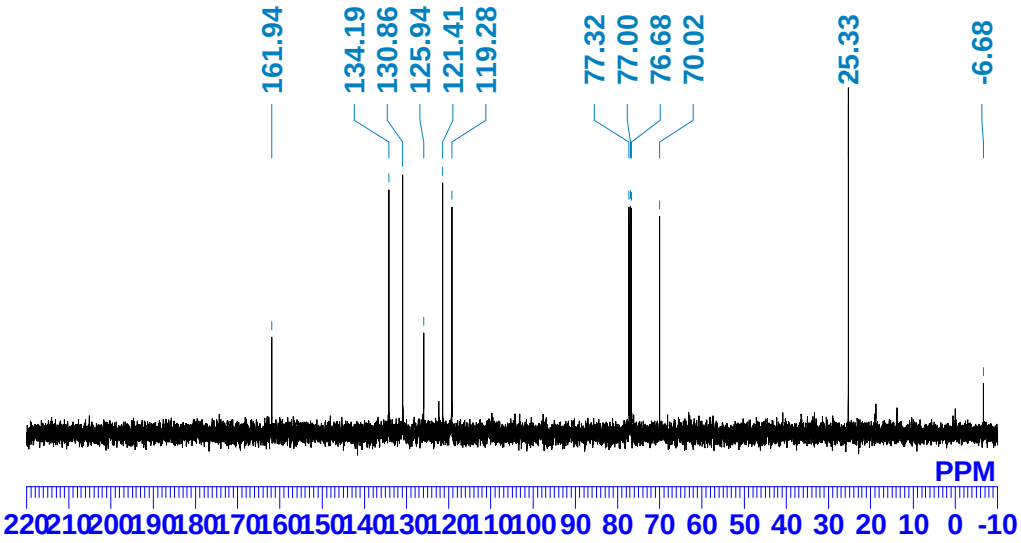
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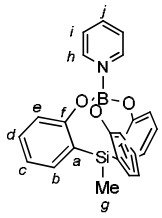
3aB·Py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Me
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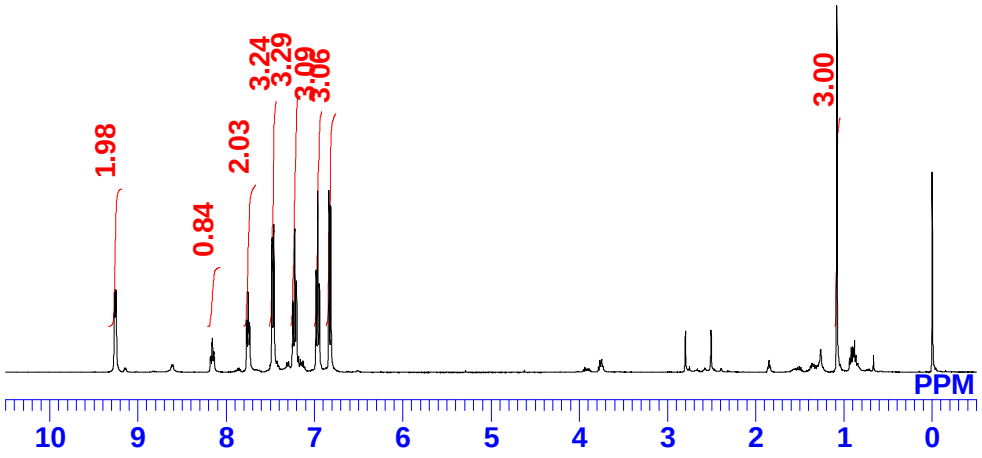
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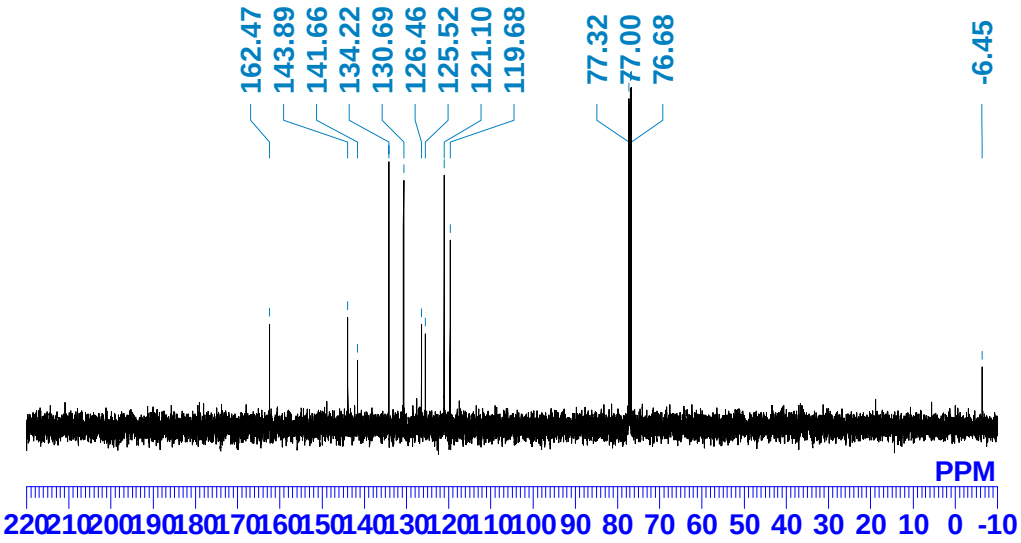
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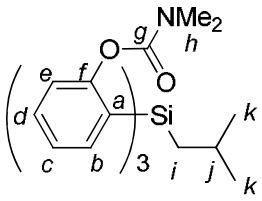
6b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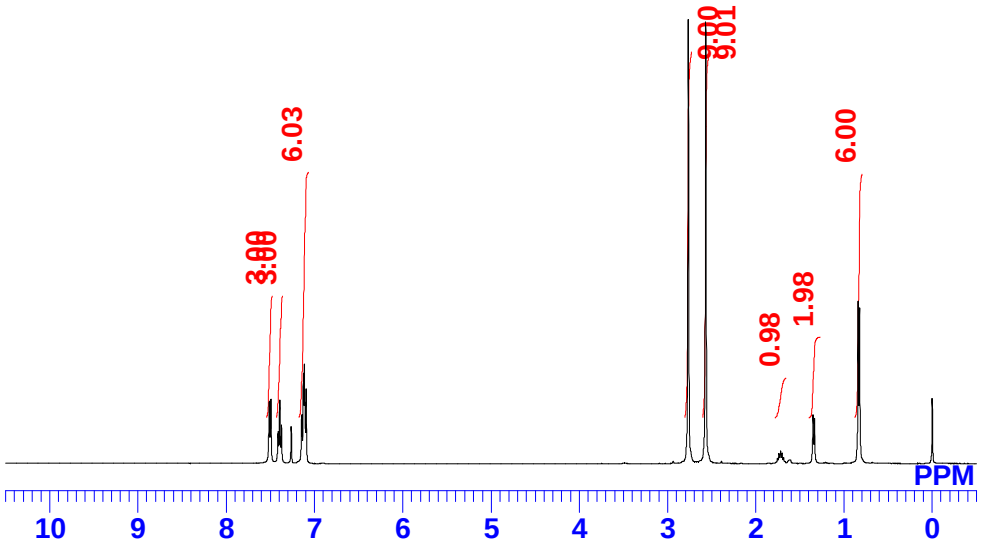
3
i
j
k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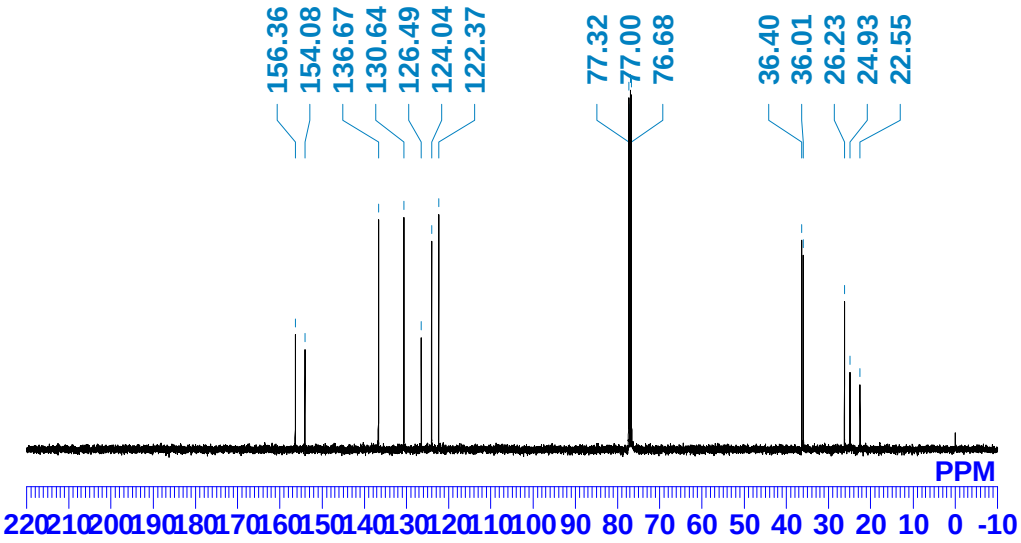
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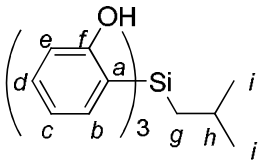
3bH_3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Si
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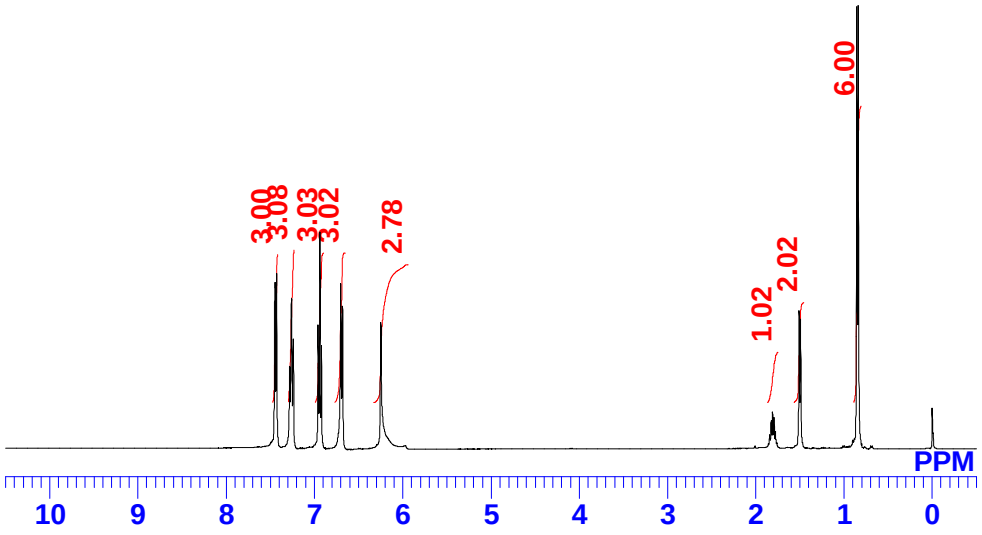
b
3
g
h
i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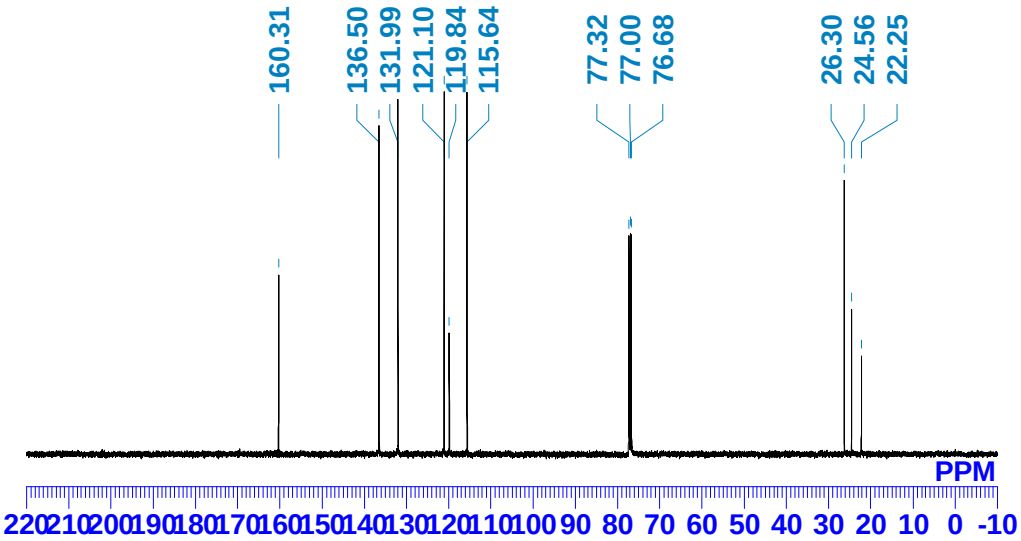
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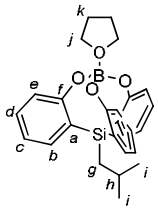
3bB·THF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Si
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h
i
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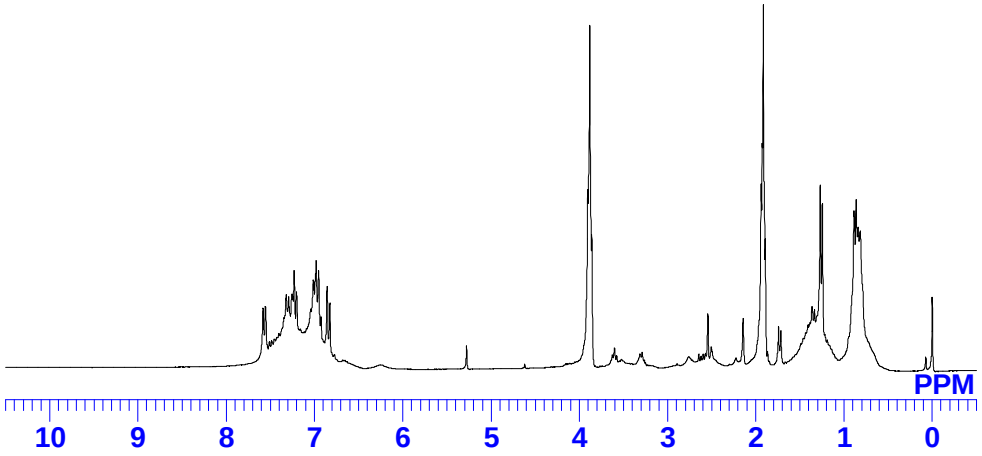
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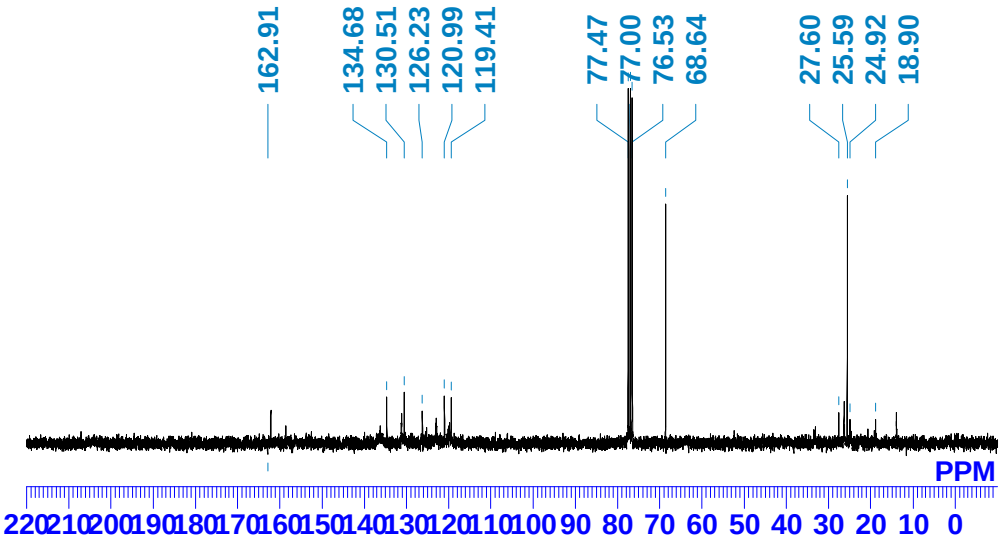
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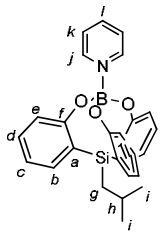
3bB·Py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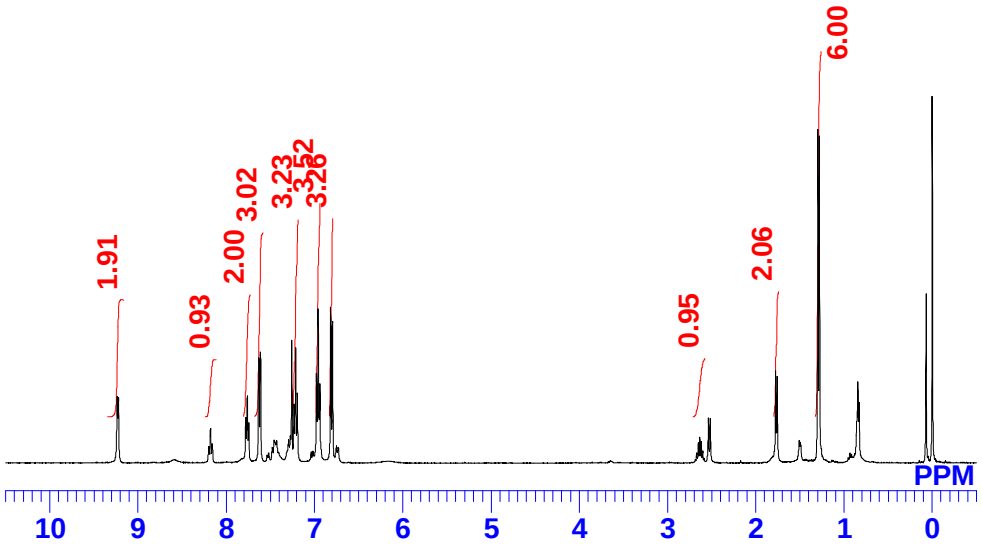
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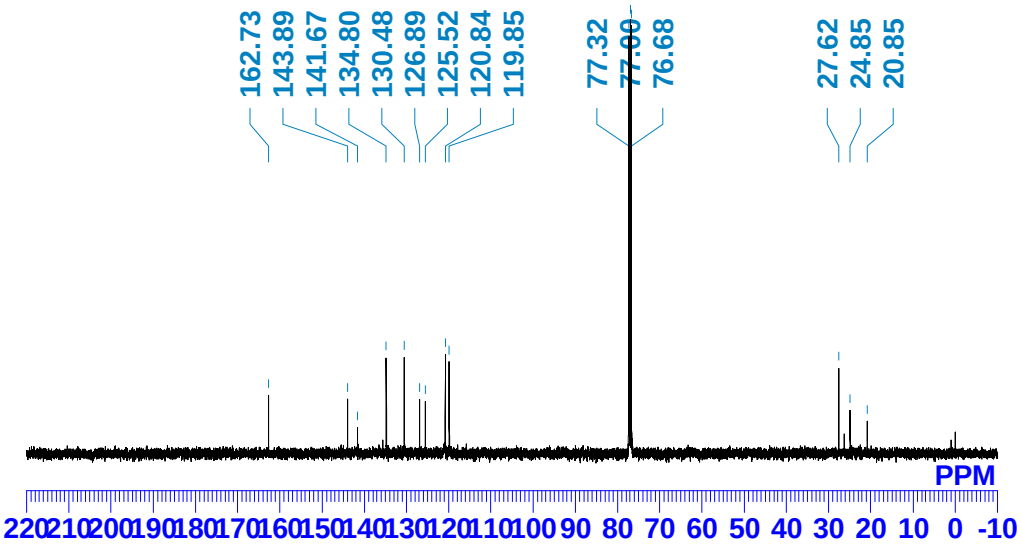
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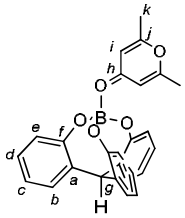
1B·**8**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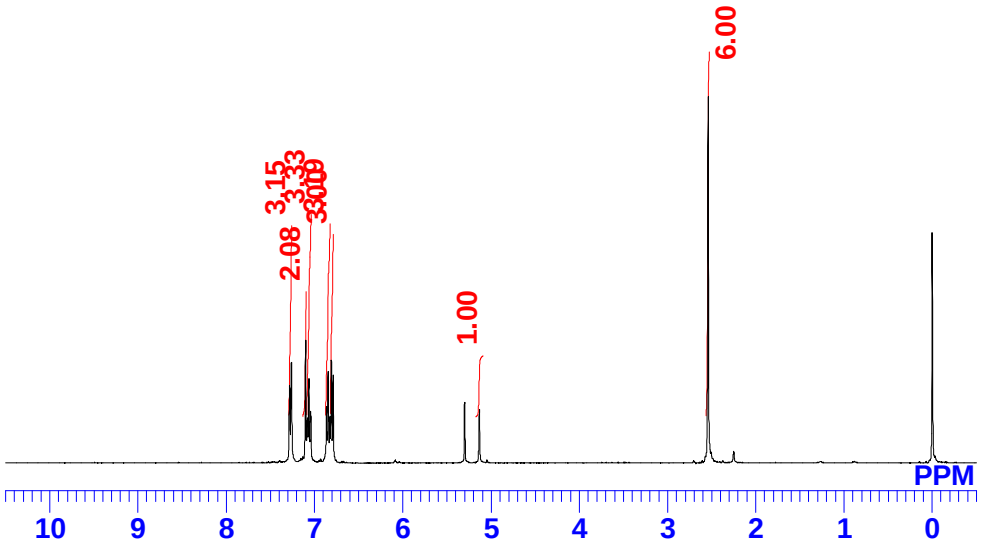
b
H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1.00
PPM
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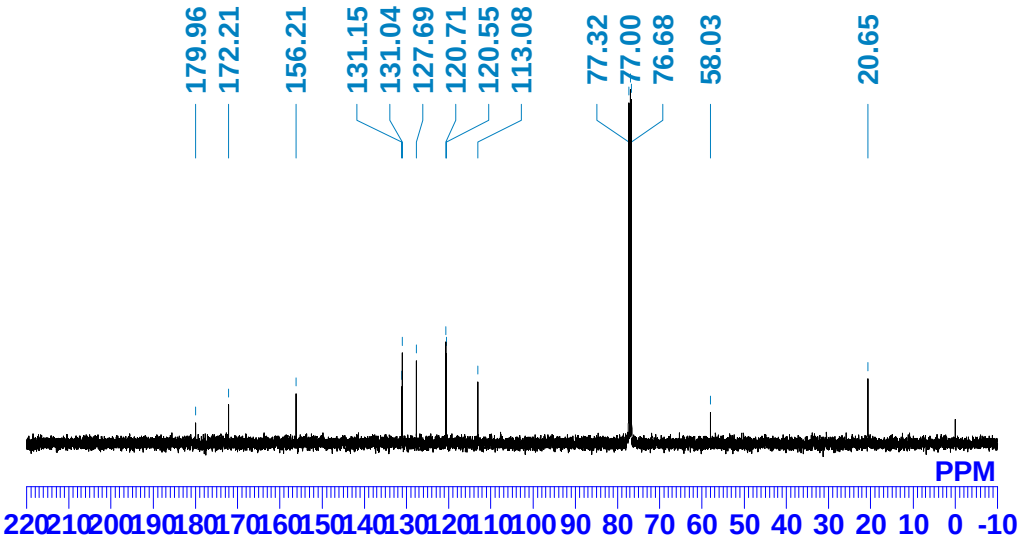
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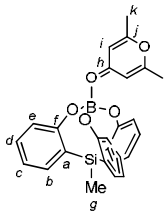
3aB·**8**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O
O
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O
e
f
d
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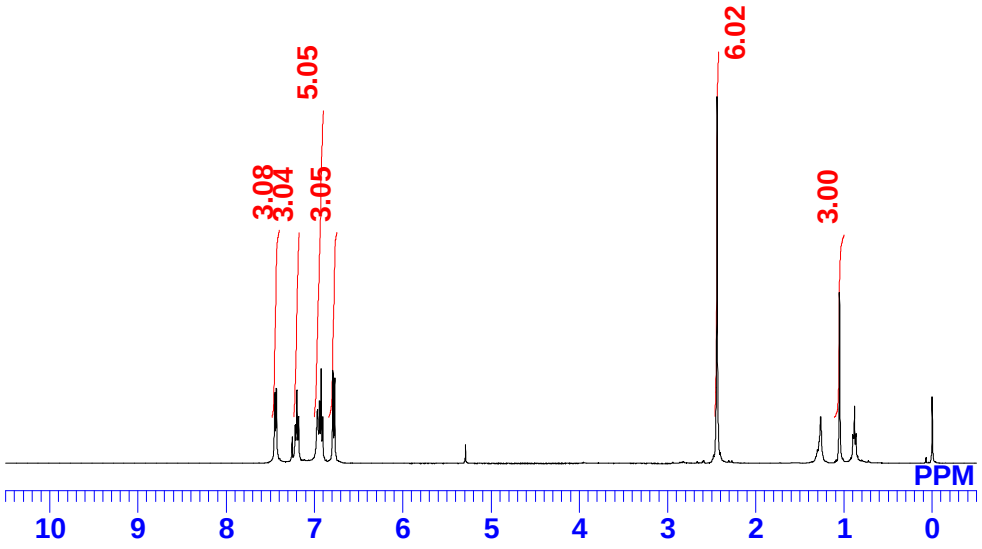
Si
Me
c
b
g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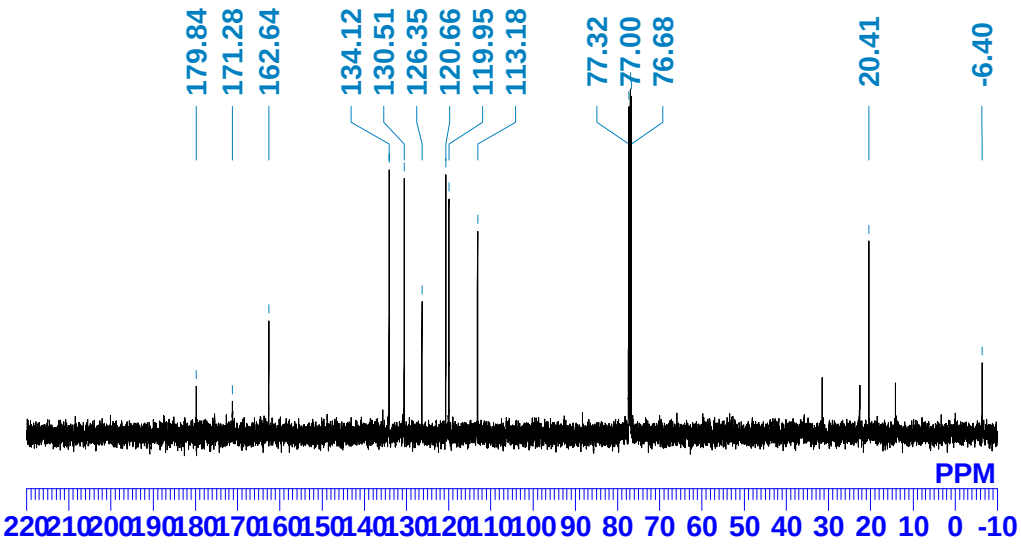
4
3
2
1
0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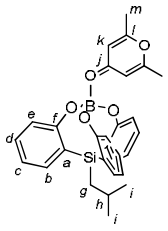
3bB·**8**


m
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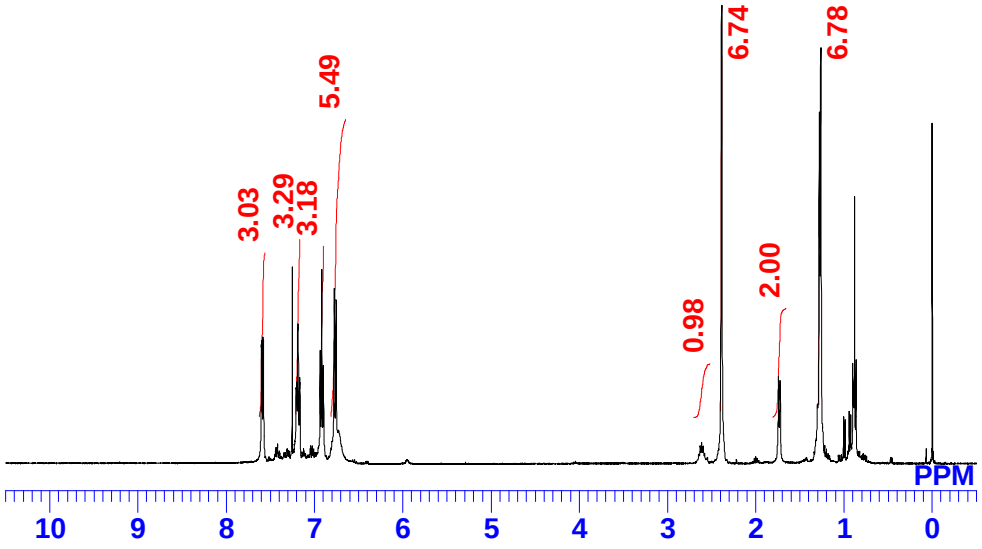
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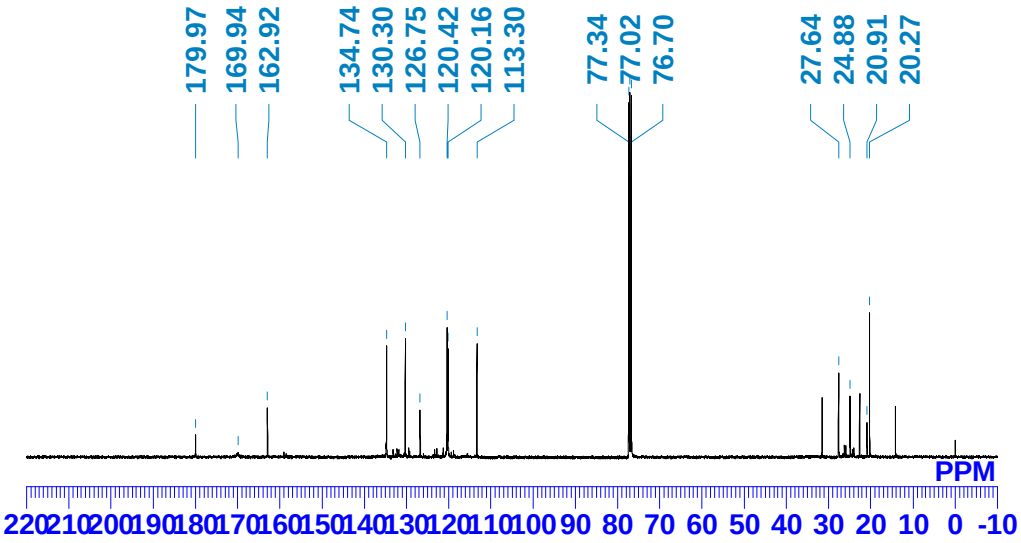
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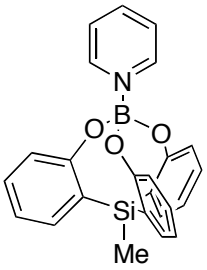
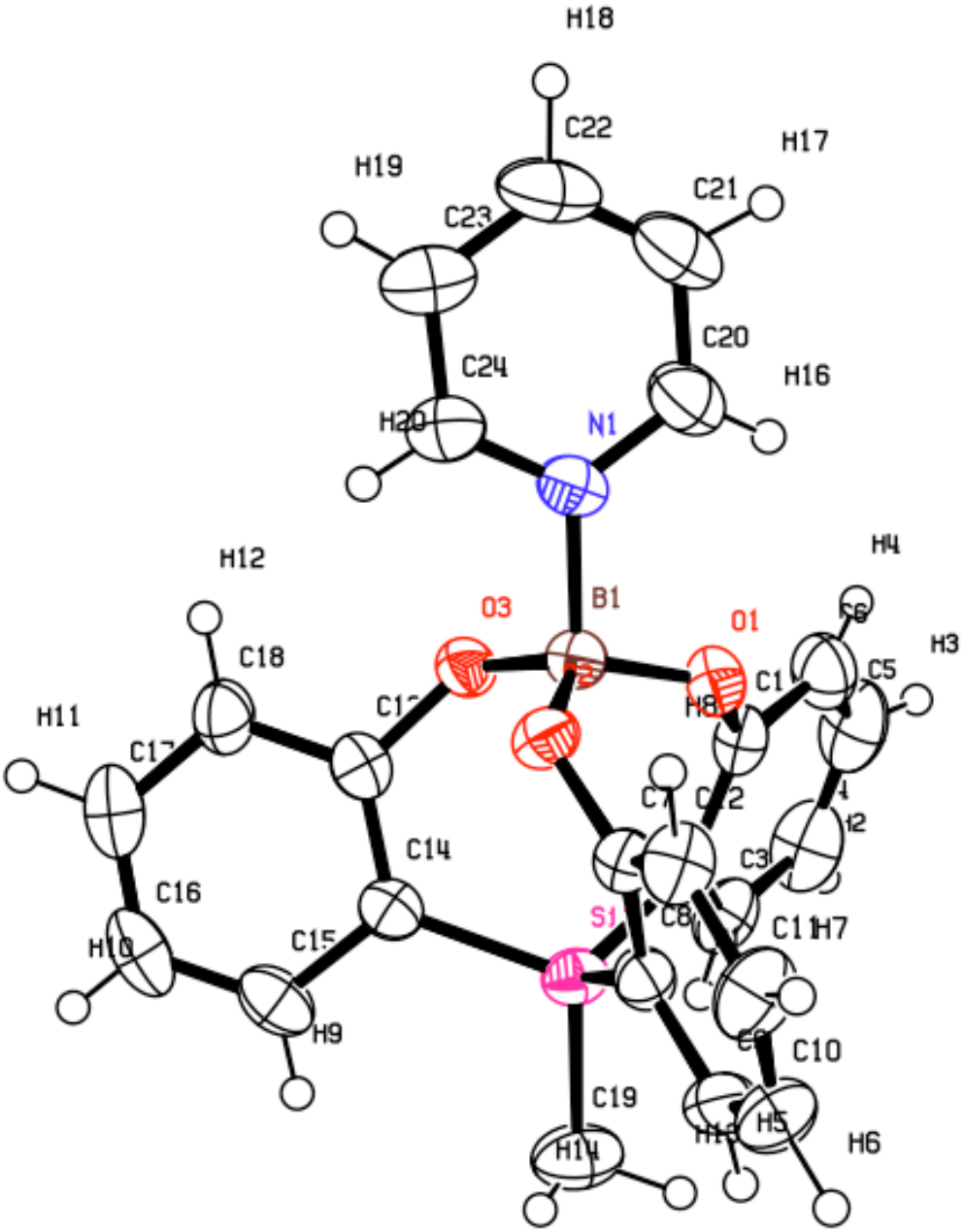
X-ray Structure Report



3aB·Py



Experimental

Data Collection

A colorless block crystal of $C_{24}H_{20}BSiNO_3$ having approximate dimensions of 0.95 x 0.40 x 0.40 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 1 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 9.1921 Å
b = 15.3839(2) Å β = 98.4086(15)^o
c = 14.4803(4) Å
V = 2025.65(6) Å^3

For Z = 4 and F.W. = 409.32, the calculated density is 1.342 g/cm^3. The systematic absences of:

h0l: h+l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of 0 $\pm$ 1^{o}C to a maximum 2θ value of 61.0^o. A total of 89 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 2.5^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 48.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 162.5^o in

2.5° step, at χ=45.0° and ϕ = 180.0°. The exposure rate was 48.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 22204 reflections that were collected, 6144 were unique (R_{int} = 0.068); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.424 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.575 to 0.945. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[3] on F was based on 4244 observed reflections ($I > 2.00\sigma(I)$) and 351 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0803$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.0906$$

The standard deviation of an observation of unit weight[4] was 1.36. Unit weights were used. Plots of Σ w (|Fo| - |Fc|)^2 versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.64 and -0.48 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" were those of

Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where w = Least Squares weights.

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

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

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

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

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

(7) 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).

(8) 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).

(9) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2006). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 11: Carruthers, J.R., Rollett,J.S., Betteridge, P.W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{24}H_{20}BSiNO_3$
Formula Weight	409.32
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.95 X 0.40 X 0.40 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	1 oscillations @ 180.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 9.1921 Å b = 15.3839(2) Å c = 14.4803(4) Å β = 98.4086(15) ^{o} V = 2025.65(6) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.342 g/cm^3
F_{000}	856.00
μ(MoKα)	1.424 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Detector Aperture	270 mm x 256 mm
Data Images	89 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	48.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.5^{o}
Exposure Rate	48.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	61.0^{o}
No. of Reflections Measured	Total: 22204 Unique: 6144 (R_{int} = 0.068)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.575 - 0.945)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1
$2\theta_{max}$ cutoff	61.0^{o}
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	4244
No. Variables	351
Reflection/Parameter Ratio	12.09
Residuals: R (I>2.00σ(I))	0.0803
Residuals: Rw (I>2.00σ(I))	0.0906
Goodness of Fit Indicator	1.363
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.64 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.48 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
S(I1)	1.01276(13)	0.19095(8)	0.56721(8)	2.81(2)
O(1)	0.7355(3)	0.2747(2)	0.4487(2)	3.21(6)
O(2)	0.9535(3)	0.36162(18)	0.4463(2)	2.91(5)
O(3)	0.8308(3)	0.36028(19)	0.58321(19)	2.82(5)
N(1)	0.7152(3)	0.4334(2)	0.4437(2)	3.06(7)
C(1)	0.7040(4)	0.2059(2)	0.5012(2)	2.95(8)
C(2)	0.8140(4)	0.1603(2)	0.5576(2)	2.93(8)
C(3)	0.7705(6)	0.0880(3)	0.6050(3)	3.78(10)
C(4)	0.6268(7)	0.0616(4)	0.5969(4)	4.83(13)
C(5)	0.5224(7)	0.1079(4)	0.5420(4)	5.00(14)
C(6)	0.5597(5)	0.1789(3)	0.4941(4)	4.11(11)
C(7)	1.0245(4)	0.2970(2)	0.4046(2)	2.64(7)
C(8)	1.0608(4)	0.2183(2)	0.4492(2)	2.77(7)
C(9)	1.1401(5)	0.1585(3)	0.4028(3)	3.40(9)
C(10)	1.1826(5)	0.1773(3)	0.3172(3)	4.09(11)
C(11)	1.1447(6)	0.2563(3)	0.2754(3)	4.24(11)
C(12)	1.0651(5)	0.3162(3)	0.3185(3)	3.48(9)
C(13)	0.9616(4)	0.3580(2)	0.6423(2)	2.78(7)
C(14)	1.0541(4)	0.2860(2)	0.6466(2)	2.77(7)
C(15)	1.1817(5)	0.2887(3)	0.7132(3)	3.66(10)
C(16)	1.2144(5)	0.3588(4)	0.7708(3)	4.37(11)
C(17)	1.1214(6)	0.4285(4)	0.7650(3)	4.41(12)
C(18)	0.9942(5)	0.4288(3)	0.7009(3)	3.59(10)
C(19)	1.1240(8)	0.0964(4)	0.6159(4)	4.63(14)
C(20)	0.5848(5)	0.4243(4)	0.3898(3)	4.17(11)
C(21)	0.4972(6)	0.4949(4)	0.3635(4)	5.03(14)
C(22)	0.5438(6)	0.5755(4)	0.3922(4)	5.10(14)
C(23)	0.6786(6)	0.5860(3)	0.4470(4)	4.46(12)
C(24)	0.7618(5)	0.5132(3)	0.4708(3)	3.57(10)
B(1)	0.8177(5)	0.3493(3)	0.4838(3)	2.71(8)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.835(6)	0.055(3)	0.640(3)	5.4(14)
H(2)	0.600(5)	0.014(3)	0.632(3)	5.0(13)
H(3)	0.441(6)	0.081(4)	0.529(4)	5.9(15)
H(4)	0.506(4)	0.206(2)	0.455(3)	2.6(10)
H(5)	1.163(4)	0.100(2)	0.431(2)	2.9(9)
H(6)	1.235(5)	0.133(3)	0.289(3)	3.7(10)
H(7)	1.173(5)	0.272(3)	0.213(3)	4.8(12)
H(8)	1.035(5)	0.371(3)	0.286(3)	3.8(10)
H(9)	1.242(4)	0.242(2)	0.714(2)	2.7(9)
H(10)	1.291(5)	0.360(3)	0.810(3)	3.5(10)
H(11)	1.139(6)	0.476(3)	0.808(3)	5.3(13)
H(12)	0.923(6)	0.475(4)	0.704(4)	6.7(16)
H(13)	1.100(7)	0.044(4)	0.570(4)	7.6(18)
H(14)	1.205(7)	0.103(4)	0.615(4)	6.5(20)
H(15)	1.099(5)	0.080(3)	0.673(4)	4.9(13)
H(16)	0.551(5)	0.370(3)	0.374(3)	4.9(13)
H(17)	0.414(6)	0.481(3)	0.322(3)	5.1(13)
H(18)	0.476(6)	0.623(3)	0.370(3)	5.6(14)
H(19)	0.700(7)	0.643(4)	0.468(4)	7.3(18)
H(20)	0.840(6)	0.519(4)	0.516(4)	6.2(16)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(I1)	0.0388(5)	0.0338(5)	0.0350(5)	0.0061(4)	0.0078(4)	0.0037(4)
O(1)	0.0409(16)	0.0439(17)	0.0353(14)	-0.0042(13)	-0.0004(12)	-0.0022(12)
O(2)	0.0371(15)	0.0326(14)	0.0419(15)	0.0026(11)	0.0095(12)	-0.0024(12)
O(3)	0.0338(14)	0.0412(16)	0.0314(13)	0.0042(12)	0.0023(10)	-0.0029(12)
N(1)	0.0347(18)	0.045(2)	0.0363(18)	0.0065(15)	0.0045(14)	0.0036(15)
C(1)	0.041(2)	0.037(2)	0.035(2)	-0.0080(17)	0.0096(16)	-0.0084(16)
C(2)	0.047(2)	0.033(2)	0.0331(19)	-0.0035(17)	0.0142(17)	-0.0046(16)
C(3)	0.066(3)	0.037(2)	0.044(2)	-0.006(2)	0.016(2)	-0.002(2)
C(4)	0.073(3)	0.057(3)	0.060(3)	-0.024(3)	0.029(2)	-0.004(2)
C(5)	0.059(3)	0.061(3)	0.075(3)	-0.029(2)	0.029(3)	-0.018(3)
C(6)	0.041(2)	0.059(3)	0.056(3)	-0.009(2)	0.006(2)	-0.009(2)

C(7)	0.0325(18)	0.034(2)	0.0341(19)	-0.0022(15)	0.0069(14)	-0.0004(15)
C(8)	0.0331(19)	0.037(2)	0.0349(19)	-0.0008(16)	0.0038(15)	-0.0010(16)
C(9)	0.041(2)	0.042(2)	0.047(2)	0.0094(19)	0.0084(18)	-0.0021(19)
C(10)	0.053(2)	0.055(3)	0.051(2)	0.009(2)	0.019(2)	-0.011(2)
C(11)	0.069(3)	0.053(3)	0.044(2)	-0.005(2)	0.024(2)	-0.005(2)
C(12)	0.054(2)	0.043(2)	0.037(2)	-0.006(2)	0.0110(19)	0.0015(19)
C(13)	0.036(2)	0.042(2)	0.0285(17)	-0.0044(17)	0.0051(14)	0.0039(16)
C(14)	0.0353(19)	0.037(2)	0.0328(19)	-0.0000(16)	0.0048(15)	0.0061(16)
C(15)	0.040(2)	0.063(3)	0.035(2)	0.002(2)	0.0001(17)	0.013(2)
C(16)	0.044(2)	0.082(4)	0.037(2)	-0.015(2)	-0.0067(19)	0.002(2)
C(17)	0.059(3)	0.066(3)	0.041(2)	-0.022(2)	0.004(2)	-0.010(2)
C(18)	0.048(2)	0.051(2)	0.037(2)	-0.004(2)	0.0037(19)	-0.009(2)
C(19)	0.069(4)	0.057(3)	0.052(3)	0.023(3)	0.014(2)	0.015(2)
C(20)	0.047(2)	0.066(3)	0.043(2)	0.007(2)	-0.002(2)	0.003(2)
C(21)	0.052(3)	0.087(4)	0.048(2)	0.014(3)	-0.007(2)	0.012(3)
C(22)	0.065(3)	0.075(4)	0.053(3)	0.032(3)	0.009(2)	0.022(2)
C(23)	0.062(3)	0.051(3)	0.060(3)	0.016(2)	0.019(2)	0.013(2)
C(24)	0.042(2)	0.042(2)	0.053(2)	0.005(2)	0.012(2)	0.005(2)
B(1)	0.033(2)	0.035(2)	0.035(2)	0.0026(18)	0.0035(17)	-0.0006(18)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
S(I1)	C(2)	1.872(4)	S(I1)	C(8)	1.875(4)
S(I1)	C(14)	1.865(4)	S(I1)	C(19)	1.857(6)
O(1)	C(1)	1.358(5)	O(1)	B(1)	1.427(5)
O(2)	C(7)	1.377(5)	O(2)	B(1)	1.445(5)
O(3)	C(13)	1.370(4)	O(3)	B(1)	1.437(5)
N(1)	C(20)	1.338(5)	N(1)	C(24)	1.340(6)
N(1)	B(1)	1.656(5)	C(1)	C(2)	1.392(5)
C(1)	C(6)	1.379(6)	C(2)	C(3)	1.396(6)
C(3)	C(4)	1.371(8)	C(4)	C(5)	1.355(8)
C(5)	C(6)	1.366(8)	C(7)	C(8)	1.389(5)
C(7)	C(12)	1.384(6)	C(8)	C(9)	1.405(6)
C(9)	C(10)	1.383(7)	C(10)	C(11)	1.380(7)

C(11)	C(12)	1.382(7)	C(13)	C(14)	1.392(5)
C(13)	C(18)	1.387(6)	C(14)	C(15)	1.405(5)
C(15)	C(16)	1.370(7)	C(16)	C(17)	1.366(8)
C(17)	C(18)	1.382(6)	C(20)	C(21)	1.372(8)
C(21)	C(22)	1.358(9)	C(22)	C(23)	1.379(8)
C(23)	C(24)	1.372(7)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.88(5)	C(4)	H(2)	0.94(5)
C(5)	H(3)	0.86(5)	C(6)	H(4)	0.81(4)
C(9)	H(5)	0.99(4)	C(10)	H(6)	0.95(4)
C(11)	H(7)	1.00(5)	C(12)	H(8)	0.99(4)
C(15)	H(9)	0.91(4)	C(16)	H(10)	0.84(4)
C(17)	H(11)	0.96(5)	C(18)	H(12)	0.97(6)
C(19)	H(13)	1.05(6)	C(19)	H(14)	0.75(6)
C(19)	H(15)	0.92(5)	C(20)	H(16)	0.91(5)
C(21)	H(17)	0.92(5)	C(22)	H(18)	0.99(5)
C(23)	H(19)	0.94(6)	C(24)	H(20)	0.91(5)

Table 6. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	S(I1)	C(8)	110.28(17)	C(2)	S(I1)	C(14)	110.59(19)
C(2)	S(I1)	C(19)	108.0(2)	C(8)	S(I1)	C(14)	109.39(18)
C(8)	S(I1)	C(19)	109.4(2)	C(14)	S(I1)	C(19)	109.2(2)
C(1)	O(1)	B(1)	124.9(3)	C(7)	O(2)	B(1)	124.2(3)
C(13)	O(3)	B(1)	124.0(3)	C(20)	N(1)	C(24)	119.2(4)
C(20)	N(1)	B(1)	122.5(4)	C(24)	N(1)	B(1)	118.1(3)
O(1)	C(1)	C(2)	121.6(3)	O(1)	C(1)	C(6)	118.3(3)
C(2)	C(1)	C(6)	120.0(4)	S(I1)	C(2)	C(1)	122.3(3)
S(I1)	C(2)	C(3)	120.7(3)	C(1)	C(2)	C(3)	117.0(4)
C(2)	C(3)	C(4)	122.4(4)	C(3)	C(4)	C(5)	119.0(5)
C(4)	C(5)	C(6)	120.7(5)	C(1)	C(6)	C(5)	120.9(4)
O(2)	C(7)	C(8)	121.5(3)	O(2)	C(7)	C(12)	116.6(3)
C(8)	C(7)	C(12)	121.8(4)	S(I1)	C(8)	C(7)	123.2(3)

S(I1)	C(8)	C(9)	119.8(3)	C(7)	C(8)	C(9)	117.0(3)
C(8)	C(9)	C(10)	121.8(4)	C(9)	C(10)	C(11)	119.4(5)
C(10)	C(11)	C(12)	120.4(5)	C(7)	C(12)	C(11)	119.7(4)
O(3)	C(13)	C(14)	121.5(3)	O(3)	C(13)	C(18)	116.9(3)
C(14)	C(13)	C(18)	121.4(3)	S(I1)	C(14)	C(13)	121.8(2)
S(I1)	C(14)	C(15)	121.4(3)	C(13)	C(14)	C(15)	116.8(3)
C(14)	C(15)	C(16)	121.8(4)	C(15)	C(16)	C(17)	120.1(4)
C(16)	C(17)	C(18)	120.3(5)	C(13)	C(18)	C(17)	119.6(4)
N(1)	C(20)	C(21)	121.2(5)	C(20)	C(21)	C(22)	119.5(5)
C(21)	C(22)	C(23)	120.0(5)	C(22)	C(23)	C(24)	118.0(5)
N(1)	C(24)	C(23)	122.1(4)	O(1)	B(1)	O(2)	114.4(3)
O(1)	B(1)	O(3)	114.4(3)	O(1)	B(1)	N(1)	105.0(3)
O(2)	B(1)	O(3)	114.3(3)	O(2)	B(1)	N(1)	104.1(3)
O(3)	B(1)	N(1)	102.7(3)				

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	122(3)	C(4)	C(3)	H(1)	116(3)
C(3)	C(4)	H(2)	120(3)	C(5)	C(4)	H(2)	120(3)
C(4)	C(5)	H(3)	113(4)	C(6)	C(5)	H(3)	124(4)
C(1)	C(6)	H(4)	112(3)	C(5)	C(6)	H(4)	126(3)
C(8)	C(9)	H(5)	119(2)	C(10)	C(9)	H(5)	119(2)
C(9)	C(10)	H(6)	117(2)	C(11)	C(10)	H(6)	123(2)
C(10)	C(11)	H(7)	122(3)	C(12)	C(11)	H(7)	117(3)
C(7)	C(12)	H(8)	122(3)	C(11)	C(12)	H(8)	119(3)
C(14)	C(15)	H(9)	116(2)	C(16)	C(15)	H(9)	122(2)
C(15)	C(16)	H(10)	121(3)	C(17)	C(16)	H(10)	119(3)
C(16)	C(17)	H(11)	121(3)	C(18)	C(17)	H(11)	119(3)
C(13)	C(18)	H(12)	121(3)	C(17)	C(18)	H(12)	119(3)
S(I1)	C(19)	H(13)	108(3)	S(I1)	C(19)	H(14)	112(5)
S(I1)	C(19)	H(15)	111(3)	H(13)	C(19)	H(14)	102(6)
H(13)	C(19)	H(15)	107(5)	H(14)	C(19)	H(15)	115(6)
N(1)	C(20)	H(16)	119(3)	C(21)	C(20)	H(16)	120(3)
C(20)	C(21)	H(17)	113(3)	C(22)	C(21)	H(17)	127(3)
C(21)	C(22)	H(18)	115(3)	C(23)	C(22)	H(18)	125(3)
C(22)	C(23)	H(19)	115(3)	C(24)	C(23)	H(19)	127(3)
N(1)	C(24)	H(20)	119(3)	C(23)	C(24)	H(20)	117(3)

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle
C(2)	S(I1)	C(8)	C(7)	77.5(3)
C(8)	S(I1)	C(2)	C(1)	-42.5(4)
C(2)	S(I1)	C(14)	C(13)	-44.0(4)
C(14)	S(I1)	C(2)	C(1)	78.7(3)
C(19)	S(I1)	C(2)	C(1)	-161.9(3)
C(8)	S(I1)	C(14)	C(13)	77.6(3)
C(14)	S(I1)	C(8)	C(7)	-44.4(3)
C(19)	S(I1)	C(8)	C(7)	-163.9(3)
C(19)	S(I1)	C(14)	C(13)	-162.7(4)
C(1)	O(1)	B(1)	O(2)	117.3(4)
C(1)	O(1)	B(1)	N(1)	-129.1(3)
B(1)	O(1)	C(1)	C(6)	128.7(4)
C(7)	O(2)	B(1)	O(3)	114.9(3)
B(1)	O(2)	C(7)	C(8)	-53.4(5)
C(13)	O(3)	B(1)	O(1)	116.8(4)
C(13)	O(3)	B(1)	N(1)	-129.9(3)
B(1)	O(3)	C(13)	C(18)	125.7(4)
C(24)	N(1)	C(20)	C(21)	-1.1(7)
C(20)	N(1)	B(1)	O(2)	120.3(4)
B(1)	N(1)	C(20)	C(21)	175.0(4)
C(24)	N(1)	B(1)	O(2)	-63.5(4)
B(1)	N(1)	C(24)	C(23)	-174.8(4)
O(1)	C(1)	C(2)	C(3)	-176.8(4)
C(2)	C(1)	C(6)	C(5)	0.3(6)
C(6)	C(1)	C(2)	C(3)	-0.1(5)
C(1)	C(2)	C(3)	C(4)	0.4(7)
C(3)	C(4)	C(5)	C(6)	1.2(9)
O(2)	C(7)	C(8)	S(I1)	1.9(5)
O(2)	C(7)	C(12)	C(11)	176.0(4)
C(12)	C(7)	C(8)	S(I1)	178.2(3)
S(I1)	C(8)	C(9)	C(10)	-177.6(3)
C(8)	C(9)	C(10)	C(11)	-0.9(7)
C(10)	C(11)	C(12)	C(7)	0.6(7)
O(3)	C(13)	C(14)	C(15)	-176.7(3)
C(14)	C(13)	C(18)	C(17)	0.3(7)
C(18)	C(13)	C(14)	C(15)	-0.0(5)
C(2)	S(I1)	C(8)	C(9)	-104.0(3)
C(8)	S(I1)	C(2)	C(3)	135.3(3)
C(2)	S(I1)	C(14)	C(15)	136.8(3)
C(14)	S(I1)	C(2)	C(3)	-103.6(3)
C(19)	S(I1)	C(2)	C(3)	15.8(4)
C(8)	S(I1)	C(14)	C(15)	-101.5(3)
C(14)	S(I1)	C(8)	C(9)	134.2(3)
C(19)	S(I1)	C(8)	C(9)	14.6(4)
C(19)	S(I1)	C(14)	C(15)	18.2(4)
C(1)	O(1)	B(1)	O(3)	-17.3(5)
B(1)	O(1)	C(1)	C(2)	-54.5(5)
C(7)	O(2)	B(1)	O(1)	-19.8(5)
C(7)	O(2)	B(1)	N(1)	-133.9(3)
B(1)	O(2)	C(7)	C(12)	130.1(4)
C(13)	O(3)	B(1)	O(2)	-17.8(5)
B(1)	O(3)	C(13)	C(14)	-57.5(5)
C(20)	N(1)	C(24)	C(23)	1.5(7)
C(20)	N(1)	B(1)	O(1)	-0.2(5)
C(20)	N(1)	B(1)	O(3)	-120.2(4)
C(24)	N(1)	B(1)	O(1)	175.9(3)
C(24)	N(1)	B(1)	O(3)	55.9(4)
O(1)	C(1)	C(2)	S(I1)	1.0(5)
O(1)	C(1)	C(6)	C(5)	177.1(5)
C(6)	C(1)	C(2)	S(I1)	177.7(3)
S(I1)	C(2)	C(3)	C(4)	-177.4(4)
C(2)	C(3)	C(4)	C(5)	-1.0(8)
C(4)	C(5)	C(6)	C(1)	-0.9(9)
O(2)	C(7)	C(8)	C(9)	-176.7(3)
C(8)	C(7)	C(12)	C(11)	-0.5(6)
C(12)	C(7)	C(8)	C(9)	-0.4(5)
C(7)	C(8)	C(9)	C(10)	1.1(6)
C(9)	C(10)	C(11)	C(12)	0.0(6)
O(3)	C(13)	C(14)	S(I1)	4.1(5)
O(3)	C(13)	C(18)	C(17)	177.2(4)
C(18)	C(13)	C(14)	S(I1)	-179.2(3)
S(I1)	C(14)	C(15)	C(16)	178.9(4)

C(13)	C(14)	C(15)	C(16)	-0.3(7)	C(14)	C(15)	C(16)	C(17)	0.4(8)
C(15)	C(16)	C(17)	C(18)	-0.1(6)	C(16)	C(17)	C(18)	C(13)	-0.2(7)
N(1)	C(20)	C(21)	C(22)	0.3(7)	C(20)	C(21)	C(22)	C(23)	0.3(7)
C(21)	C(22)	C(23)	C(24)	0.0(8)	C(22)	C(23)	C(24)	N(1)	-0.9(8)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
O(1)	C(15)[1)]	3.513(5)	O(1)	C(16)[1)]	3.278(6)
O(2)	C(23)[2)]	3.598(6)	O(2)	C(24)[2)]	3.329(5)
C(1)	C(16)[1)]	3.497(6)	C(4)	C(5)[3)]	3.451(8)
C(5)	C(4)[3)]	3.451(8)	C(5)	C(5)[3)]	3.538(8)
C(14)	C(23)[2)]	3.568(7)	C(15)	O(1)[4)]	3.513(5)
C(15)	C(23)[2)]	3.408(8)	C(16)	O(1)[4)]	3.278(6)
C(16)	C(1)[4)]	3.497(6)	C(16)	C(23)[2)]	3.542(8)
C(20)	C(22)[5)]	3.528(8)	C(22)	C(20)[5)]	3.528(8)
C(23)	O(2)[2)]	3.598(6)	C(23)	C(14)[2)]	3.568(7)
C(23)	C(15)[2)]	3.408(8)	C(23)	C(16)[2)]	3.542(8)
C(24)	O(2)[2)]	3.329(5)			

Symmetry Operators:

(1) X+1/2-1,-Y+1/2,Z+1/2-1
(2) -X+2,-Y+1,-Z+1
(3) -X+1,-Y,-Z+1
(4) X+1/2,-Y+1/2,Z+1/2
(5) -X+1,-Y+1,-Z+1

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O(1)	H(9)[1)]	3.41(4)	O(1)	H(10)[1)]	2.97(4)
O(2)	H(19)[2)]	3.24(6)	O(2)	H(20)[2)]	2.64(6)
O(3)	H(6)[3)]	3.23(4)	O(3)	H(7)[3)]	3.26(5)
O(3)	H(18)[4)]	3.00(6)	N(1)	H(18)[4)]	3.53(6)

C(1)	H(7)[3)]	3.14(5)	C(1)	H(10)[1)]	3.15(4)
C(2)	H(7)[3)]	2.95(5)	C(2)	H(10)[1)]	3.57(4)
C(3)	H(5)[5)]	3.02(4)	C(3)	H(7)[3)]	2.88(5)
C(3)	H(13)[5)]	3.58(7)	C(3)	H(17)[6)]	3.40(5)
C(4)	H(3)[7)]	2.86(6)	C(4)	H(5)[5)]	3.21(4)
C(4)	H(6)[5)]	3.57(4)	C(4)	H(7)[3)]	3.06(5)
C(4)	H(8)[3)]	3.15(5)	C(4)	H(11)[8)]	3.25(5)
C(4)	H(12)[8)]	3.27(6)	C(5)	H(2)[7)]	3.21(5)
C(5)	H(3)[7)]	3.11(6)	C(5)	H(5)[9)]	3.46(4)
C(5)	H(7)[3)]	3.23(5)	C(5)	H(8)[3)]	3.53(4)
C(5)	H(11)[8)]	3.46(5)	C(5)	H(14)[9)]	3.25(7)
C(6)	H(7)[3)]	3.28(5)	C(7)	H(9)[1)]	3.55(3)
C(7)	H(10)[1)]	3.38(4)	C(7)	H(19)[2)]	3.05(6)
C(7)	H(20)[2)]	3.24(6)	C(8)	H(10)[1)]	3.19(4)
C(8)	H(19)[2)]	3.16(6)	C(9)	H(1)[5)]	3.36(5)
C(9)	H(3)[10)]	3.31(5)	C(9)	H(4)[10)]	3.42(4)
C(9)	H(10)[1)]	3.30(4)	C(10)	H(2)[5)]	3.57(5)
C(10)	H(4)[10)]	3.36(4)	C(10)	H(18)[11)]	3.00(5)
C(11)	H(18)[11)]	3.03(5)	C(12)	H(9)[1)]	3.25(4)
C(12)	H(12)[2)]	3.23(6)	C(12)	H(19)[2)]	3.56(6)
C(12)	H(20)[2)]	3.51(6)	C(13)	H(6)[3)]	3.19(5)
C(13)	H(7)[3)]	3.60(5)	C(14)	H(19)[2)]	3.18(7)
C(15)	H(19)[2)]	3.16(7)	C(17)	H(2)[12)]	3.00(5)
C(17)	H(8)[2)]	3.44(4)	C(17)	H(14)[13)]	3.46(6)
C(17)	H(15)[13)]	3.48(5)	C(18)	H(2)[12)]	2.99(5)
C(18)	H(6)[3)]	3.02(5)	C(18)	H(8)[2)]	3.10(4)
C(19)	H(3)[10)]	3.35(6)	C(19)	H(11)[14)]	2.95(5)
C(20)	H(15)[1)]	3.17(5)	C(21)	H(1)[1)]	3.45(5)
C(21)	H(6)[15)]	3.55(4)	C(21)	H(15)[1)]	3.26(6)
C(22)	H(6)[15)]	3.51(4)	H(1)	C(9)[5)]	3.36(5)
H(1)	C(21)[6)]	3.45(5)	H(1)	H(5)[5)]	2.60(7)
H(1)	H(6)[5)]	3.17(7)	H(1)	H(7)[3)]	3.30(8)
H(1)	H(13)[5)]	3.53(9)	H(1)	H(17)[6)]	2.70(7)
H(2)	C(5)[7)]	3.21(5)	H(2)	C(10)[5)]	3.57(5)
H(2)	C(17)[8)]	3.00(5)	H(2)	C(18)[8)]	2.99(5)
H(2)	H(3)[7)]	2.73(8)	H(2)	H(5)[5)]	3.04(7)
H(2)	H(6)[5)]	2.87(7)	H(2)	H(7)[3)]	3.52(7)
H(2)	H(8)[3)]	2.97(7)	H(2)	H(11)[8)]	2.55(8)
H(2)	H(12)[8)]	2.49(8)	H(3)	C(4)[7)]	2.86(6)
H(3)	C(5)[7)]	3.11(6)	H(3)	C(9)[9)]	3.31(5)
H(3)	C(19)[9)]	3.35(6)	H(3)	H(2)[7)]	2.73(8)
H(3)	H(3)[7)]	2.88(8)	H(3)	H(5)[9)]	2.75(7)

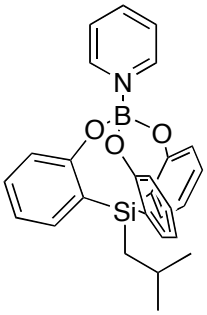
H(3)	H(11)[8)]	3.03(8)	H(3)	H(13)[9)]	3.32(9)
H(3)	H(14)[9)]	2.68(9)	H(4)	C(9)[9)]	3.42(4)
H(4)	C(10)[9)]	3.36(4)	H(4)	H(5)[9)]	3.52(6)
H(4)	H(6)[9)]	3.39(6)	H(4)	H(19)[4)]	3.29(8)
H(5)	C(3)[5)]	3.02(4)	H(5)	C(4)[5)]	3.21(4)
H(5)	C(5)[10)]	3.46(4)	H(5)	H(1)[5)]	2.60(7)
H(5)	H(2)[5)]	3.04(7)	H(5)	H(3)[10)]	2.75(7)
H(5)	H(4)[10)]	3.52(6)	H(5)	H(13)[5)]	3.28(8)
H(6)	O(3)[16)]	3.23(4)	H(6)	C(4)[5)]	3.57(4)
H(6)	C(13)[16)]	3.19(5)	H(6)	C(18)[16)]	3.02(5)
H(6)	C(21)[11)]	3.55(4)	H(6)	C(22)[11)]	3.51(4)
H(6)	H(1)[5)]	3.17(7)	H(6)	H(2)[5)]	2.87(7)
H(6)	H(4)[10)]	3.39(6)	H(6)	H(12)[16)]	2.81(8)
H(6)	H(17)[11)]	3.05(7)	H(6)	H(18)[11)]	2.79(6)
H(7)	O(3)[16)]	3.26(5)	H(7)	C(1)[16)]	3.14(5)
H(7)	C(2)[16)]	2.95(5)	H(7)	C(3)[16)]	2.88(5)
H(7)	C(4)[16)]	3.06(5)	H(7)	C(5)[16)]	3.23(5)
H(7)	C(6)[16)]	3.28(5)	H(7)	C(13)[16)]	3.60(5)
H(7)	H(1)[16)]	3.30(8)	H(7)	H(2)[16)]	3.52(7)
H(7)	H(18)[11)]	2.85(7)	H(8)	C(4)[16)]	3.15(5)
H(8)	C(5)[16)]	3.53(4)	H(8)	C(17)[2)]	3.44(4)
H(8)	C(18)[2)]	3.10(4)	H(8)	H(2)[16)]	2.97(7)
H(8)	H(9)[1)]	3.24(6)	H(8)	H(11)[2)]	3.05(7)
H(8)	H(12)[2)]	2.40(8)	H(8)	H(20)[2)]	3.38(7)
H(9)	O(1)[6)]	3.41(4)	H(9)	C(7)[6)]	3.55(3)
H(9)	C(12)[6)]	3.25(4)	H(9)	H(8)[6)]	3.24(6)
H(9)	H(16)[6)]	3.54(7)	H(9)	H(19)[2)]	3.28(8)
H(10)	O(1)[6)]	2.97(4)	H(10)	C(1)[6)]	3.15(4)
H(10)	C(2)[6)]	3.57(4)	H(10)	C(7)[6)]	3.38(4)
H(10)	C(8)[6)]	3.19(4)	H(10)	C(9)[6)]	3.30(4)
H(10)	H(13)[13)]	3.39(8)	H(10)	H(15)[13)]	3.53(7)
H(11)	C(4)[12)]	3.25(5)	H(11)	C(5)[12)]	3.46(5)
H(11)	C(19)[13)]	2.95(5)	H(11)	H(2)[12)]	2.55(8)
H(11)	H(3)[12)]	3.03(8)	H(11)	H(8)[2)]	3.05(7)
H(11)	H(13)[13)]	2.95(8)	H(11)	H(14)[13)]	2.57(8)
H(11)	H(15)[13)]	2.87(7)	H(12)	C(4)[12)]	3.27(6)
H(12)	C(12)[2)]	3.23(6)	H(12)	H(2)[12)]	2.49(8)
H(12)	H(6)[3)]	2.81(8)	H(12)	H(8)[2)]	2.40(7)
H(12)	H(17)[4)]	3.14(8)	H(13)	C(3)[5)]	3.58(7)
H(13)	H(1)[5)]	3.53(9)	H(13)	H(3)[10)]	3.32(9)
H(13)	H(5)[5)]	3.28(8)	H(13)	H(10)[14)]	3.39(8)
H(13)	H(11)[14)]	2.95(8)	H(13)	H(13)[5)]	2.87(9)

H(14)	C(5)[10)]	3.25(7)	H(14)	C(17)[14)]	3.46(6)
H(14)	H(3)[10)]	2.68(9)	H(14)	H(11)[14)]	2.57(8)
H(15)	C(17)[14)]	3.48(5)	H(15)	C(20)[6)]	3.17(5)
H(15)	C(21)[6)]	3.26(6)	H(15)	H(10)[14)]	3.53(7)
H(15)	H(11)[14)]	2.87(7)	H(15)	H(16)[6)]	3.11(8)
H(15)	H(17)[6)]	3.10(8)	H(16)	H(9)[1)]	3.54(7)
H(16)	H(15)[1)]	3.11(8)	H(16)	H(19)[4)]	3.50(9)
H(17)	C(3)[1)]	3.40(5)	H(17)	H(1)[1)]	2.70(7)
H(17)	H(6)[15)]	3.05(7)	H(17)	H(12)[4)]	3.14(8)
H(17)	H(15)[1)]	3.10(8)	H(17)	H(20)[4)]	3.53(8)
H(18)	O(3)[4)]	3.00(5)	H(18)	N(1)[4)]	3.53(6)
H(18)	C(10)[15)]	3.00(5)	H(18)	C(11)[15)]	3.03(5)
H(18)	H(6)[15)]	2.79(6)	H(18)	H(7)[15)]	2.85(7)
H(19)	O(2)[2)]	3.24(6)	H(19)	C(7)[2)]	3.05(6)
H(19)	C(8)[2)]	3.16(6)	H(19)	C(12)[2)]	3.56(6)
H(19)	C(14)[2)]	3.18(7)	H(19)	C(15)[2)]	3.16(6)
H(19)	H(4)[4)]	3.29(8)	H(19)	H(9)[2)]	3.28(8)
H(19)	H(16)[4)]	3.50(9)	H(20)	O(2)[2)]	2.64(5)
H(20)	C(7)[2)]	3.24(5)	H(20)	C(12)[2)]	3.51(5)
H(20)	H(8)[2)]	3.38(7)	H(20)	H(17)[4)]	3.53(8)
H(20)	H(20)[2)]	3.10(8)			

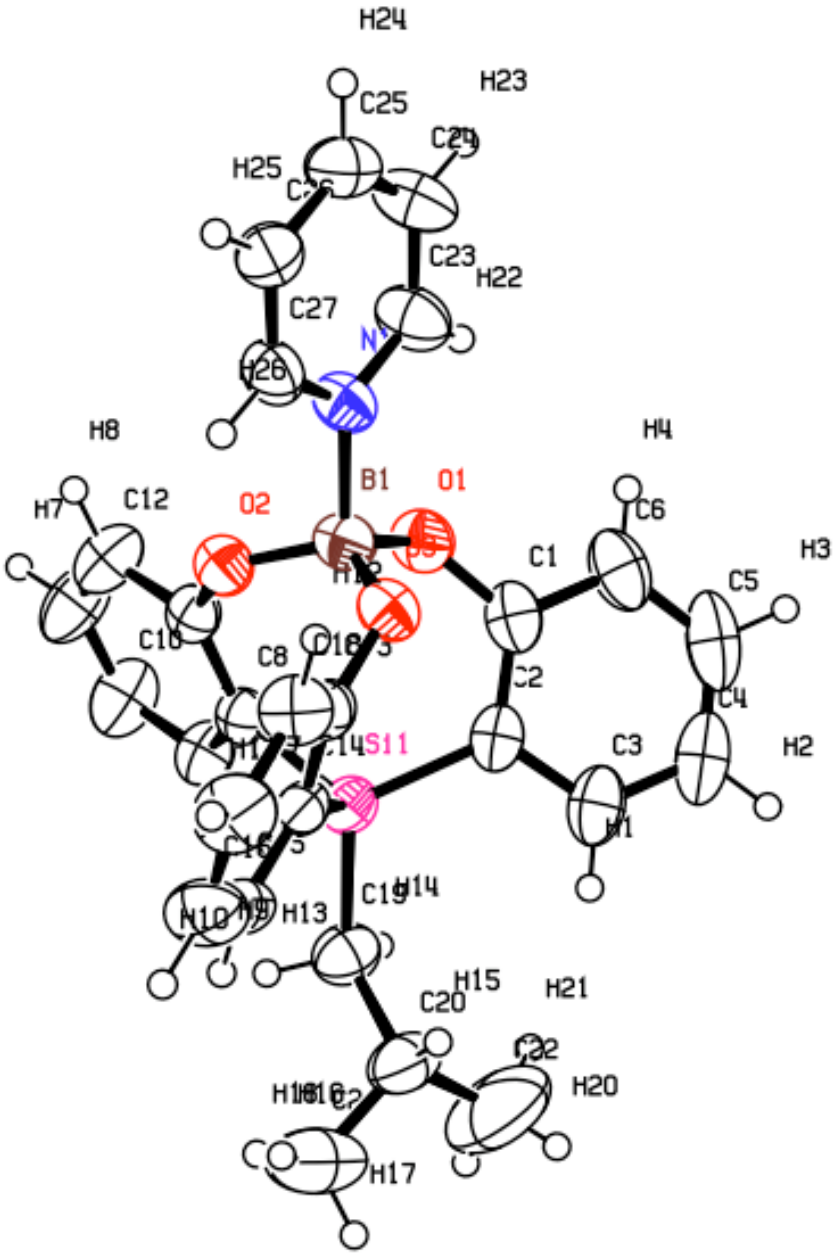
Symmetry Operators:

(1) X+1/2-1,-Y+1/2,Z+1/2-1
(2) -X+2,-Y+1,-Z+1
(3) X+1/2-1,-Y+1/2,Z+1/2
(4) -X+1,-Y+1,-Z+1
(5) -X+2,-Y,-Z+1
(6) X+1/2,-Y+1/2,Z+1/2
(7) -X+1,-Y,-Z+1
(8) -X+1/2+1,Y+1/2-1,-Z+1/2+1
(9) X-1,Y,Z
(10) X+1,Y,Z
(11) -X+1/2+1,Y+1/2-1,-Z+1/2
(12) -X+1/2+1,Y+1/2,-Z+1/2+1
(13) -X+1/2+2,Y+1/2,-Z+1/2+1
(14) -X+1/2+2,Y+1/2-1,-Z+1/2+1
(15) -X+1/2+1,Y+1/2,-Z+1/2
(16) X+1/2,-Y+1/2,Z+1/2-1

X-ray Structure Report



3bB·Py



Experimental

Data Collection

A colorless prism crystal of $C_{27}H_{26}BNO_3Si$ having approximate dimensions of 0.80 x 0.50 x 0.30 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive orthorhombic cell with dimensions:

a = 9.1369(3) Å
b = 20.4629(5) Å
c = 25.7290(6) Å
V = 4810.5(2) Å^3

For Z = 8 and F.W. = 451.40, the calculated density is 1.246 g/cm^3. The systematic absences of:

0kl: k ± 2n
h0l: l ± 2n
hk0: h ± 2n

uniquely determine the space group to be:

Pbca (#61)

The data were collected at a temperature of 23 ± 1°C to a maximum 2θ value of 61.0°. A total of 90 oscillation images were collected. A sweep of data was done using ω scans from 0.0 to 180.0° in 4.0° step, at χ=45.0° and ϕ = 0.0°. The exposure rate was 60.0 [sec./°]. A second sweep was performed using ω scans from 0.0 to 180.0° in

4.0° step, at χ=45.0° and ϕ = 180.0°. The exposure rate was 60.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 89471 reflections that were collected, 7305 were unique (R_{int} = 0.039); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.263 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F was based on 2402 observed reflections ($I > 2.00\sigma(I)$) and 324 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0462$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.0553$$

The standard deviation of an observation of unit weight[4] was 1.02. A Sheldrick weighting scheme was used. Plots of Σ w (|Fo| - |Fc|)^2 versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.51 and -0.53 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of

Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$$\Sigma w(|F_o|-|F_c|)^2 \qquad \text{where w = Least Squares weights.}$$

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

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

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

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

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(7) 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).

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(9) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC

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(10) CRYSTALS Issue 11: Carruthers, J.R., Rollett,J.S., Betteridge, P.W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{26}BNO_3Si$
Formula Weight	451.40
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.80 X 0.50 X 0.30 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 180.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 9.1369(3) Å b = 20.4629(5) Å c = 25.7290(6) Å V = 4810.5(2) Å^3
Space Group	Pbca (#61)
Z value	8
D_{calc}	1.246 g/cm^3
F_{000}	1904.00
μ(MoKα)	1.263 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated

Detector Aperture	280 mm x 256 mm
Data Images	90 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	0.0 - 180.0^o
Exposure Rate	60.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 180.0^o
Exposure Rate	60.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	61.0^o
No. of Reflections Measured	Total: 89471 Unique: 7305 (R_{int} = 0.039)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1/[0.0013Fo^2+1.0000σ(Fo^2)]
$2\theta_{max}$ cutoff	61.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	2402
No. Variables	324
Reflection/Parameter Ratio	7.41
Residuals: R (I>2.00σ(I))	0.0462
Residuals: Rw (I>2.00σ(I))	0.0553
Goodness of Fit Indicator	1.016
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.51 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.53 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Si(1)	0.09397(11)	0.16954(4)	0.63767(3)	3.409(19)
O(1)	0.3077(2)	0.05096(10)	0.62222(8)	4.13(5)
O(2)	0.0686(2)	0.03046(10)	0.58585(8)	3.69(5)
O(3)	0.2350(2)	0.10272(10)	0.54149(7)	3.75(5)
N(1)	0.2843(3)	-0.01337(12)	0.54219(10)	3.81(6)
C(1)	0.3761(4)	0.10716(17)	0.63836(11)	3.94(8)
C(2)	0.2976(3)	0.16534(15)	0.64542(10)	3.60(7)
C(3)	0.3798(4)	0.21945(19)	0.66161(13)	4.87(9)
C(4)	0.5274(5)	0.2160(2)	0.67090(15)	5.98(12)
C(5)	0.5983(5)	0.1577(2)	0.66563(15)	6.39(12)
C(6)	0.5237(4)	0.1030(2)	0.64965(13)	5.16(10)
C(7)	0.0057(3)	0.03427(14)	0.63428(12)	3.44(7)
C(8)	0.0104(3)	0.09197(14)	0.66346(11)	3.32(7)
C(9)	-0.0580(4)	0.09014(16)	0.71234(12)	4.13(8)
C(10)	-0.1312(5)	0.03580(18)	0.73015(14)	5.46(10)
C(11)	-0.1381(5)	-0.01882(17)	0.69954(14)	5.74(10)
C(12)	-0.0695(4)	-0.02012(16)	0.65193(13)	4.92(9)
C(13)	0.1215(3)	0.14339(14)	0.52919(12)	3.40(7)
C(14)	0.0448(3)	0.17810(13)	0.56697(12)	3.36(7)
C(15)	-0.0667(4)	0.21885(14)	0.54938(14)	4.30(8)
C(16)	-0.0991(5)	0.22616(17)	0.49738(15)	5.49(10)
C(17)	-0.0197(5)	0.19262(18)	0.46112(15)	5.39(10)
C(18)	0.0901(4)	0.15094(16)	0.47668(13)	4.36(8)
C(19)	0.0147(4)	0.23871(15)	0.67660(13)	4.53(9)
C(20)	0.0315(5)	0.31136(16)	0.66110(15)	5.29(10)
C(21)	-0.1163(6)	0.3438(2)	0.65419(19)	8.21(14)
C(22)	0.1151(8)	0.3497(2)	0.7011(2)	11.7(2)
C(23)	0.4025(4)	-0.04718(17)	0.55671(13)	4.88(9)
C(24)	0.4585(4)	-0.09684(17)	0.52620(15)	5.47(10)
C(25)	0.3912(4)	-0.11194(17)	0.48039(14)	4.92(9)
C(26)	0.2692(4)	-0.07737(16)	0.46555(14)	4.63(9)
C(27)	0.2187(4)	-0.02877(16)	0.49700(12)	4.19(8)
B(1)	0.2181(5)	0.04781(18)	0.57639(13)	3.66(9)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.3314	0.2601	0.6663	5.83
H(2)	0.5799	0.2540	0.6810	7.18
H(3)	0.7000	0.1550	0.6730	7.66
H(4)	0.5734	0.0625	0.6464	6.19
H(5)	-0.0536	0.1278	0.7339	4.94
H(6)	-0.1765	0.0362	0.7634	6.54
H(7)	-0.1907	-0.0561	0.7112	6.89
H(8)	-0.0737	-0.0584	0.6311	5.88
H(9)	-0.1226	0.2425	0.5742	5.16
H(10)	-0.1761	0.2544	0.4868	6.58
H(11)	-0.0404	0.1980	0.4252	6.47
H(12)	0.1445	0.1273	0.4515	5.22
H(13)	-0.0877	0.2307	0.6783	5.45
H(14)	0.0558	0.2349	0.7104	5.45
H(15)	0.0829	0.3135	0.6291	6.34
H(16)	-0.1471	0.3393	0.6191	9.88
H(17)	-0.1087	0.3889	0.6626	9.86
H(18)	-0.1857	0.3236	0.6765	9.87
H(19)	0.0490	0.3672	0.7259	14.05
H(20)	0.1662	0.3844	0.6845	14.04
H(21)	0.1831	0.3217	0.7180	14.04
H(22)	0.4491	-0.0369	0.5887	5.85
H(23)	0.5431	-0.1202	0.5370	6.56
H(24)	0.4282	-0.1460	0.4590	5.90
H(25)	0.2209	-0.0872	0.4338	5.55
H(26)	0.1343	-0.0050	0.4867	5.03

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si(1)	0.0474(6)	0.0424(4)	0.0398(4)	-0.0032(4)	-0.0013(4)	-0.0010(3)
O(1)	0.0528(16)	0.0589(13)	0.0453(12)	0.0062(13)	-0.0125(11)	-0.0017(9)
O(2)	0.0452(16)	0.0531(12)	0.0418(11)	0.0019(12)	-0.0018(11)	-0.0037(9)
O(3)	0.0439(15)	0.0544(12)	0.0441(11)	0.0051(12)	-0.0004(11)	0.0013(9)
N(1)	0.045(2)	0.0546(15)	0.0449(14)	0.0091(15)	-0.0019(14)	0.0003(12)

C(1)	0.044(2)	0.072(2)	0.0340(15)	-0.0050(19)	-0.0042(17)	0.0033(15)
C(2)	0.046(2)	0.0566(18)	0.0337(15)	-0.0118(19)	-0.0008(15)	0.0008(13)
C(3)	0.059(3)	0.076(2)	0.0502(19)	-0.022(2)	0.002(2)	0.0042(17)
C(4)	0.062(3)	0.102(3)	0.063(2)	-0.038(2)	-0.004(2)	0.004(2)
C(5)	0.045(2)	0.136(4)	0.062(2)	-0.025(3)	-0.009(2)	0.010(2)
C(6)	0.045(2)	0.102(3)	0.050(2)	0.002(2)	-0.0064(19)	0.006(2)
C(7)	0.044(2)	0.0448(16)	0.0420(16)	-0.0013(16)	-0.0072(17)	0.0039(14)
C(8)	0.041(2)	0.0452(17)	0.0405(16)	-0.0006(16)	-0.0046(16)	0.0020(14)
C(9)	0.060(2)	0.0559(19)	0.0413(17)	-0.0092(19)	-0.0001(17)	-0.0020(14)
C(10)	0.087(3)	0.076(2)	0.0445(18)	-0.024(2)	0.008(2)	0.0034(18)
C(11)	0.103(3)	0.061(2)	0.054(2)	-0.034(2)	0.002(2)	0.0099(18)
C(12)	0.086(3)	0.0498(18)	0.051(2)	-0.015(2)	-0.007(2)	0.0023(15)
C(13)	0.043(2)	0.0411(15)	0.0447(17)	-0.0037(17)	-0.0039(16)	0.0036(13)
C(14)	0.044(2)	0.0343(15)	0.0488(17)	-0.0047(16)	-0.0042(15)	-0.0013(13)
C(15)	0.060(2)	0.0390(15)	0.065(2)	0.0065(18)	-0.008(2)	-0.0015(15)
C(16)	0.085(3)	0.055(2)	0.069(2)	0.015(2)	-0.023(2)	0.0101(18)
C(17)	0.087(3)	0.069(2)	0.049(2)	0.002(2)	-0.015(2)	0.0112(18)
C(18)	0.065(2)	0.0589(19)	0.0420(16)	0.003(2)	-0.0026(19)	0.0043(15)
C(19)	0.068(2)	0.0522(19)	0.052(2)	-0.001(2)	0.0051(19)	-0.0048(15)
C(20)	0.082(3)	0.0462(19)	0.073(2)	-0.004(2)	0.014(2)	-0.0091(17)
C(21)	0.128(4)	0.066(2)	0.117(4)	0.025(3)	0.036(3)	0.007(2)
C(22)	0.196(7)	0.080(3)	0.168(5)	-0.021(4)	-0.045(5)	-0.043(3)
C(23)	0.062(2)	0.070(2)	0.053(2)	0.020(2)	-0.010(2)	0.0015(17)
C(24)	0.071(3)	0.072(2)	0.065(2)	0.032(2)	0.002(2)	0.002(2)
C(25)	0.070(2)	0.0531(19)	0.064(2)	0.009(2)	0.009(2)	-0.0057(17)
C(26)	0.058(2)	0.0586(19)	0.059(2)	0.000(2)	-0.001(2)	-0.0138(16)
C(27)	0.044(2)	0.061(2)	0.0542(19)	0.0060(19)	-0.0063(18)	-0.0021(15)
B(1)	0.049(3)	0.050(2)	0.0398(19)	0.008(2)	-0.0058(19)	-0.0055(15)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Si(1)	C(2)	1.874(3)	Si(1)	C(8)	1.882(3)
Si(1)	C(14)	1.882(3)	Si(1)	C(19)	1.879(3)
O(1)	C(1)	1.373(4)	O(1)	B(1)	1.437(4)

O(2)	C(7)	1.374(3)	O(2)	B(1)	1.432(5)
O(3)	C(13)	1.367(3)	O(3)	B(1)	1.447(4)
N(1)	C(23)	1.336(4)	N(1)	C(27)	1.345(4)
N(1)	B(1)	1.645(4)	C(1)	C(2)	1.402(4)
C(1)	C(6)	1.382(5)	C(2)	C(3)	1.401(5)
C(3)	C(4)	1.372(6)	C(4)	C(5)	1.363(7)
C(5)	C(6)	1.374(6)	C(7)	C(8)	1.400(4)
C(7)	C(12)	1.385(4)	C(8)	C(9)	1.405(4)
C(9)	C(10)	1.376(5)	C(10)	C(11)	1.369(5)
C(11)	C(12)	1.376(5)	C(13)	C(14)	1.393(4)
C(13)	C(18)	1.390(4)	C(14)	C(15)	1.392(4)
C(15)	C(16)	1.378(5)	C(16)	C(17)	1.366(5)
C(17)	C(18)	1.376(5)	C(19)	C(20)	1.547(4)
C(20)	C(21)	1.515(7)	C(20)	C(22)	1.502(7)
C(23)	C(24)	1.382(5)	C(24)	C(25)	1.365(5)
C(25)	C(26)	1.374(5)	C(26)	C(27)	1.363(4)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.950	C(4)	H(2)	0.950
C(5)	H(3)	0.950	C(6)	H(4)	0.950
C(9)	H(5)	0.950	C(10)	H(6)	0.950
C(11)	H(7)	0.950	C(12)	H(8)	0.950
C(15)	H(9)	0.950	C(16)	H(10)	0.950
C(17)	H(11)	0.950	C(18)	H(12)	0.950
C(19)	H(13)	0.950	C(19)	H(14)	0.950
C(20)	H(15)	0.950	C(21)	H(16)	0.950
C(21)	H(17)	0.950	C(21)	H(18)	0.950
C(22)	H(19)	0.950	C(22)	H(20)	0.950
C(22)	H(21)	0.950	C(23)	H(22)	0.950
C(24)	H(23)	0.950	C(25)	H(24)	0.950
C(26)	H(25)	0.950	C(27)	H(26)	0.950

Table 6. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle

C(2)	Si(1)	C(8)	109.08(14)	C(2)	Si(1)	C(14)	110.14(14)
C(2)	Si(1)	C(19)	111.15(15)	C(8)	Si(1)	C(14)	108.80(13)
C(8)	Si(1)	C(19)	106.90(14)	C(14)	Si(1)	C(19)	110.67(14)
C(1)	O(1)	B(1)	123.0(2)	C(7)	O(2)	B(1)	122.6(2)
C(13)	O(3)	B(1)	122.4(2)	C(23)	N(1)	C(27)	118.7(2)
C(23)	N(1)	B(1)	122.8(2)	C(27)	N(1)	B(1)	118.5(2)
O(1)	C(1)	C(2)	121.2(3)	O(1)	C(1)	C(6)	117.2(3)
C(2)	C(1)	C(6)	121.6(3)	Si(1)	C(2)	C(1)	122.2(2)
Si(1)	C(2)	C(3)	121.8(2)	C(1)	C(2)	C(3)	115.8(3)
C(2)	C(3)	C(4)	122.5(3)	C(3)	C(4)	C(5)	119.7(4)
C(4)	C(5)	C(6)	120.4(4)	C(1)	C(6)	C(5)	119.8(4)
O(2)	C(7)	C(8)	121.4(2)	O(2)	C(7)	C(12)	117.3(2)
C(8)	C(7)	C(12)	121.1(2)	Si(1)	C(8)	C(7)	122.3(2)
Si(1)	C(8)	C(9)	121.2(2)	C(7)	C(8)	C(9)	116.4(2)
C(8)	C(9)	C(10)	122.4(3)	C(9)	C(10)	C(11)	119.4(3)
C(10)	C(11)	C(12)	120.5(3)	C(7)	C(12)	C(11)	120.2(3)
O(3)	C(13)	C(14)	122.1(2)	O(3)	C(13)	C(18)	116.7(2)
C(14)	C(13)	C(18)	121.2(3)	Si(1)	C(14)	C(13)	120.5(2)
Si(1)	C(14)	C(15)	123.0(2)	C(13)	C(14)	C(15)	116.5(2)
C(14)	C(15)	C(16)	122.5(3)	C(15)	C(16)	C(17)	119.6(3)
C(16)	C(17)	C(18)	120.0(3)	C(13)	C(18)	C(17)	120.2(3)
Si(1)	C(19)	C(20)	123.2(2)	C(19)	C(20)	C(21)	111.3(3)
C(19)	C(20)	C(22)	112.1(3)	C(21)	C(20)	C(22)	107.7(3)
N(1)	C(23)	C(24)	121.4(3)	C(23)	C(24)	C(25)	119.4(3)
C(24)	C(25)	C(26)	119.3(3)	C(25)	C(26)	C(27)	119.0(3)
N(1)	C(27)	C(26)	122.2(3)	O(1)	B(1)	O(2)	114.5(2)
O(1)	B(1)	O(3)	114.4(2)	O(1)	B(1)	N(1)	105.3(2)
O(2)	B(1)	O(3)	113.6(3)	O(2)	B(1)	N(1)	104.6(2)
O(3)	B(1)	N(1)	102.7(2)				

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	118.8	C(4)	C(3)	H(1)	118.7
C(3)	C(4)	H(2)	120.1	C(5)	C(4)	H(2)	120.2
C(4)	C(5)	H(3)	119.8	C(6)	C(5)	H(3)	119.8
C(1)	C(6)	H(4)	120.1	C(5)	C(6)	H(4)	120.1
C(8)	C(9)	H(5)	118.8	C(10)	C(9)	H(5)	118.8
C(9)	C(10)	H(6)	120.3	C(11)	C(10)	H(6)	120.3

C(10)	C(11)	H(7)	119.8	C(12)	C(11)	H(7)	119.8
C(7)	C(12)	H(8)	119.9	C(11)	C(12)	H(8)	119.9
C(14)	C(15)	H(9)	118.7	C(16)	C(15)	H(9)	118.7
C(15)	C(16)	H(10)	120.2	C(17)	C(16)	H(10)	120.2
C(16)	C(17)	H(11)	120.0	C(18)	C(17)	H(11)	120.0
C(13)	C(18)	H(12)	119.9	C(17)	C(18)	H(12)	119.9
Si(1)	C(19)	H(13)	105.9	Si(1)	C(19)	H(14)	105.9
C(20)	C(19)	H(13)	105.9	C(20)	C(19)	H(14)	105.9
H(13)	C(19)	H(14)	109.5	C(19)	C(20)	H(15)	108.5
C(21)	C(20)	H(15)	108.5	C(22)	C(20)	H(15)	108.6
C(20)	C(21)	H(16)	109.4	C(20)	C(21)	H(17)	109.5
C(20)	C(21)	H(18)	109.5	H(16)	C(21)	H(17)	109.5
H(16)	C(21)	H(18)	109.5	H(17)	C(21)	H(18)	109.5
C(20)	C(22)	H(19)	109.5	C(20)	C(22)	H(20)	109.5
C(20)	C(22)	H(21)	109.4	H(19)	C(22)	H(20)	109.5
H(19)	C(22)	H(21)	109.5	H(20)	C(22)	H(21)	109.5
N(1)	C(23)	H(22)	119.3	C(24)	C(23)	H(22)	119.3
C(23)	C(24)	H(23)	120.3	C(25)	C(24)	H(23)	120.3
C(24)	C(25)	H(24)	120.4	C(26)	C(25)	H(24)	120.4
C(25)	C(26)	H(25)	120.5	C(27)	C(26)	H(25)	120.5
N(1)	C(27)	H(26)	118.9	C(26)	C(27)	H(26)	118.9

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(2)	Si(1)	C(8)	C(7)	-80.9(3)	C(2)	Si(1)	C(8)	C(9)	102.5(2)
C(8)	Si(1)	C(2)	C(1)	37.1(2)	C(8)	Si(1)	C(2)	C(3)	-139.1(2)
C(2)	Si(1)	C(14)	C(13)	39.6(2)	C(2)	Si(1)	C(14)	C(15)	-139.8(2)
C(14)	Si(1)	C(2)	C(1)	-82.2(2)	C(14)	Si(1)	C(2)	C(3)	101.6(2)
C(2)	Si(1)	C(19)	C(20)	73.2(3)	C(19)	Si(1)	C(2)	C(1)	154.8(2)
C(19)	Si(1)	C(2)	C(3)	-21.4(2)	C(8)	Si(1)	C(14)	C(13)	-79.9(2)
C(8)	Si(1)	C(14)	C(15)	100.7(2)	C(14)	Si(1)	C(8)	C(7)	39.3(3)
C(14)	Si(1)	C(8)	C(9)	-137.3(2)	C(8)	Si(1)	C(19)	C(20)	-167.8(3)
C(19)	Si(1)	C(8)	C(7)	158.8(2)	C(19)	Si(1)	C(8)	C(9)	-17.7(3)
C(14)	Si(1)	C(19)	C(20)	-49.5(3)	C(19)	Si(1)	C(14)	C(13)	162.9(2)
C(19)	Si(1)	C(14)	C(15)	-16.5(3)	C(1)	O(1)	B(1)	O(2)	-118.5(3)
C(1)	O(1)	B(1)	O(3)	15.1(4)	C(1)	O(1)	B(1)	N(1)	127.1(2)
B(1)	O(1)	C(1)	C(2)	53.3(4)	B(1)	O(1)	C(1)	C(6)	-129.7(3)
C(7)	O(2)	B(1)	O(1)	17.2(4)	C(7)	O(2)	B(1)	O(3)	-116.8(2)

C(7)	O(2)	B(1)	N(1)	132.0(2)	B(1)	O(2)	C(7)	C(8)	53.5(4)
B(1)	O(2)	C(7)	C(12)	-130.0(3)	C(13)	O(3)	B(1)	O(1)	-119.0(3)
C(13)	O(3)	B(1)	O(2)	15.0(3)	C(13)	O(3)	B(1)	N(1)	127.4(2)
B(1)	O(3)	C(13)	C(14)	58.4(4)	B(1)	O(3)	C(13)	C(18)	-124.5(3)
C(23)	N(1)	C(27)	C(26)	-0.3(5)	C(27)	N(1)	C(23)	C(24)	0.4(5)
C(23)	N(1)	B(1)	O(1)	-3.3(4)	C(23)	N(1)	B(1)	O(2)	-124.3(3)
C(23)	N(1)	B(1)	O(3)	116.8(3)	B(1)	N(1)	C(23)	C(24)	-177.7(3)
C(27)	N(1)	B(1)	O(1)	178.6(2)	C(27)	N(1)	B(1)	O(2)	57.6(3)
C(27)	N(1)	B(1)	O(3)	-61.3(3)	B(1)	N(1)	C(27)	C(26)	177.9(3)
O(1)	C(1)	C(2)	Si(1)	4.0(3)	O(1)	C(1)	C(2)	C(3)	-179.6(2)
O(1)	C(1)	C(6)	C(5)	179.5(3)	C(2)	C(1)	C(6)	C(5)	-3.5(4)
C(6)	C(1)	C(2)	Si(1)	-172.9(2)	C(6)	C(1)	C(2)	C(3)	3.6(4)
Si(1)	C(2)	C(3)	C(4)	175.4(2)	C(1)	C(2)	C(3)	C(4)	-1.0(4)
C(2)	C(3)	C(4)	C(5)	-1.7(5)	C(3)	C(4)	C(5)	C(6)	1.9(5)
C(4)	C(5)	C(6)	C(1)	0.6(5)	O(2)	C(7)	C(8)	Si(1)	3.1(4)
O(2)	C(7)	C(8)	C(9)	179.8(3)	O(2)	C(7)	C(12)	C(11)	-178.3(3)
C(8)	C(7)	C(12)	C(11)	-1.8(5)	C(12)	C(7)	C(8)	Si(1)	-173.3(2)
C(12)	C(7)	C(8)	C(9)	3.4(5)	Si(1)	C(8)	C(9)	C(10)	174.1(3)
C(7)	C(8)	C(9)	C(10)	-2.7(5)	C(8)	C(9)	C(10)	C(11)	0.2(4)
C(9)	C(10)	C(11)	C(12)	1.6(6)	C(10)	C(11)	C(12)	C(7)	-0.8(6)
O(3)	C(13)	C(14)	Si(1)	-0.6(4)	O(3)	C(13)	C(14)	C(15)	178.8(2)
O(3)	C(13)	C(18)	C(17)	-178.0(3)	C(14)	C(13)	C(18)	C(17)	-0.8(5)
C(18)	C(13)	C(14)	Si(1)	-177.7(2)	C(18)	C(13)	C(14)	C(15)	1.8(4)
Si(1)	C(14)	C(15)	C(16)	178.1(2)	C(13)	C(14)	C(15)	C(16)	-1.3(5)
C(14)	C(15)	C(16)	C(17)	-0.1(4)	C(15)	C(16)	C(17)	C(18)	1.2(6)
C(16)	C(17)	C(18)	C(13)	-0.7(5)	Si(1)	C(19)	C(20)	C(21)	121.9(3)
Si(1)	C(19)	C(20)	C(22)	-117.3(4)	N(1)	C(23)	C(24)	C(25)	-0.3(5)
C(23)	C(24)	C(25)	C(26)	0.1(4)	C(24)	C(25)	C(26)	C(27)	0.1(4)
C(25)	C(26)	C(27)	N(1)	0.0(4)					

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
O(2)	C(26)[1)]	3.493(4)	O(2)	C(27)[1)]	3.382(4)
O(3)	C(24)[2)]	3.300(4)	O(3)	C(25)[2)]	3.466(5)
C(6)	C(25)[2)]	3.440(4)	C(6)	C(26)[2)]	3.556(5)

C(15)	C(26)[1)]	3.458(4)	C(16)	C(25)[1)]	3.594(5)
C(16)	C(26)[1)]	3.549(5)	C(24)	O(3)[2)]	3.300(4)
C(25)	O(3)[2)]	3.466(5)	C(25)	C(6)[2)]	3.440(4)
C(25)	C(16)[1)]	3.594(5)	C(26)	O(2)[1)]	3.493(4)
C(26)	C(6)[2)]	3.556(5)	C(26)	C(15)[1)]	3.458(4)
C(26)	C(16)[1)]	3.549(5)	C(27)	O(2)[1)]	3.382(4)

Symmetry Operators:

(1) -X,-Y,-Z+1 (2) -X+1,-Y,-Z+1

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O(1)	H(6)[1)]	2.962	O(2)	H(25)[2)]	2.933
O(2)	H(26)[2)]	2.682	O(3)	H(10)[3)]	3.121
O(3)	H(23)[4)]	2.884	O(3)	H(24)[4)]	3.202
C(1)	H(5)[1)]	3.376	C(1)	H(6)[1)]	2.955
C(1)	H(24)[4)]	3.180	C(2)	H(5)[1)]	3.476
C(2)	H(6)[1)]	3.542	C(3)	H(5)[1)]	3.334
C(3)	H(11)[3)]	2.893	C(4)	H(5)[1)]	3.131
C(4)	H(11)[3)]	3.097	C(4)	H(13)[5)]	3.535
C(4)	H(14)[1)]	3.090	C(4)	H(18)[5)]	3.427
C(5)	H(5)[1)]	2.997	C(5)	H(13)[5)]	3.251
C(5)	H(14)[1)]	3.581	C(5)	H(24)[4)]	3.226
C(5)	H(25)[4)]	3.370	C(6)	H(5)[1)]	3.120
C(6)	H(6)[1)]	3.197	C(6)	H(24)[4)]	2.964
C(6)	H(25)[4)]	3.188	C(7)	H(25)[2)]	2.921
C(7)	H(26)[2)]	3.418	C(8)	H(3)[6)]	3.125
C(8)	H(25)[2)]	3.277	C(9)	H(3)[6)]	2.770
C(10)	H(3)[6)]	3.238	C(10)	H(4)[6)]	3.497
C(11)	H(4)[6)]	3.404	C(11)	H(17)[7)]	3.134
C(11)	H(19)[8)]	3.127	C(11)	H(20)[8)]	3.590
C(12)	H(12)[2)]	3.515	C(12)	H(17)[7)]	3.491
C(12)	H(25)[2)]	3.406	C(13)	H(10)[3)]	2.822
C(13)	H(23)[4)]	3.538	C(13)	H(25)[2)]	3.467
C(14)	H(10)[3)]	3.214	C(14)	H(25)[2)]	3.059
C(15)	H(23)[9)]	3.316	C(15)	H(25)[2)]	3.071
C(16)	H(23)[9)]	3.344	C(16)	H(24)[9)]	3.202

C(16)	H(25)[2)]	3.530	C(17)	H(10)[3)]	3.582
C(17)	H(24)[9)]	3.407	C(18)	H(8)[2)]	3.362
C(18)	H(10)[3)]	3.034	C(18)	H(16)[3)]	3.447
C(18)	H(23)[4)]	3.429	C(19)	H(3)[6)]	3.348
C(20)	H(23)[9)]	3.553	C(21)	H(2)[6)]	3.400
C(21)	H(7)[10)]	3.076	C(21)	H(8)[10)]	3.518
C(21)	H(12)[11)]	3.538	C(21)	H(22)[9)]	3.336
C(21)	H(23)[9)]	3.176	C(22)	H(7)[12)]	3.048
C(23)	H(15)[13)]	3.407	C(23)	H(17)[13)]	3.561
C(24)	H(15)[13)]	3.242	C(24)	H(16)[13)]	3.224
C(25)	H(4)[4)]	3.431	C(26)	H(4)[4)]	3.234
C(27)	H(26)[2)]	3.325	H(1)	H(11)[3)]	2.766
H(2)	C(21)[5)]	3.400	H(2)	H(5)[1)]	3.599
H(2)	H(11)[3)]	3.104	H(2)	H(13)[5)]	3.075
H(2)	H(14)[1)]	2.830	H(2)	H(16)[5)]	3.435
H(2)	H(18)[5)]	2.575	H(2)	H(19)[1)]	3.344
H(2)	H(21)[1)]	3.093	H(3)	C(8)[5)]	3.125
H(3)	C(9)[5)]	2.770	H(3)	C(10)[5)]	3.238
H(3)	C(19)[5)]	3.348	H(3)	H(5)[5)]	2.798
H(3)	H(5)[1)]	3.378	H(3)	H(6)[5)]	3.548
H(3)	H(9)[5)]	3.508	H(3)	H(13)[5)]	2.487
H(3)	H(24)[4)]	3.599	H(3)	H(25)[4)]	3.163
H(4)	C(10)[5)]	3.497	H(4)	C(11)[5)]	3.404
H(4)	C(25)[4)]	3.431	H(4)	C(26)[4)]	3.234
H(4)	H(5)[1)]	3.553	H(4)	H(6)[1)]	3.300
H(4)	H(17)[13)]	3.591	H(4)	H(24)[4)]	3.206
H(4)	H(25)[4)]	2.836	H(5)	C(1)[14)]	3.376
H(5)	C(2)[14)]	3.476	H(5)	C(3)[14)]	3.334
H(5)	C(4)[14)]	3.131	H(5)	C(5)[14)]	2.997
H(5)	C(6)[14)]	3.120	H(5)	H(2)[14)]	3.599
H(5)	H(3)[6)]	2.798	H(5)	H(3)[14)]	3.378
H(5)	H(4)[14)]	3.553	H(6)	O(1)[14)]	2.962
H(6)	C(1)[14)]	2.955	H(6)	C(2)[14)]	3.542
H(6)	C(6)[14)]	3.197	H(6)	H(3)[6)]	3.548
H(6)	H(4)[14)]	3.300	H(6)	H(20)[8)]	3.385
H(7)	C(21)[7)]	3.076	H(7)	C(22)[8)]	3.048
H(7)	H(16)[7)]	3.522	H(7)	H(17)[7)]	2.489
H(7)	H(18)[7)]	2.853	H(7)	H(19)[8)]	2.599
H(7)	H(20)[8)]	2.955	H(7)	H(21)[8)]	3.094
H(8)	C(18)[2)]	3.362	H(8)	C(21)[7)]	3.518
H(8)	H(11)[2)]	3.369	H(8)	H(12)[2)]	2.631
H(8)	H(16)[7)]	3.315	H(8)	H(17)[7)]	3.200

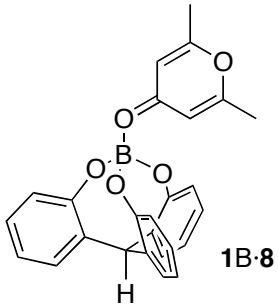
H(8)	H(18)[7)]	3.467	H(8)	H(26)[2)]	3.344
H(9)	H(3)[6)]	3.508	H(9)	H(12)[11)]	3.473
H(9)	H(23)[9)]	3.056	H(9)	H(24)[2)]	3.525
H(9)	H(25)[2)]	3.309	H(10)	O(3)[11)]	3.121
H(10)	C(13)[11)]	2.822	H(10)	C(14)[11)]	3.214
H(10)	C(17)[11)]	3.582	H(10)	C(18)[11)]	3.034
H(10)	H(12)[11)]	3.327	H(10)	H(23)[9)]	3.119
H(10)	H(24)[9)]	3.129	H(10)	H(24)[2)]	3.488
H(11)	C(3)[11)]	2.893	H(11)	C(4)[11)]	3.097
H(11)	H(1)[11)]	2.766	H(11)	H(2)[11)]	3.104
H(11)	H(8)[2)]	3.369	H(11)	H(24)[9)]	3.463
H(12)	C(12)[2)]	3.515	H(12)	C(21)[3)]	3.538
H(12)	H(8)[2)]	2.631	H(12)	H(9)[3)]	3.473
H(12)	H(10)[3)]	3.327	H(12)	H(16)[3)]	2.719
H(12)	H(23)[4)]	2.874	H(13)	C(4)[6)]	3.535
H(13)	C(5)[6)]	3.251	H(13)	H(2)[6)]	3.075
H(13)	H(3)[6)]	2.487	H(14)	C(4)[14)]	3.090
H(14)	C(5)[14)]	3.581	H(14)	H(2)[14)]	2.830
H(15)	C(23)[9)]	3.407	H(15)	C(24)[9)]	3.242
H(15)	H(22)[9)]	3.245	H(15)	H(23)[9)]	2.962
H(16)	C(18)[11)]	3.447	H(16)	C(24)[9)]	3.224
H(16)	H(2)[6)]	3.435	H(16)	H(7)[10)]	3.522
H(16)	H(8)[10)]	3.315	H(16)	H(12)[11)]	2.719
H(16)	H(22)[9)]	3.211	H(16)	H(23)[9)]	2.461
H(17)	C(11)[10)]	3.134	H(17)	C(12)[10)]	3.491
H(17)	C(23)[9)]	3.561	H(17)	H(4)[9)]	3.591
H(17)	H(7)[10)]	2.489	H(17)	H(8)[10)]	3.200
H(17)	H(22)[9)]	2.837	H(17)	H(23)[9)]	3.293
H(18)	C(4)[6)]	3.427	H(18)	H(2)[6)]	2.575
H(18)	H(7)[10)]	2.853	H(18)	H(8)[10)]	3.467
H(18)	H(21)[14)]	2.968	H(19)	C(11)[12)]	3.127
H(19)	H(2)[14)]	3.344	H(19)	H(7)[12)]	2.599
H(20)	C(11)[12)]	3.590	H(20)	H(6)[12)]	3.385
H(20)	H(7)[12)]	2.955	H(20)	H(22)[9)]	3.128
H(21)	H(2)[14)]	3.093	H(21)	H(7)[12)]	3.094
H(21)	H(18)[1)]	2.968	H(22)	C(21)[13)]	3.336
H(22)	H(15)[13)]	3.245	H(22)	H(16)[13)]	3.211
H(22)	H(17)[13)]	2.837	H(22)	H(20)[13)]	3.128
H(23)	O(3)[4)]	2.884	H(23)	C(13)[4)]	3.538
H(23)	C(15)[13)]	3.316	H(23)	C(16)[13)]	3.344
H(23)	C(18)[4)]	3.429	H(23)	C(20)[13)]	3.553
H(23)	C(21)[13)]	3.176	H(23)	H(9)[13)]	3.056

H(23)	H(10)[13)]	3.119	H(23)	H(12)[4)]	2.874
H(23)	H(15)[13)]	2.962	H(23)	H(16)[13)]	2.461
H(23)	H(17)[13)]	3.293	H(24)	O(3)[4)]	3.202
H(24)	C(1)[4)]	3.180	H(24)	C(5)[4)]	3.226
H(24)	C(6)[4)]	2.964	H(24)	C(16)[13)]	3.202
H(24)	C(17)[13)]	3.407	H(24)	H(3)[4)]	3.599
H(24)	H(4)[4)]	3.206	H(24)	H(9)[2)]	3.525
H(24)	H(10)[13)]	3.129	H(24)	H(10)[2)]	3.488
H(24)	H(11)[13)]	3.463	H(25)	O(2)[2)]	2.933
H(25)	C(5)[4)]	3.370	H(25)	C(6)[4)]	3.188
H(25)	C(7)[2)]	2.921	H(25)	C(8)[2)]	3.277
H(25)	C(12)[2)]	3.406	H(25)	C(13)[2)]	3.467
H(25)	C(14)[2)]	3.059	H(25)	C(15)[2)]	3.071
H(25)	C(16)[2)]	3.530	H(25)	H(3)[4)]	3.163
H(25)	H(4)[4)]	2.836	H(25)	H(9)[2)]	3.309
H(26)	O(2)[2)]	2.682	H(26)	C(7)[2)]	3.418
H(26)	C(27)[2)]	3.325	H(26)	H(8)[2)]	3.344
H(26)	H(26)[2)]	2.557			

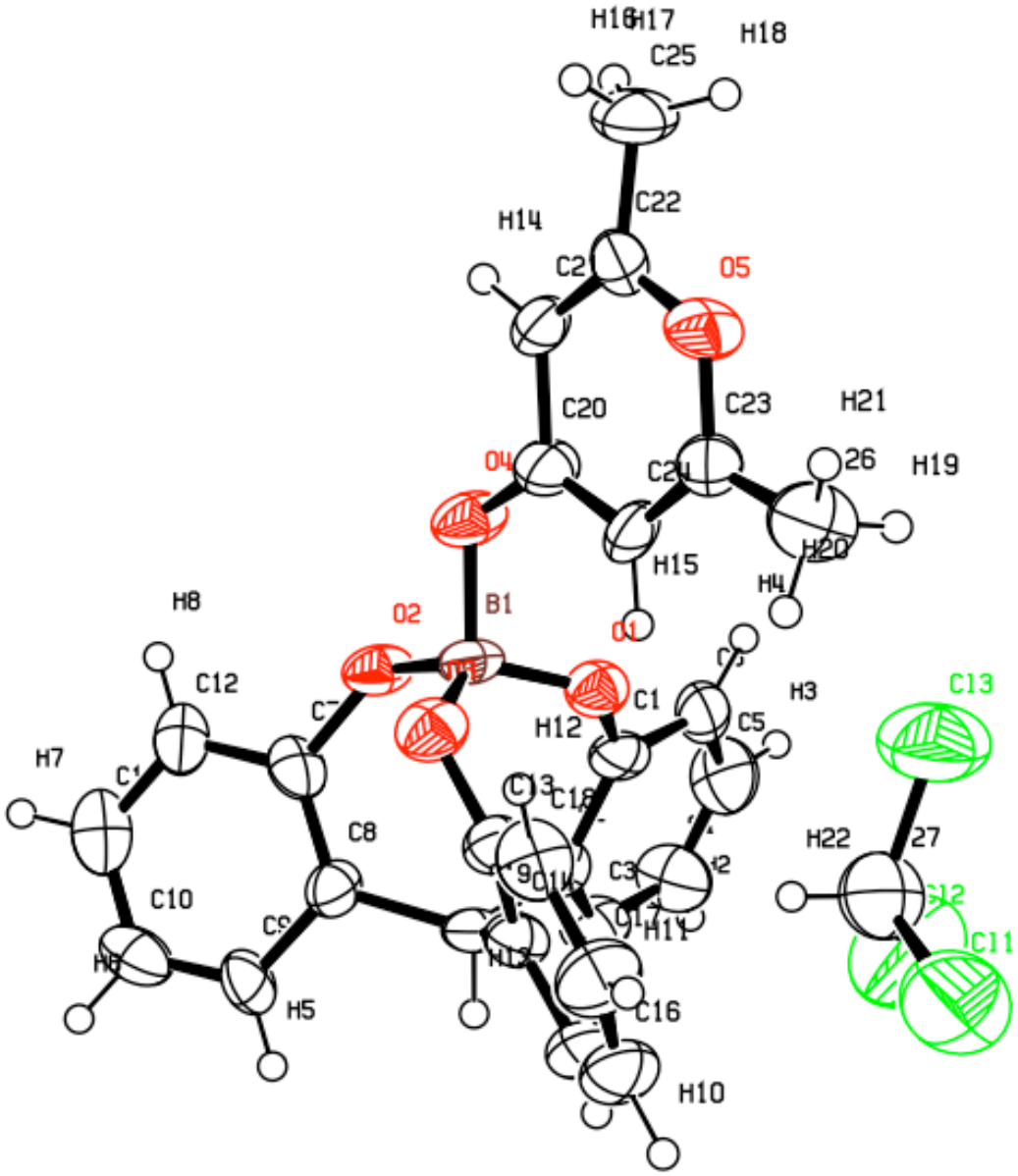
Symmetry Operators:

(1) X+1/2,Y,-Z+1/2+1	(2) -X,-Y,-Z+1
(3) X+1/2,-Y+1/2,-Z+1	(4) -X+1,-Y,-Z+1
(5) X+1,Y,Z	(6) X-1,Y,Z
(7) -X+1/2-1,Y+1/2-1,Z	(8) -X,Y+1/2-1,-Z+1/2+1
(9) -X+1/2,Y+1/2,Z	(10) -X+1/2-1,Y+1/2,Z
(11) X+1/2-1,-Y+1/2,-Z+1	(12) -X,Y+1/2,-Z+1/2+1
(13) -X+1/2,Y+1/2-1,Z	(14) X+1/2-1,Y,-Z+1/2+1

X-ray Structure Report



1B·8



Experimental

Data Collection

A colorless prism crystal of $C_{27}H_{22}BO_5Cl_3$ having approximate dimensions of 0.60 x 0.20 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 8.8892(12) Å	α	= 75.822(4)^o
b	= 9.3224(13) Å	β	= 83.017(4)^o
c	= 16.548(2) Å	γ	= 73.858(3)^o
V	= 1275.0(3) Å^3		

For Z = 2 and F.W. = 543.64, the calculated density is 1.416 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of 0 $\pm$ 1^{o}C to a maximum 2θ value of 61.0^o. A total of 57 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 4.0^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 90.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 168.0^o in 4.0^o step, at χ=45.0^o and ϕ = 210.0^o. The exposure rate was 90.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.200 mm pixel mode.

Data Reduction

Of the 16553 reflections that were collected, 7414 were unique (R_{int} = 0.116).

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.958 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F was based on 3561 observed reflections ($I > 3.00\sigma(I)$) and 347 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0846$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.1477$$

The standard deviation of an observation of unit weight[4] was 1.00. A Sheldrick weighting scheme was used. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.23 and -0.97 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$$\Sigma w(|F_o|-|F_c|)^2 \qquad \text{where w = Least Squares weights.}$$

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

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

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

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

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

(7) 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).

(8) 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).

(9) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2006). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 11: Carruthers, J.R., Rollett,J.S., Betteridge, P.W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{22}BO_5Cl_3$
Formula Weight	543.64
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.60 X 0.20 X 0.20 mm
Crystal System	triclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 180.0 seconds
Detector Position	127.40 mm
Pixel Size	0.200 mm
Lattice Parameters	a = 8.8892(12) Å b = 9.3224(13) Å c = 16.548(2) Å α = 75.822(4) ^{o} β = 83.017(4) ^{o} γ = 73.858(3) ^{o} V = 1275.0(3) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.416 g/cm^3
F_{000}	560.00
μ(MoKα)	3.958 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID

Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	57 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^o
Exposure Rate	90.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=210.0)	0.0 - 168.0^o
Exposure Rate	90.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.200 mm
$2\theta_{max}$	61.0^o
No. of Reflections Measured	Total: 16553 Unique: 7414 (R_{int} = 0.116)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1/[0.0194Fo^2+1.0000σ(Fo^2)]
$2\theta_{max}$ cutoff	61.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	3561
No. Variables	347
Reflection/Parameter Ratio	10.26
Residuals: R (I>3.00σ(I))	0.0846
Residuals: Rw (I>3.00σ(I))	0.1477
Goodness of Fit Indicator	1.000
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.23 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.97 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Cl(1)	0.1864(4)	0.0522(3)	0.0120(2)	10.48(12)
Cl(2)	0.3337(5)	0.2778(3)	0.0168(2)	11.07(12)
Cl(3)	0.3974(4)	0.0003(3)	0.1395(2)	10.22(11)
O(1)	0.1996(6)	0.2525(5)	0.2856(3)	3.45(12)
O(2)	0.0475(6)	0.4179(4)	0.3767(3)	3.62(12)
O(3)	-0.0575(6)	0.2312(4)	0.3416(3)	3.95(13)
O(4)	0.1567(6)	0.1582(4)	0.4305(3)	4.13(13)
O(5)	0.3196(6)	-0.2991(4)	0.4566(3)	3.88(13)
C(1)	0.2353(9)	0.3730(7)	0.2302(4)	3.28(19)
C(2)	0.1189(8)	0.4945(7)	0.1888(4)	3.30(18)
C(3)	0.1691(11)	0.6129(7)	0.1313(5)	4.3(2)
C(4)	0.3240(11)	0.6132(9)	0.1149(5)	5.0(2)
C(5)	0.4309(11)	0.4948(10)	0.1549(6)	5.2(2)
C(6)	0.3913(9)	0.3726(9)	0.2115(5)	4.1(2)
C(7)	-0.0875(8)	0.5322(6)	0.3556(5)	3.44(18)
C(8)	-0.1423(8)	0.5724(7)	0.2768(4)	3.31(18)
C(9)	-0.2758(8)	0.6929(7)	0.2587(5)	3.59(18)
C(10)	-0.3463(9)	0.7697(8)	0.3150(5)	4.4(2)
C(11)	-0.2863(9)	0.7297(8)	0.3947(5)	4.5(2)
C(12)	-0.1564(9)	0.6131(7)	0.4143(5)	3.83(19)
C(13)	-0.0955(8)	0.2330(8)	0.2622(4)	3.35(19)
C(14)	-0.0926(8)	0.3544(7)	0.1951(4)	3.31(18)
C(15)	-0.1327(9)	0.3428(8)	0.1195(5)	4.0(2)
C(16)	-0.1778(9)	0.2175(10)	0.1106(5)	4.7(2)
C(17)	-0.1815(10)	0.0976(10)	0.1764(6)	5.4(2)
C(18)	-0.1384(9)	0.1045(8)	0.2531(5)	4.4(2)
C(19)	-0.0529(8)	0.5010(7)	0.2009(4)	3.44(18)
C(20)	0.2091(9)	0.0131(7)	0.4334(4)	3.9(2)
C(21)	0.2844(8)	-0.0803(7)	0.5094(4)	3.44(19)
C(22)	0.3379(8)	-0.2313(8)	0.5164(5)	3.70(19)
C(23)	0.2490(9)	-0.2150(7)	0.3864(4)	3.59(19)
C(24)	0.1942(9)	-0.0636(7)	0.3746(4)	3.51(19)
C(25)	0.4276(10)	-0.3397(8)	0.5849(5)	5.2(2)
C(26)	0.2451(11)	-0.3094(8)	0.3286(6)	5.5(2)
C(27)	0.2612(12)	0.1338(9)	0.0774(6)	6.5(2)
B(1)	0.0833(11)	0.2722(8)	0.3526(5)	3.1(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.0922	0.6969	0.1029	4.92
H(2)	0.3539	0.6953	0.0759	5.92
H(3)	0.5385	0.4942	0.1443	6.32
H(4)	0.4717	0.2889	0.2373	5.05
H(5)	-0.3159	0.7198	0.2048	4.20
H(6)	-0.4376	0.8515	0.3023	4.93
H(7)	-0.3377	0.7854	0.4356	5.52
H(8)	-0.1146	0.5891	0.4676	4.40
H(9)	-0.1294	0.4238	0.0722	4.99
H(10)	-0.2064	0.2151	0.0576	5.88
H(11)	-0.2126	0.0116	0.1700	6.85
H(12)	-0.1385	0.0213	0.2996	5.33
H(13)	-0.0966	0.5736	0.1531	3.94
H(14)	0.2952	-0.0345	0.5530	4.09
H(15)	0.1447	-0.0073	0.3246	4.21
H(16)	0.3578	-0.3806	0.6264	5.83
H(17)	0.4835	-0.2883	0.6087	5.84
H(18)	0.4997	-0.4204	0.5640	5.84
H(19)	0.3369	-0.3165	0.2922	6.94
H(20)	0.1550	-0.2640	0.2967	6.94
H(21)	0.2409	-0.4090	0.3590	6.94
H(22)	0.1769	0.1771	0.1125	7.88

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.126(2)	0.128(2)	0.167(3)	-0.018(2)	-0.051(2)	-0.070(2)
Cl(2)	0.220(4)	0.092(2)	0.112(3)	-0.071(2)	0.003(2)	0.0009(18)
Cl(3)	0.170(3)	0.089(2)	0.108(2)	0.005(2)	-0.058(2)	-0.0043(17)

O(1)	0.052(3)	0.035(2)	0.041(3)	-0.009(2)	-0.007(2)	-0.004(2)
O(2)	0.069(3)	0.031(2)	0.038(3)	-0.010(2)	-0.019(2)	-0.003(2)
O(3)	0.065(4)	0.039(2)	0.042(3)	-0.016(2)	-0.004(2)	0.002(2)
O(4)	0.086(4)	0.032(2)	0.038(3)	-0.010(2)	-0.018(2)	-0.004(2)
O(5)	0.068(3)	0.023(2)	0.052(3)	-0.009(2)	-0.015(3)	0.003(2)
C(1)	0.050(5)	0.040(4)	0.040(5)	-0.005(3)	-0.019(4)	-0.017(3)
C(2)	0.043(5)	0.046(4)	0.034(4)	-0.010(3)	0.002(3)	-0.008(3)
C(3)	0.069(6)	0.040(4)	0.046(5)	-0.014(4)	-0.008(4)	0.005(3)
C(4)	0.049(6)	0.069(5)	0.070(7)	-0.026(4)	-0.002(5)	0.003(4)
C(5)	0.051(6)	0.080(6)	0.069(7)	-0.029(5)	0.013(5)	-0.013(5)
C(6)	0.039(5)	0.066(5)	0.054(6)	-0.004(4)	-0.008(4)	-0.032(4)
C(7)	0.045(5)	0.024(3)	0.051(5)	-0.004(3)	0.004(4)	0.002(3)
C(8)	0.054(5)	0.033(3)	0.035(4)	-0.005(3)	-0.002(4)	-0.009(3)
C(9)	0.042(4)	0.032(3)	0.059(5)	0.002(3)	-0.003(4)	-0.018(3)
C(10)	0.046(5)	0.044(4)	0.066(6)	-0.005(3)	-0.013(4)	0.004(4)
C(11)	0.059(5)	0.040(4)	0.076(7)	-0.022(4)	0.019(5)	-0.021(4)
C(12)	0.055(5)	0.034(3)	0.050(5)	-0.011(3)	0.014(4)	-0.008(3)
C(13)	0.040(4)	0.054(4)	0.036(5)	-0.014(3)	-0.004(3)	-0.011(3)
C(14)	0.045(4)	0.035(3)	0.045(5)	-0.006(3)	-0.012(4)	-0.007(3)
C(15)	0.055(5)	0.059(4)	0.044(5)	-0.008(4)	-0.016(4)	-0.021(4)
C(16)	0.058(6)	0.079(6)	0.050(6)	-0.023(4)	-0.015(4)	-0.020(5)
C(17)	0.077(7)	0.076(6)	0.064(7)	-0.027(5)	-0.014(5)	-0.026(5)
C(18)	0.060(5)	0.041(4)	0.068(6)	-0.021(3)	0.003(5)	-0.008(4)
C(19)	0.042(4)	0.050(4)	0.033(4)	-0.005(3)	-0.014(3)	-0.000(3)
C(20)	0.070(6)	0.032(3)	0.037(5)	0.001(3)	-0.009(4)	-0.003(3)
C(21)	0.055(5)	0.045(4)	0.030(4)	-0.009(3)	-0.002(4)	-0.012(3)
C(22)	0.040(4)	0.044(4)	0.048(5)	0.000(3)	0.002(4)	-0.010(3)
C(23)	0.050(5)	0.041(4)	0.040(5)	-0.008(3)	-0.002(4)	-0.004(3)
C(24)	0.062(5)	0.043(4)	0.028(4)	-0.006(3)	-0.001(4)	-0.017(3)
C(25)	0.093(7)	0.042(4)	0.050(5)	-0.001(4)	-0.025(5)	0.006(4)
C(26)	0.086(7)	0.052(4)	0.082(7)	-0.014(4)	-0.030(5)	-0.027(4)
C(27)	0.097(8)	0.059(5)	0.093(8)	-0.017(5)	-0.012(6)	-0.023(5)
B(1)	0.053(6)	0.035(4)	0.032(5)	-0.008(4)	-0.018(5)	-0.004(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Cl(1)	C(27)	1.747(13)	Cl(2)	C(27)	1.699(10)
Cl(3)	C(27)	1.705(9)	O(1)	C(1)	1.351(8)
O(1)	B(1)	1.431(10)	O(2)	C(7)	1.380(7)
O(2)	B(1)	1.450(10)	O(3)	C(13)	1.390(10)
O(3)	B(1)	1.450(12)	O(4)	C(20)	1.294(8)
O(4)	B(1)	1.538(9)	O(5)	C(22)	1.345(10)
O(5)	C(23)	1.346(8)	C(1)	C(2)	1.402(9)
C(1)	C(6)	1.383(12)	C(2)	C(3)	1.406(10)
C(2)	C(19)	1.502(11)	C(3)	C(4)	1.371(14)
C(4)	C(5)	1.331(11)	C(5)	C(6)	1.384(12)
C(7)	C(8)	1.376(11)	C(7)	C(12)	1.359(11)
C(8)	C(9)	1.393(8)	C(8)	C(19)	1.589(10)
C(9)	C(10)	1.307(12)	C(10)	C(11)	1.409(13)
C(11)	C(12)	1.356(9)	C(13)	C(14)	1.381(9)
C(13)	C(18)	1.400(12)	C(14)	C(15)	1.379(12)
C(14)	C(19)	1.530(11)	C(15)	C(16)	1.381(14)
C(16)	C(17)	1.361(12)	C(17)	C(18)	1.390(15)
C(20)	C(21)	1.459(9)	C(20)	C(24)	1.379(12)
C(21)	C(22)	1.335(9)	C(22)	C(25)	1.468(10)
C(23)	C(24)	1.332(9)	C(23)	C(26)	1.460(13)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.950	C(4)	H(2)	0.950
C(5)	H(3)	0.950	C(6)	H(4)	0.950
C(9)	H(5)	0.950	C(10)	H(6)	0.950
C(11)	H(7)	0.950	C(12)	H(8)	0.950
C(15)	H(9)	0.950	C(16)	H(10)	0.950
C(17)	H(11)	0.950	C(18)	H(12)	0.950
C(19)	H(13)	0.950	C(21)	H(14)	0.950
C(24)	H(15)	0.950	C(25)	H(16)	0.950
C(25)	H(17)	0.950	C(25)	H(18)	0.950
C(26)	H(19)	0.950	C(26)	H(20)	0.950
C(26)	H(21)	0.950	C(27)	H(22)	0.950

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	O(1)	B(1)	121.9(5)	C(7)	O(2)	B(1)	122.8(6)
C(13)	O(3)	B(1)	120.2(6)	C(20)	O(4)	B(1)	122.1(6)
C(22)	O(5)	C(23)	120.4(5)	O(1)	C(1)	C(2)	121.7(7)
O(1)	C(1)	C(6)	118.9(6)	C(2)	C(1)	C(6)	119.4(6)
C(1)	C(2)	C(3)	117.1(7)	C(1)	C(2)	C(19)	123.4(6)
C(3)	C(2)	C(19)	119.5(6)	C(2)	C(3)	C(4)	123.0(6)
C(3)	C(4)	C(5)	118.0(8)	C(4)	C(5)	C(6)	122.6(9)
C(1)	C(6)	C(5)	119.9(6)	O(2)	C(7)	C(8)	122.1(6)
O(2)	C(7)	C(12)	116.5(7)	C(8)	C(7)	C(12)	121.1(6)
C(7)	C(8)	C(9)	119.2(7)	C(7)	C(8)	C(19)	123.9(5)
C(9)	C(8)	C(19)	116.6(6)	C(8)	C(9)	C(10)	120.7(8)
C(9)	C(10)	C(11)	119.5(6)	C(10)	C(11)	C(12)	121.3(8)
C(7)	C(12)	C(11)	118.2(8)	O(3)	C(13)	C(14)	122.6(7)
O(3)	C(13)	C(18)	116.5(6)	C(14)	C(13)	C(18)	120.8(8)
C(13)	C(14)	C(15)	117.2(7)	C(13)	C(14)	C(19)	123.9(7)
C(15)	C(14)	C(19)	118.9(6)	C(14)	C(15)	C(16)	122.1(7)
C(15)	C(16)	C(17)	121.1(9)	C(16)	C(17)	C(18)	118.2(9)
C(13)	C(18)	C(17)	120.6(7)	C(2)	C(19)	C(8)	115.0(7)
C(2)	C(19)	C(14)	114.5(5)	C(8)	C(19)	C(14)	114.1(6)
O(4)	C(20)	C(21)	116.2(7)	O(4)	C(20)	C(24)	127.0(6)
C(21)	C(20)	C(24)	116.7(6)	C(20)	C(21)	C(22)	118.7(7)
O(5)	C(22)	C(21)	121.6(6)	O(5)	C(22)	C(25)	112.6(6)
C(21)	C(22)	C(25)	125.7(8)	O(5)	C(23)	C(24)	121.3(7)
O(5)	C(23)	C(26)	111.9(5)	C(24)	C(23)	C(26)	126.8(7)
C(20)	C(24)	C(23)	121.2(6)	Cl(1)	C(27)	Cl(2)	108.1(5)
Cl(1)	C(27)	Cl(3)	111.7(5)	Cl(2)	C(27)	Cl(3)	112.7(6)
O(1)	B(1)	O(2)	116.0(6)	O(1)	B(1)	O(3)	113.0(7)
O(1)	B(1)	O(4)	105.7(5)	O(2)	B(1)	O(3)	111.9(6)
O(2)	B(1)	O(4)	102.7(6)	O(3)	B(1)	O(4)	106.4(5)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	118.5	C(4)	C(3)	H(1)	118.4
C(3)	C(4)	H(2)	120.9	C(5)	C(4)	H(2)	121.1
C(4)	C(5)	H(3)	118.6	C(6)	C(5)	H(3)	118.8

C(1)	C(6)	H(4)	120.3	C(5)	C(6)	H(4)	119.8
C(8)	C(9)	H(5)	119.7	C(10)	C(9)	H(5)	119.7
C(9)	C(10)	H(6)	120.3	C(11)	C(10)	H(6)	120.2
C(10)	C(11)	H(7)	119.4	C(12)	C(11)	H(7)	119.3
C(7)	C(12)	H(8)	120.9	C(11)	C(12)	H(8)	120.9
C(14)	C(15)	H(9)	118.8	C(16)	C(15)	H(9)	119.1
C(15)	C(16)	H(10)	119.3	C(17)	C(16)	H(10)	119.6
C(16)	C(17)	H(11)	120.8	C(18)	C(17)	H(11)	121.0
C(13)	C(18)	H(12)	119.9	C(17)	C(18)	H(12)	119.5
C(2)	C(19)	H(13)	103.8	C(8)	C(19)	H(13)	103.8
C(14)	C(19)	H(13)	103.7	C(20)	C(21)	H(14)	120.6
C(22)	C(21)	H(14)	120.7	C(20)	C(24)	H(15)	119.4
C(23)	C(24)	H(15)	119.4	C(22)	C(25)	H(16)	109.4
C(22)	C(25)	H(17)	109.6	C(22)	C(25)	H(18)	109.4
H(16)	C(25)	H(17)	109.5	H(16)	C(25)	H(18)	109.5
H(17)	C(25)	H(18)	109.5	C(23)	C(26)	H(19)	109.4
C(23)	C(26)	H(20)	109.4	C(23)	C(26)	H(21)	109.6
H(19)	C(26)	H(20)	109.5	H(19)	C(26)	H(21)	109.5
H(20)	C(26)	H(21)	109.5	Cl(1)	C(27)	H(22)	108.1
Cl(2)	C(27)	H(22)	108.1	Cl(3)	C(27)	H(22)	108.1

Table 8. Torsion Angles(^{o})

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(1)	O(1)	B(1)	O(2)	-21.6(11)	C(1)	O(1)	B(1)	O(3)	109.6(7)
C(1)	O(1)	B(1)	O(4)	-134.5(7)	B(1)	O(1)	C(1)	C(2)	-50.5(12)
B(1)	O(1)	C(1)	C(6)	132.3(8)	C(7)	O(2)	B(1)	O(1)	104.2(8)
C(7)	O(2)	B(1)	O(3)	-27.4(9)	C(7)	O(2)	B(1)	O(4)	-141.1(6)
B(1)	O(2)	C(7)	C(8)	-44.1(10)	B(1)	O(2)	C(7)	C(12)	141.7(7)
C(13)	O(3)	B(1)	O(1)	-23.4(7)	C(13)	O(3)	B(1)	O(2)	109.7(6)
C(13)	O(3)	B(1)	O(4)	-138.9(5)	B(1)	O(3)	C(13)	C(14)	-47.6(8)
B(1)	O(3)	C(13)	C(18)	132.6(6)	C(20)	O(4)	B(1)	O(1)	-56.3(9)
C(20)	O(4)	B(1)	O(2)	-178.2(6)	C(20)	O(4)	B(1)	O(3)	64.1(8)
B(1)	O(4)	C(20)	C(21)	176.4(6)	B(1)	O(4)	C(20)	C(24)	-7.3(12)
C(22)	O(5)	C(23)	C(24)	-0.7(11)	C(22)	O(5)	C(23)	C(26)	178.2(6)
C(23)	O(5)	C(22)	C(21)	1.5(10)	C(23)	O(5)	C(22)	C(25)	-175.6(6)
O(1)	C(1)	C(2)	C(3)	-178.9(7)	O(1)	C(1)	C(2)	C(19)	-0.9(13)
O(1)	C(1)	C(6)	C(5)	180.0(7)	C(2)	C(1)	C(6)	C(5)	2.7(14)
C(6)	C(1)	C(2)	C(3)	-1.8(12)	C(6)	C(1)	C(2)	C(19)	176.2(8)

C(1)	C(2)	C(3)	C(4)	0.1(11)	C(1)	C(2)	C(19)	C(8)	86.7(9)
C(1)	C(2)	C(19)	C(14)	-48.4(10)	C(3)	C(2)	C(19)	C(8)	-95.4(8)
C(3)	C(2)	C(19)	C(14)	129.6(7)	C(19)	C(2)	C(3)	C(4)	-178.0(8)
C(2)	C(3)	C(4)	C(5)	0.6(14)	C(3)	C(4)	C(5)	C(6)	0.4(12)
C(4)	C(5)	C(6)	C(1)	-2.1(16)	O(2)	C(7)	C(8)	C(9)	-177.5(6)
O(2)	C(7)	C(8)	C(19)	-4.0(11)	O(2)	C(7)	C(12)	C(11)	177.9(7)
C(8)	C(7)	C(12)	C(11)	3.6(12)	C(12)	C(7)	C(8)	C(9)	-3.5(12)
C(12)	C(7)	C(8)	C(19)	170.0(7)	C(7)	C(8)	C(9)	C(10)	1.7(12)
C(7)	C(8)	C(19)	C(2)	-47.3(9)	C(7)	C(8)	C(19)	C(14)	87.9(9)
C(9)	C(8)	C(19)	C(2)	126.3(7)	C(9)	C(8)	C(19)	C(14)	-98.5(7)
C(19)	C(8)	C(9)	C(10)	-172.2(7)	C(8)	C(9)	C(10)	C(11)	-0.1(10)
C(9)	C(10)	C(11)	C(12)	0.2(10)	C(10)	C(11)	C(12)	C(7)	-1.9(12)
O(3)	C(13)	C(14)	C(15)	180.0(6)	O(3)	C(13)	C(14)	C(19)	-2.1(10)
O(3)	C(13)	C(18)	C(17)	178.7(6)	C(14)	C(13)	C(18)	C(17)	-1.1(11)
C(18)	C(13)	C(14)	C(15)	-0.3(8)	C(18)	C(13)	C(14)	C(19)	177.7(6)
C(13)	C(14)	C(15)	C(16)	1.5(10)	C(13)	C(14)	C(19)	C(2)	88.1(8)
C(13)	C(14)	C(19)	C(8)	-47.3(9)	C(15)	C(14)	C(19)	C(2)	-93.9(7)
C(15)	C(14)	C(19)	C(8)	130.6(6)	C(19)	C(14)	C(15)	C(16)	-176.6(6)
C(14)	C(15)	C(16)	C(17)	-1.4(12)	C(15)	C(16)	C(17)	C(18)	-0.0(11)
C(16)	C(17)	C(18)	C(13)	1.2(12)	O(4)	C(20)	C(21)	C(22)	178.7(7)
O(4)	C(20)	C(24)	C(23)	-177.6(7)	C(21)	C(20)	C(24)	C(23)	-1.3(11)
C(24)	C(20)	C(21)	C(22)	2.0(11)	C(20)	C(21)	C(22)	O(5)	-2.2(11)

Table 8. Torsion angles (^{o}) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(20)	C(21)	C(22)	C(25)	174.6(7)	O(5)	C(23)	C(24)	C(20)	0.7(11)
C(26)	C(23)	C(24)	C(20)	-178.1(8)					

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
Cl(1)	C(16)	3.563(8)	O(2)	C(26)[1)]	3.366(10)

O(3)	C(21)[2)]	3.285(8)	O(3)	C(22)[2)]	3.211(9)
O(3)	C(25)[2)]	3.333(10)	O(5)	C(11)[3)]	3.593(10)
C(7)	C(26)[1)]	3.592(13)	C(11)	O(5)[4)]	3.593(10)
C(15)	C(27)	3.581(12)	C(16)	Cl(1)	3.563(8)
C(21)	O(3)[2)]	3.285(8)	C(22)	O(3)[2)]	3.211(9)
C(25)	O(3)[2)]	3.333(10)	C(26)	O(2)[5)]	3.366(10)
C(26)	C(7)[5)]	3.592(13)	C(27)	C(15)	3.581(12)

Symmetry Operators:

(1)	X,Y+1,Z	(2)	-X,-Y,-Z+1
(3)	X+1,Y-1,Z	(4)	X-1,Y+1,Z
(5)	X,Y-1,Z		

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl(1)	H(1)[1)]	3.568	Cl(1)	H(1)[2)]	3.311
Cl(1)	H(2)[1)]	3.211	Cl(1)	H(10)	3.470
Cl(1)	H(10)[3)]	2.945	Cl(1)	H(11)[3)]	3.180
Cl(2)	H(2)[4)]	3.048	Cl(2)	H(3)[4)]	3.278
Cl(2)	H(9)[2)]	3.006	Cl(2)	H(13)[2)]	3.489
Cl(3)	H(2)[1)]	3.393	Cl(3)	H(5)[5)]	3.175
Cl(3)	H(6)[5)]	3.056	Cl(3)	H(11)[6)]	3.598
Cl(3)	H(15)	3.569	Cl(3)	H(19)	3.506
O(1)	H(22)	3.154	O(2)	H(8)[7)]	2.695
O(2)	H(20)[8)]	3.287	O(2)	H(21)[8)]	2.614
O(3)	H(14)[9)]	3.250	O(3)	H(16)[9)]	2.701
O(4)	H(7)[7)]	3.111	O(4)	H(8)[7)]	3.136
O(5)	H(6)[5)]	3.426	O(5)	H(7)[5)]	3.311
O(5)	H(8)[9)]	3.567	O(5)	H(18)[10)]	2.739
C(1)	H(21)[8)]	3.298	C(1)	H(22)	3.149
C(2)	H(20)[8)]	3.297	C(2)	H(21)[8)]	3.527
C(2)	H(22)	3.383	C(3)	H(9)[2)]	3.536
C(3)	H(10)[2)]	3.169	C(3)	H(19)[8)]	3.479
C(3)	H(20)[8)]	3.193	C(4)	H(10)[2)]	3.059
C(4)	H(19)[8)]	3.180	C(4)	H(20)[8)]	3.501
C(5)	H(19)[8)]	3.103	C(6)	H(17)[11)]	3.143
C(6)	H(19)[8)]	3.372	C(6)	H(21)[8)]	3.466

C(7)	H(8)[7)]	3.405	C(7)	H(16)[9)]	3.061
C(7)	H(20)[8)]	3.172	C(7)	H(21)[8)]	3.125
C(8)	H(16)[9)]	3.031	C(8)	H(20)[8)]	3.482
C(9)	H(11)[8)]	3.144	C(9)	H(16)[9)]	3.279
C(9)	H(19)[12)]	3.442	C(10)	H(11)[8)]	3.225
C(10)	H(12)[8)]	3.314	C(10)	H(16)[9)]	3.545
C(10)	H(19)[12)]	3.223	C(11)	H(12)[8)]	3.314
C(11)	H(14)[7)]	3.146	C(11)	H(16)[9)]	3.588
C(11)	H(18)[12)]	3.419	C(12)	H(8)[7)]	3.160
C(12)	H(16)[9)]	3.395	C(12)	H(20)[8)]	3.482
C(12)	H(21)[8)]	3.501	C(13)	H(16)[9)]	3.023
C(13)	H(22)	3.279	C(14)	H(3)[13)]	3.305
C(14)	H(16)[9)]	3.560	C(14)	H(22)	2.907
C(15)	H(3)[13)]	2.899	C(15)	H(22)	2.761
C(16)	H(1)[2)]	3.464	C(16)	H(2)[2)]	3.446
C(16)	H(3)[13)]	3.173	C(16)	H(4)[13)]	3.534
C(16)	H(22)	3.073	C(17)	H(4)[13)]	3.282
C(17)	H(22)	3.453	C(18)	H(4)[13)]	3.424
C(18)	H(14)[9)]	3.326	C(18)	H(22)	3.525
C(21)	H(7)[5)]	3.428	C(21)	H(7)[7)]	3.266
C(21)	H(12)[9)]	3.382	C(22)	H(7)[5)]	3.055
C(23)	H(6)[5)]	3.111	C(23)	H(18)[10)]	3.475
C(24)	H(6)[5)]	3.293	C(25)	H(4)[11)]	3.352
C(25)	H(7)[5)]	3.241	C(25)	H(19)[10)]	3.592
C(25)	H(21)[10)]	3.285	C(26)	H(6)[5)]	3.483
C(26)	H(18)[10)]	3.203	B(1)	H(8)[7)]	3.590
H(1)	Cl(1)[8)]	3.568	H(1)	Cl(1)[2)]	3.311
H(1)	C(16)[2)]	3.464	H(1)	H(9)[2)]	3.305
H(1)	H(10)[2)]	2.737	H(1)	H(20)[8)]	3.443
H(2)	Cl(1)[8)]	3.211	H(2)	Cl(2)[4)]	3.048
H(2)	Cl(3)[8)]	3.393	H(2)	C(16)[2)]	3.446
H(2)	H(10)[2)]	2.547	H(2)	H(19)[8)]	3.539
H(3)	Cl(2)[4)]	3.278	H(3)	C(14)[6)]	3.305
H(3)	C(15)[6)]	2.899	H(3)	C(16)[6)]	3.173
H(3)	H(5)[6)]	3.157	H(3)	H(9)[6)]	3.004
H(3)	H(10)[6)]	3.425	H(3)	H(13)[6)]	3.549
H(3)	H(19)[8)]	3.407	H(4)	C(16)[6)]	3.534
H(4)	C(17)[6)]	3.282	H(4)	C(18)[6)]	3.424
H(4)	C(25)[11)]	3.352	H(4)	H(11)[6)]	3.524
H(4)	H(16)[11)]	3.258	H(4)	H(17)[11)]	2.625
H(5)	Cl(3)[12)]	3.175	H(5)	H(3)[13)]	3.157
H(5)	H(11)[8)]	3.011	H(5)	H(19)[12)]	3.315

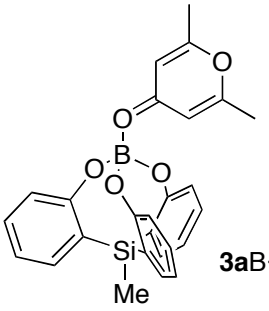
H(6)	Cl(3)[12)]	3.056	H(6)	O(5)[12)]	3.426
H(6)	C(23)[12)]	3.111	H(6)	C(24)[12)]	3.293
H(6)	C(26)[12)]	3.483	H(6)	H(11)[8)]	3.165
H(6)	H(12)[8)]	3.443	H(6)	H(15)[12)]	3.584
H(6)	H(19)[12)]	2.908	H(7)	O(4)[7)]	3.111
H(7)	O(5)[12)]	3.311	H(7)	C(21)[12)]	3.428
H(7)	C(21)[7)]	3.266	H(7)	C(22)[12)]	3.055
H(7)	C(25)[12)]	3.241	H(7)	H(12)[8)]	3.437
H(7)	H(14)[7)]	2.508	H(7)	H(17)[12)]	3.120
H(7)	H(18)[12)]	3.013	H(8)	O(2)[7)]	2.695
H(8)	O(4)[7)]	3.136	H(8)	O(5)[9)]	3.567
H(8)	C(7)[7)]	3.405	H(8)	C(12)[7)]	3.160
H(8)	B(1)[7)]	3.590	H(8)	H(8)[7)]	2.415
H(8)	H(21)[8)]	3.443	H(8)	H(21)[9)]	3.197
H(9)	Cl(2)[2)]	3.006	H(9)	C(3)[2)]	3.536
H(9)	H(1)[2)]	3.305	H(9)	H(3)[13)]	3.004
H(9)	H(9)[2)]	3.440	H(9)	H(22)	3.059
H(10)	Cl(1)	3.470	H(10)	Cl(1)[3)]	2.945
H(10)	C(3)[2)]	3.169	H(10)	C(4)[2)]	3.059
H(10)	H(1)[2)]	2.737	H(10)	H(2)[2)]	2.547
H(10)	H(3)[13)]	3.425	H(10)	H(22)	3.533
H(11)	Cl(1)[3)]	3.180	H(11)	Cl(3)[13)]	3.598
H(11)	C(9)[1)]	3.144	H(11)	C(10)[1)]	3.225
H(11)	H(4)[13)]	3.524	H(11)	H(5)[1)]	3.011
H(11)	H(6)[1)]	3.165	H(12)	C(10)[1)]	3.314
H(12)	C(11)[1)]	3.314	H(12)	C(21)[9)]	3.382
H(12)	H(6)[1)]	3.443	H(12)	H(7)[1)]	3.437
H(12)	H(14)[9)]	2.671	H(13)	Cl(2)[2)]	3.489
H(13)	H(3)[13)]	3.549	H(14)	O(3)[9)]	3.250
H(14)	C(11)[7)]	3.146	H(14)	C(18)[9)]	3.326
H(14)	H(7)[7)]	2.508	H(14)	H(12)[9)]	2.671
H(15)	Cl(3)	3.569	H(15)	H(6)[5)]	3.584
H(15)	H(22)	3.526	H(16)	O(3)[9)]	2.701
H(16)	C(7)[9)]	3.061	H(16)	C(8)[9)]	3.031
H(16)	C(9)[9)]	3.279	H(16)	C(10)[9)]	3.545
H(16)	C(11)[9)]	3.588	H(16)	C(12)[9)]	3.395
H(16)	C(13)[9)]	3.023	H(16)	C(14)[9)]	3.560
H(16)	H(4)[11)]	3.258	H(16)	H(19)[10)]	3.452
H(16)	H(21)[10)]	3.566	H(17)	C(6)[11)]	3.143
H(17)	H(4)[11)]	2.625	H(17)	H(7)[5)]	3.120
H(17)	H(21)[10)]	3.160	H(18)	O(5)[10)]	2.739
H(18)	C(11)[5)]	3.419	H(18)	C(23)[10)]	3.475

H(18)	C(26)[10)]	3.203	H(18)	H(7)[5)]	3.013
H(18)	H(18)[10)]	2.868	H(18)	H(19)[10)]	3.129
H(18)	H(21)[10)]	2.675	H(19)	Cl(3)	3.506
H(19)	C(3)[1)]	3.479	H(19)	C(4)[1)]	3.180
H(19)	C(5)[1)]	3.103	H(19)	C(6)[1)]	3.372
H(19)	C(9)[5)]	3.442	H(19)	C(10)[5)]	3.223
H(19)	C(25)[10)]	3.592	H(19)	H(2)[1)]	3.539
H(19)	H(3)[1)]	3.407	H(19)	H(5)[5)]	3.315
H(19)	H(6)[5)]	2.908	H(19)	H(16)[10)]	3.452
H(19)	H(18)[10)]	3.129	H(20)	O(2)[1)]	3.287
H(20)	C(2)[1)]	3.297	H(20)	C(3)[1)]	3.193
H(20)	C(4)[1)]	3.501	H(20)	C(7)[1)]	3.172
H(20)	C(8)[1)]	3.482	H(20)	C(12)[1)]	3.482
H(20)	H(1)[1)]	3.443	H(21)	O(2)[1)]	2.614
H(21)	C(1)[1)]	3.298	H(21)	C(2)[1)]	3.527
H(21)	C(6)[1)]	3.466	H(21)	C(7)[1)]	3.125
H(21)	C(12)[1)]	3.501	H(21)	C(25)[10)]	3.285
H(21)	H(8)[1)]	3.443	H(21)	H(8)[9)]	3.197
H(21)	H(16)[10)]	3.566	H(21)	H(17)[10)]	3.160
H(21)	H(18)[10)]	2.675	H(22)	O(1)	3.154
H(22)	C(1)	3.149	H(22)	C(2)	3.383
H(22)	C(13)	3.279	H(22)	C(14)	2.907
H(22)	C(15)	2.761	H(22)	C(16)	3.073
H(22)	C(17)	3.453	H(22)	C(18)	3.525
H(22)	H(9)	3.059	H(22)	H(10)	3.533
H(22)	H(15)	3.526			

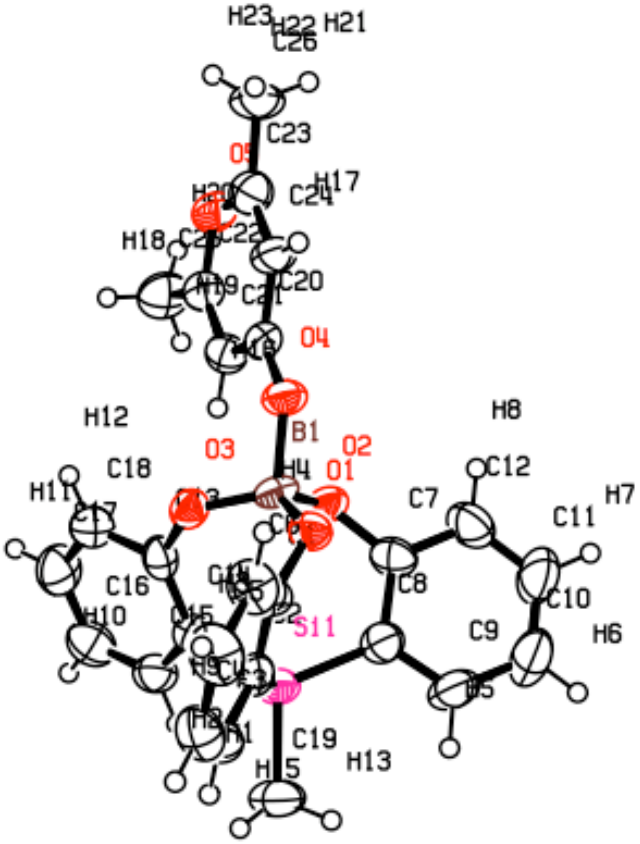
Symmetry Operators:

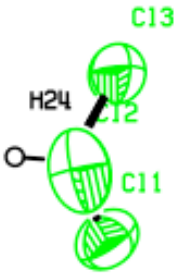
(1) X,Y-1,Z	(2) -X,-Y+1,-Z
(3) -X,-Y,-Z	(4) -X+1,-Y+1,-Z
(5) X+1,Y-1,Z	(6) X+1,Y,Z
(7) -X,-Y+1,-Z+1	(8) X,Y+1,Z
(9) -X,-Y,-Z+1	(10) -X+1,-Y-1,-Z+1
(11) -X+1,-Y,-Z+1	(12) X-1,Y+1,Z
(13) X-1,Y,Z	

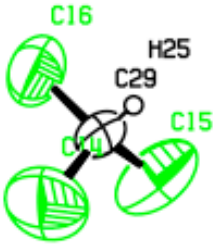
X-ray Structure Report



3aB·**8**







Experimental

Data Collection

A colorless prism crystal of $C_{28}H_{25}BO_5SiCl_6$ having approximate dimensions of 0.70 x 0.40 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 12.7774(13) Å
b = 18.6212(18) Å β = 109.020(3)^o
c = 14.6414(17) Å
V = 3293.5(6) Å^3

For Z = 4 and F.W. = 693.12, the calculated density is 1.398 g/cm^3. The systematic absences of:

h0l: h+l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of 0 $\pm$ 1^{o}C to a maximum 2θ value of 61.0^o. A total of 74 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 3.0^o step, at χ=45.0^o and ϕ = 90.0^o. The exposure rate was 60.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 162.0^o in

3.0° step, at χ=45.0° and ϕ = 270.0°. The exposure rate was 60.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.200 mm pixel mode.

Data Reduction

Of the 40786 reflections that were collected, 9988 were unique (R_{int} = 0.130).

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.924 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 9556 observed reflections and 395 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0867$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.2471$$

The standard deviation of an observation of unit weight[4] was 1.00. A Sheldrick weighting scheme was used. Plots of Σ w (|Fo| - |Fc|)^2 versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 3.28 and -2.12 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10]

crystallographic software package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) 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

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

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(7) 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).

(8) 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).

(9) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2006). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 11: Carruthers, J.R., Rollett,J.S., Betteridge, P.W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{28}H_{25}BO_5SiCl_6$
Formula Weight	693.12
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.70 X 0.40 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 180.0 seconds
Detector Position	127.40 mm
Pixel Size	0.200 mm
Lattice Parameters	a = 12.7774(13) Å b = 18.6212(18) Å c = 14.6414(17) Å β = 109.020(3) ^{o} V = 3293.5(6) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.398 g/cm^3
F_{000}	1416.00
μ(MoKα)	5.924 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated

Detector Aperture	280 mm x 256 mm
Data Images	74 exposures
ω oscillation Range (χ=45.0, ϕ=90.0)	130.0 - 190.0^{o}
Exposure Rate	60.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=270.0)	0.0 - 162.0^{o}
Exposure Rate	60.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.200 mm
$2\theta_{max}$	61.0^{o}
No. of Reflections Measured	Total: 40786 Unique: 9988 (R_{int} = 0.130)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	$1/[0.0111Fo^2+1.0000\sigma(Fo^2)]/(4Fo^2)$
$2\theta_{max}$ cutoff	61.0^{o}
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	9556
No. Variables	395
Reflection/Parameter Ratio	24.19
Residuals: R1 (I>3.00σ(I))	0.0867
Residuals: wR2 (I>3.00σ(I))	0.2471
Goodness of Fit Indicator	1.002
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	3.28 $e^-/Å^3$
Minimum peak in Final Diff. Map	-2.12 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Cl(1)	0.94261(18)	0.64410(10)	0.00033(16)	9.49(6)
Cl(2)	0.82429(15)	0.51285(10)	-0.00022(19)	10.66(7)
Cl(3)	1.00638(15)	0.55282(13)	0.16412(16)	10.45(6)
Cl(4)	0.1498(2)	0.8703(2)	0.0451(2)	17.14(11)
Cl(5)	0.3694(2)	0.92981(16)	0.1189(2)	15.44(11)
Cl(6)	0.25319(19)	0.89409(16)	0.24573(19)	13.20(9)
Si(1)	0.86888(10)	0.26433(6)	0.25550(9)	3.63(2)
O(1)	0.8660(2)	0.10783(13)	0.3289(2)	3.46(6)
O(2)	1.0062(2)	0.18358(14)	0.4398(2)	3.59(6)
O(3)	0.8145(2)	0.19057(14)	0.4328(2)	3.27(6)
O(4)	0.9218(2)	0.08535(14)	0.4936(2)	3.65(7)
O(5)	1.0191(2)	0.10652(18)	0.7840(2)	4.63(8)
C(1)	0.7748(3)	0.1239(2)	0.2529(3)	3.29(10)
C(2)	0.7643(3)	0.1917(2)	0.2071(3)	3.54(10)
C(3)	0.6721(3)	0.2027(2)	0.1256(3)	4.18(11)
C(4)	0.5943(4)	0.1507(2)	0.0914(4)	5.07(13)
C(5)	0.6063(3)	0.0850(2)	0.1378(3)	5.23(13)
C(6)	0.6965(3)	0.0727(2)	0.2175(3)	4.63(12)
C(7)	1.0597(3)	0.1880(2)	0.3724(3)	3.85(10)
C(8)	1.0097(3)	0.2243(2)	0.2844(3)	3.96(11)
C(9)	1.0719(4)	0.2262(2)	0.2226(3)	5.18(13)
C(10)	1.1768(4)	0.1963(3)	0.2440(4)	6.20(17)
C(11)	1.2204(4)	0.1619(3)	0.3286(4)	6.50(17)
C(12)	1.1648(3)	0.1581(2)	0.3941(4)	5.03(13)
C(13)	0.8158(3)	0.2648(2)	0.4322(3)	3.39(10)
C(14)	0.8410(3)	0.3053(2)	0.3626(3)	3.19(10)
C(15)	0.8356(3)	0.3793(2)	0.3712(3)	4.06(12)
C(16)	0.8053(4)	0.4118(2)	0.4409(4)	4.97(13)
C(17)	0.7795(4)	0.3717(2)	0.5097(4)	5.07(14)
C(18)	0.7830(3)	0.2977(2)	0.5042(3)	4.37(12)
C(19)	0.8521(4)	0.3360(2)	0.1625(3)	5.36(13)
C(20)	0.9560(3)	0.0954(2)	0.5850(3)	3.60(11)
C(21)	0.9736(3)	0.1624(2)	0.6325(3)	3.50(10)
C(22)	1.0045(3)	0.1668(2)	0.7287(3)	4.10(12)
C(23)	1.0044(4)	0.0387(2)	0.7417(3)	4.48(13)
C(24)	0.9723(3)	0.0341(2)	0.6456(3)	4.21(12)
C(25)	1.0222(4)	0.2328(2)	0.7887(3)	5.25(13)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(26)	1.0253(4)	-0.0187(2)	0.8153(3)	5.95(15)
C(28)	0.8934(4)	0.5843(3)	0.0658(5)	7.50(19)
C(29)	0.2739(5)	0.8691(4)	0.1376(4)	9.1(2)
B(1)	0.8998(4)	0.1465(2)	0.4195(3)	3.22(12)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.6632	0.2476	0.0932	4.84
H(2)	0.5320	0.1595	0.0357	5.79
H(3)	0.5520	0.0486	0.1144	5.77
H(4)	0.7046	0.0274	0.2488	5.24
H(5)	1.0409	0.2493	0.1619	6.29
H(6)	1.2168	0.2001	0.1997	7.94
H(7)	1.2910	0.1399	0.3432	8.09
H(8)	1.1981	0.1350	0.4545	5.69
H(9)	0.8542	0.4086	0.3256	4.78
H(10)	0.8017	0.4627	0.4427	5.83
H(11)	0.7597	0.3945	0.5598	6.15
H(12)	0.7631	0.2690	0.5497	5.29
H(13)	0.8969	0.3250	0.1237	6.33
H(14)	0.8741	0.3809	0.1936	6.32
H(15)	0.7767	0.3384	0.1228	6.35
H(16)	0.9633	0.2052	0.5954	4.08
H(17)	0.9599	-0.0121	0.6166	5.22
H(18)	0.9540	0.2473	0.7959	6.15
H(19)	1.0493	0.2700	0.7581	6.16
H(20)	1.0745	0.2233	0.8505	6.14
H(21)	1.1013	-0.0319	0.8352	7.30
H(22)	0.9810	-0.0594	0.7886	7.29
H(23)	1.0072	-0.0018	0.8695	7.29
H(24)	0.8440	0.6092	0.0911	9.52

H(25)	0.3041	0.8220	0.1440	11.36

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.1491(17)	0.1106(13)	0.1196(17)	-0.0017(11)	0.0695(14)	0.0108(11)
Cl(2)	0.1006(13)	0.1096(13)	0.194(2)	-0.0166(11)	0.0476(15)	-0.0324(14)
Cl(3)	0.0946(12)	0.192(2)	0.1169(18)	0.0211(12)	0.0435(12)	0.0296(15)
Cl(4)	0.174(2)	0.334(4)	0.106(2)	0.046(2)	-0.0054(19)	-0.008(2)
Cl(5)	0.234(3)	0.221(2)	0.171(3)	-0.052(2)	0.120(2)	0.012(2)
Cl(6)	0.1228(17)	0.273(3)	0.120(2)	0.0225(18)	0.0588(15)	0.001(2)
Si(1)	0.0479(7)	0.0517(7)	0.0355(8)	0.0007(5)	0.0098(5)	0.0076(6)
O(1)	0.0451(16)	0.0481(16)	0.0347(18)	0.0046(13)	0.0084(14)	0.0028(14)
O(2)	0.0442(16)	0.0620(18)	0.0287(18)	-0.0014(15)	0.0096(14)	0.0033(14)
O(3)	0.0475(16)	0.0427(17)	0.0371(17)	0.0007(14)	0.0179(13)	-0.0031(13)
O(4)	0.0609(18)	0.0461(17)	0.033(2)	0.0050(14)	0.0165(15)	0.0055(14)
O(5)	0.060(2)	0.081(2)	0.036(2)	0.0116(17)	0.0162(15)	0.0102(18)
C(1)	0.051(2)	0.039(2)	0.034(2)	0.008(2)	0.012(2)	-0.001(2)
C(2)	0.036(2)	0.065(2)	0.032(2)	0.006(2)	0.009(2)	-0.006(2)
C(3)	0.050(2)	0.066(3)	0.038(2)	0.005(2)	0.007(2)	-0.000(2)
C(4)	0.054(3)	0.074(3)	0.056(3)	0.009(2)	0.005(2)	-0.014(2)
C(5)	0.048(2)	0.071(3)	0.064(3)	-0.012(2)	-0.004(2)	-0.028(2)
C(6)	0.049(2)	0.057(2)	0.060(3)	-0.009(2)	0.005(2)	-0.015(2)
C(7)	0.042(2)	0.057(2)	0.039(2)	-0.001(2)	-0.000(2)	0.002(2)
C(8)	0.052(2)	0.054(2)	0.045(3)	-0.001(2)	0.017(2)	0.002(2)
C(9)	0.066(3)	0.093(3)	0.040(3)	-0.004(2)	0.020(2)	0.013(2)
C(10)	0.070(3)	0.103(4)	0.079(4)	0.001(3)	0.046(3)	-0.008(3)
C(11)	0.052(3)	0.126(5)	0.078(4)	0.010(3)	0.034(3)	0.004(4)
C(12)	0.051(2)	0.072(3)	0.057(3)	0.013(2)	0.003(2)	0.007(2)
C(13)	0.033(2)	0.051(2)	0.041(2)	0.005(2)	0.008(2)	-0.009(2)
C(14)	0.038(2)	0.039(2)	0.043(2)	-0.0045(19)	0.012(2)	-0.001(2)
C(15)	0.052(2)	0.056(3)	0.043(3)	0.002(2)	0.011(2)	0.006(2)
C(16)	0.070(3)	0.045(2)	0.070(4)	0.006(2)	0.017(3)	0.003(2)
C(17)	0.070(3)	0.062(3)	0.062(3)	0.005(2)	0.025(2)	-0.013(2)
C(18)	0.056(2)	0.055(3)	0.057(3)	0.004(2)	0.021(2)	0.009(2)
C(19)	0.076(3)	0.071(3)	0.053(3)	-0.000(2)	0.016(2)	0.024(2)
C(20)	0.044(2)	0.059(2)	0.037(3)	0.009(2)	0.018(2)	0.008(2)
C(21)	0.042(2)	0.044(2)	0.043(3)	-0.001(2)	0.009(2)	0.001(2)

C(22)	0.053(2)	0.060(2)	0.044(3)	0.008(2)	0.018(2)	0.007(2)
C(23)	0.069(3)	0.057(3)	0.047(3)	0.011(2)	0.024(2)	0.001(2)
C(24)	0.074(3)	0.053(2)	0.038(3)	0.011(2)	0.025(2)	0.008(2)
C(25)	0.079(3)	0.075(3)	0.041(3)	-0.004(2)	0.013(2)	-0.009(2)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(26)	0.113(4)	0.074(3)	0.044(3)	0.030(3)	0.032(3)	0.022(2)
C(28)	0.081(4)	0.083(3)	0.137(6)	0.010(3)	0.057(4)	-0.006(3)
C(29)	0.100(4)	0.193(7)	0.067(4)	0.037(4)	0.044(4)	0.035(4)
B(1)	0.057(3)	0.039(2)	0.027(3)	-0.005(2)	0.016(2)	0.003(2)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Cl(1)	C(28)	1.716(7)	Cl(2)	C(28)	1.711(6)
Cl(3)	C(28)	1.774(6)	Cl(4)	C(29)	1.717(6)
Cl(5)	C(29)	1.750(8)	Cl(6)	C(29)	1.752(8)
Si(1)	C(2)	1.870(4)	Si(1)	C(8)	1.865(4)
Si(1)	C(14)	1.880(5)	Si(1)	C(19)	1.868(5)
O(1)	C(1)	1.357(4)	O(1)	B(1)	1.446(5)
O(2)	C(7)	1.374(6)	O(2)	B(1)	1.467(5)
O(3)	C(13)	1.382(5)	O(3)	B(1)	1.428(6)
O(4)	C(20)	1.280(5)	O(4)	B(1)	1.533(5)
O(5)	C(22)	1.360(5)	O(5)	C(23)	1.391(5)
C(1)	C(2)	1.416(5)	C(1)	C(6)	1.357(5)
C(2)	C(3)	1.391(5)	C(3)	C(4)	1.361(6)
C(4)	C(5)	1.384(7)	C(5)	C(6)	1.366(6)
C(7)	C(8)	1.410(6)	C(7)	C(12)	1.392(6)
C(8)	C(9)	1.386(8)	C(9)	C(10)	1.390(8)
C(10)	C(11)	1.344(8)	C(11)	C(12)	1.369(9)
C(13)	C(14)	1.387(6)	C(13)	C(18)	1.397(7)

C(14)	C(15)	1.388(5)	C(15)	C(16)	1.348(8)
C(16)	C(17)	1.377(8)	C(17)	C(18)	1.383(6)
C(20)	C(21)	1.409(6)	C(20)	C(24)	1.419(6)
C(21)	C(22)	1.336(7)	C(22)	C(25)	1.485(6)
C(23)	C(24)	1.334(7)	C(23)	C(26)	1.480(7)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.950	C(4)	H(2)	0.950
C(5)	H(3)	0.950	C(6)	H(4)	0.950
C(9)	H(5)	0.950	C(10)	H(6)	0.950
C(11)	H(7)	0.950	C(12)	H(8)	0.950
C(15)	H(9)	0.950	C(16)	H(10)	0.950
C(17)	H(11)	0.950	C(18)	H(12)	0.950
C(19)	H(13)	0.950	C(19)	H(14)	0.950
C(19)	H(15)	0.950	C(21)	H(16)	0.950
C(24)	H(17)	0.950	C(25)	H(18)	0.950
C(25)	H(19)	0.950	C(25)	H(20)	0.950
C(26)	H(21)	0.950	C(26)	H(22)	0.950
C(26)	H(23)	0.950	C(28)	H(24)	0.950
C(29)	H(25)	0.950			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	Si(1)	C(8)	108.34(18)	C(2)	Si(1)	C(14)	107.7(2)
C(2)	Si(1)	C(19)	109.96(19)	C(8)	Si(1)	C(14)	113.83(19)
C(8)	Si(1)	C(19)	108.9(2)	C(14)	Si(1)	C(19)	108.1(2)
C(1)	O(1)	B(1)	124.2(3)	C(7)	O(2)	B(1)	121.9(3)
C(13)	O(3)	B(1)	124.2(3)	C(20)	O(4)	B(1)	123.5(3)
C(22)	O(5)	C(23)	120.7(3)	O(1)	C(1)	C(2)	120.6(3)
O(1)	C(1)	C(6)	119.2(3)	C(2)	C(1)	C(6)	120.1(3)
Si(1)	C(2)	C(1)	121.3(2)	Si(1)	C(2)	C(3)	121.3(3)
C(1)	C(2)	C(3)	117.4(3)	C(2)	C(3)	C(4)	121.6(4)
C(3)	C(4)	C(5)	119.8(4)	C(4)	C(5)	C(6)	119.7(4)
C(1)	C(6)	C(5)	121.4(4)	O(2)	C(7)	C(8)	120.1(3)

O(2)	C(7)	C(12)	118.8(4)	C(8)	C(7)	C(12)	121.1(5)
Si(1)	C(8)	C(7)	121.0(4)	Si(1)	C(8)	C(9)	123.9(3)
C(7)	C(8)	C(9)	115.1(4)	C(8)	C(9)	C(10)	123.9(5)
C(9)	C(10)	C(11)	118.6(6)	C(10)	C(11)	C(12)	121.2(5)
C(7)	C(12)	C(11)	120.1(4)	O(3)	C(13)	C(14)	123.7(4)
O(3)	C(13)	C(18)	115.2(4)	C(14)	C(13)	C(18)	121.0(4)
Si(1)	C(14)	C(13)	123.0(3)	Si(1)	C(14)	C(15)	120.5(3)
C(13)	C(14)	C(15)	116.4(4)	C(14)	C(15)	C(16)	123.3(4)
C(15)	C(16)	C(17)	120.5(4)	C(16)	C(17)	C(18)	118.6(5)
C(13)	C(18)	C(17)	120.2(5)	O(4)	C(20)	C(21)	126.2(4)
O(4)	C(20)	C(24)	117.8(3)	C(21)	C(20)	C(24)	115.9(4)
C(20)	C(21)	C(22)	121.3(4)	O(5)	C(22)	C(21)	120.9(4)
O(5)	C(22)	C(25)	111.4(4)	C(21)	C(22)	C(25)	127.6(4)
O(5)	C(23)	C(24)	118.6(4)	O(5)	C(23)	C(26)	111.4(4)
C(24)	C(23)	C(26)	130.0(4)	C(20)	C(24)	C(23)	122.7(4)
Cl(1)	C(28)	Cl(2)	113.9(4)	Cl(1)	C(28)	Cl(3)	108.6(3)
Cl(2)	C(28)	Cl(3)	109.5(3)	Cl(4)	C(29)	Cl(5)	112.3(4)
Cl(4)	C(29)	Cl(6)	109.7(4)	Cl(5)	C(29)	Cl(6)	106.7(4)
O(1)	B(1)	O(2)	113.6(4)	O(1)	B(1)	O(3)	113.5(3)
O(1)	B(1)	O(4)	102.2(3)	O(2)	B(1)	O(3)	113.5(3)
O(2)	B(1)	O(4)	105.2(3)	O(3)	B(1)	O(4)	107.6(4)

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	119.2	C(4)	C(3)	H(1)	119.2
C(3)	C(4)	H(2)	120.1	C(5)	C(4)	H(2)	120.1
C(4)	C(5)	H(3)	120.2	C(6)	C(5)	H(3)	120.2
C(1)	C(6)	H(4)	119.3	C(5)	C(6)	H(4)	119.3
C(8)	C(9)	H(5)	118.0	C(10)	C(9)	H(5)	118.0
C(9)	C(10)	H(6)	120.7	C(11)	C(10)	H(6)	120.7
C(10)	C(11)	H(7)	119.4	C(12)	C(11)	H(7)	119.4
C(7)	C(12)	H(8)	120.0	C(11)	C(12)	H(8)	120.0
C(14)	C(15)	H(9)	118.3	C(16)	C(15)	H(9)	118.4
C(15)	C(16)	H(10)	119.8	C(17)	C(16)	H(10)	119.8
C(16)	C(17)	H(11)	120.7	C(18)	C(17)	H(11)	120.7
C(13)	C(18)	H(12)	119.9	C(17)	C(18)	H(12)	119.9
Si(1)	C(19)	H(13)	109.5	Si(1)	C(19)	H(14)	109.5
Si(1)	C(19)	H(15)	109.5	H(13)	C(19)	H(14)	109.5

H(13)	C(19)	H(15)	109.5	H(14)	C(19)	H(15)	109.5
C(20)	C(21)	H(16)	119.4	C(22)	C(21)	H(16)	119.4
C(20)	C(24)	H(17)	118.7	C(23)	C(24)	H(17)	118.7
C(22)	C(25)	H(18)	109.5	C(22)	C(25)	H(19)	109.5
C(22)	C(25)	H(20)	109.5	H(18)	C(25)	H(19)	109.5
H(18)	C(25)	H(20)	109.5	H(19)	C(25)	H(20)	109.5
C(23)	C(26)	H(21)	109.5	C(23)	C(26)	H(22)	109.5
C(23)	C(26)	H(23)	109.5	H(21)	C(26)	H(22)	109.5
H(21)	C(26)	H(23)	109.5	H(22)	C(26)	H(23)	109.5
Cl(1)	C(28)	H(24)	108.2	Cl(2)	C(28)	H(24)	108.2
Cl(3)	C(28)	H(24)	108.2	Cl(4)	C(29)	H(25)	109.3
Cl(5)	C(29)	H(25)	109.3	Cl(6)	C(29)	H(25)	109.3

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(2)	Si(1)	C(8)	C(7)	-82.4(3)	C(2)	Si(1)	C(8)	C(9)	96.3(4)
C(8)	Si(1)	C(2)	C(1)	46.0(4)	C(8)	Si(1)	C(2)	C(3)	-135.2(4)
C(2)	Si(1)	C(14)	C(13)	42.7(3)	C(2)	Si(1)	C(14)	C(15)	-131.8(3)
C(14)	Si(1)	C(2)	C(1)	-77.5(4)	C(14)	Si(1)	C(2)	C(3)	101.3(4)
C(19)	Si(1)	C(2)	C(1)	165.0(4)	C(19)	Si(1)	C(2)	C(3)	-16.2(5)
C(8)	Si(1)	C(14)	C(13)	-77.5(3)	C(8)	Si(1)	C(14)	C(15)	108.1(3)
C(14)	Si(1)	C(8)	C(7)	37.3(4)	C(14)	Si(1)	C(8)	C(9)	-144.0(3)
C(19)	Si(1)	C(8)	C(7)	158.0(3)	C(19)	Si(1)	C(8)	C(9)	-23.3(4)
C(19)	Si(1)	C(14)	C(13)	161.4(3)	C(19)	Si(1)	C(14)	C(15)	-13.1(3)
C(1)	O(1)	B(1)	O(2)	-115.7(4)	C(1)	O(1)	B(1)	O(3)	15.9(6)
C(1)	O(1)	B(1)	O(4)	131.5(3)	B(1)	O(1)	C(1)	C(2)	61.4(6)
B(1)	O(1)	C(1)	C(6)	-122.5(5)	C(7)	O(2)	B(1)	O(1)	7.9(4)
C(7)	O(2)	B(1)	O(3)	-123.8(4)	C(7)	O(2)	B(1)	O(4)	118.8(3)
B(1)	O(2)	C(7)	C(8)	62.6(5)	B(1)	O(2)	C(7)	C(12)	-119.4(4)
C(13)	O(3)	B(1)	O(1)	-110.7(4)	C(13)	O(3)	B(1)	O(2)	21.0(5)
C(13)	O(3)	B(1)	O(4)	137.0(3)	B(1)	O(3)	C(13)	C(14)	46.9(5)
B(1)	O(3)	C(13)	C(18)	-136.9(3)	C(20)	O(4)	B(1)	O(1)	178.8(3)
C(20)	O(4)	B(1)	O(2)	59.9(5)	C(20)	O(4)	B(1)	O(3)	-61.5(4)
B(1)	O(4)	C(20)	C(21)	3.3(7)	B(1)	O(4)	C(20)	C(24)	179.6(4)
C(22)	O(5)	C(23)	C(24)	-2.1(7)	C(22)	O(5)	C(23)	C(26)	179.6(4)
C(23)	O(5)	C(22)	C(21)	1.4(6)	C(23)	O(5)	C(22)	C(25)	178.9(4)
O(1)	C(1)	C(2)	Si(1)	-5.4(6)	O(1)	C(1)	C(2)	C(3)	175.8(4)
O(1)	C(1)	C(6)	C(5)	-176.3(5)	C(2)	C(1)	C(6)	C(5)	-0.2(6)

C(6)	C(1)	C(2)	Si(1)	178.6(4)	C(6)	C(1)	C(2)	C(3)	-0.3(7)
Si(1)	C(2)	C(3)	C(4)	-178.4(4)	C(1)	C(2)	C(3)	C(4)	0.4(7)
C(2)	C(3)	C(4)	C(5)	-0.1(6)	C(3)	C(4)	C(5)	C(6)	-0.4(8)
C(4)	C(5)	C(6)	C(1)	0.5(9)	O(2)	C(7)	C(8)	Si(1)	-2.1(5)
O(2)	C(7)	C(8)	C(9)	179.2(3)	O(2)	C(7)	C(12)	C(11)	-179.7(4)
C(8)	C(7)	C(12)	C(11)	-1.8(6)	C(12)	C(7)	C(8)	Si(1)	-180.0(2)
C(12)	C(7)	C(8)	C(9)	1.2(6)	Si(1)	C(8)	C(9)	C(10)	-179.9(3)
C(7)	C(8)	C(9)	C(10)	-1.2(6)	C(8)	C(9)	C(10)	C(11)	1.6(8)
C(9)	C(10)	C(11)	C(12)	-2.1(8)	C(10)	C(11)	C(12)	C(7)	2.2(8)
O(3)	C(13)	C(14)	Si(1)	3.6(5)	O(3)	C(13)	C(14)	C(15)	178.3(3)
O(3)	C(13)	C(18)	C(17)	-179.0(3)	C(14)	C(13)	C(18)	C(17)	-2.7(5)
C(18)	C(13)	C(14)	Si(1)	-172.4(2)	C(18)	C(13)	C(14)	C(15)	2.3(5)
Si(1)	C(14)	C(15)	C(16)	173.3(3)	C(13)	C(14)	C(15)	C(16)	-1.6(5)
C(14)	C(15)	C(16)	C(17)	1.1(6)	C(15)	C(16)	C(17)	C(18)	-1.4(6)
C(16)	C(17)	C(18)	C(13)	2.2(6)	O(4)	C(20)	C(21)	C(22)	176.8(4)
O(4)	C(20)	C(24)	C(23)	-177.9(4)	C(21)	C(20)	C(24)	C(23)	-1.2(7)
C(24)	C(20)	C(21)	C(22)	0.4(6)	C(20)	C(21)	C(22)	O(5)	-0.5(7)
C(20)	C(21)	C(22)	C(25)	-177.6(4)	O(5)	C(23)	C(24)	C(20)	2.1(7)
C(26)	C(23)	C(24)	C(20)	-180.0(5)					

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
Cl(2)	O(4)[1)]	3.453(3)	Cl(3)	C(6)[1)]	3.576(6)
Cl(5)	C(4)[2)]	3.587(6)	Cl(6)	O(5)[3)]	3.362(4)
Cl(6)	C(23)[3)]	3.581(6)	O(1)	C(23)[4)]	3.518(5)
O(1)	C(24)[4)]	3.300(5)	O(1)	C(26)[4)]	3.325(6)
O(2)	C(3)[5)]	3.552(4)	O(3)	C(28)[6)]	3.318(6)
O(4)	Cl(2)[6)]	3.453(3)	O(4)	C(24)[4)]	3.568(6)
O(5)	Cl(6)[3)]	3.362(4)	C(3)	O(2)[7)]	3.552(4)
C(3)	C(21)[7)]	3.594(6)	C(4)	Cl(5)[2)]	3.587(6)
C(6)	Cl(3)[6)]	3.576(6)	C(9)	C(29)[6)]	3.539(8)
C(21)	C(3)[5)]	3.594(6)	C(23)	Cl(6)[3)]	3.581(6)
C(23)	O(1)[4)]	3.518(6)	C(24)	O(1)[4)]	3.300(5)
C(24)	O(4)[4)]	3.568(6)	C(26)	O(1)[4)]	3.325(6)
C(28)	O(3)[1)]	3.318(6)	C(29)	C(9)[1)]	3.539(8)

Symmetry Operators:

(1) -X+1/2+1,Y+1/2,-Z+1/2 (2) -X+1,-Y+1,-Z
(3) -X+1,-Y+1,-Z+1 (4) -X+2,-Y,-Z+1
(5) X+1/2,-Y+1/2,Z+1/2 (6) -X+1/2+1,Y+1/2-1,-Z+1/2
(7) X+1/2-1,-Y+1/2,Z+1/2-1

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl(1)	H(5)[1)]	3.155	Cl(1)	H(7)[2)]	3.429
Cl(1)	H(12)[3)]	3.406	Cl(1)	H(13)[1)]	3.204
Cl(1)	H(18)[4)]	3.487	Cl(1)	H(20)[4)]	3.351
Cl(2)	H(7)[5)]	3.590	Cl(2)	H(8)[5)]	3.150
Cl(2)	H(17)[3)]	3.503	Cl(3)	H(3)[3)]	3.557
Cl(3)	H(4)[3)]	3.370	Cl(3)	H(7)[2)]	3.086
Cl(4)	H(21)[6)]	3.451	Cl(4)	H(23)[6)]	3.543
Cl(5)	H(2)[7)]	3.366	Cl(5)	H(3)[8)]	3.231
Cl(5)	H(9)[3)]	3.378	Cl(5)	H(10)[9)]	3.154
Cl(5)	H(11)[9)]	3.554	O(1)	H(17)[10)]	2.758
O(1)	H(21)[10)]	2.933	O(1)	H(22)[10)]	3.128
O(1)	H(24)[11)]	3.259	O(2)	H(1)[12)]	2.788
O(2)	H(2)[12)]	3.212	O(2)	H(17)[10)]	3.362
O(3)	H(19)[5)]	3.594	O(3)	H(20)[5)]	3.320
O(3)	H(24)[11)]	2.461	O(4)	H(17)[10)]	2.887
O(4)	H(24)[11)]	3.244	C(1)	H(19)[5)]	3.514
C(1)	H(21)[10)]	2.905	C(1)	H(22)[10)]	3.576
C(1)	H(24)[11)]	3.139	C(2)	H(19)[5)]	3.154
C(2)	H(21)[10)]	3.590	C(3)	H(16)[5)]	3.079
C(3)	H(19)[5)]	2.909	C(4)	H(16)[5)]	3.173
C(4)	H(19)[5)]	3.063	C(5)	H(9)[11)]	3.341
C(5)	H(10)[11)]	2.976	C(5)	H(19)[5)]	3.429
C(6)	H(9)[11)]	3.145	C(6)	H(10)[11)]	3.119
C(6)	H(21)[10)]	3.025	C(6)	H(24)[11)]	3.087
C(7)	H(1)[12)]	3.293	C(7)	H(17)[10)]	3.293
C(7)	H(22)[10)]	3.281	C(7)	H(25)[11)]	3.096
C(8)	H(22)[10)]	3.267	C(8)	H(25)[11)]	2.905
C(9)	H(22)[10)]	3.172	C(9)	H(25)[11)]	2.737

C(10)	H(12)[13)]	3.430	C(10)	H(18)[13)]	3.532
C(10)	H(22)[10)]	3.189	C(10)	H(25)[11)]	2.822
C(11)	H(18)[13)]	3.596	C(11)	H(22)[10)]	3.214
C(11)	H(25)[11)]	3.038	C(12)	H(1)[12)]	3.408
C(12)	H(15)[12)]	3.183	C(12)	H(17)[10)]	3.130
C(12)	H(22)[10)]	3.280	C(12)	H(25)[11)]	3.151
C(13)	H(2)[12)]	3.030	C(13)	H(19)[5)]	3.585
C(13)	H(20)[5)]	2.930	C(13)	H(24)[11)]	3.497
C(14)	H(2)[12)]	2.962	C(14)	H(20)[5)]	3.394
C(15)	H(2)[12)]	2.947	C(15)	H(3)[3)]	3.442
C(15)	H(4)[3)]	3.218	C(16)	H(2)[12)]	3.076
C(16)	H(3)[3)]	3.381	C(16)	H(3)[12)]	3.422
C(16)	H(4)[3)]	3.483	C(16)	H(21)[5)]	3.400
C(17)	H(2)[12)]	3.176	C(17)	H(6)[14)]	3.409
C(17)	H(20)[5)]	3.383	C(18)	H(2)[12)]	3.165
C(18)	H(6)[14)]	3.238	C(18)	H(20)[5)]	2.900
C(19)	H(8)[5)]	3.087	C(21)	H(1)[12)]	3.150
C(25)	H(24)[4)]	3.567	C(26)	H(10)[12)]	3.570
C(28)	H(4)[3)]	3.505	B(1)	H(17)[10)]	3.221
B(1)	H(24)[11)]	3.145	H(1)	O(2)[5)]	2.788
H(1)	C(7)[5)]	3.293	H(1)	C(12)[5)]	3.408
H(1)	C(21)[5)]	3.150	H(1)	H(8)[5)]	3.112
H(1)	H(16)[5)]	2.711	H(1)	H(19)[5)]	3.216
H(2)	Cl(5)[7)]	3.366	H(2)	O(2)[5)]	3.212
H(2)	C(13)[5)]	3.030	H(2)	C(14)[5)]	2.962
H(2)	C(15)[5)]	2.947	H(2)	C(16)[5)]	3.076
H(2)	C(17)[5)]	3.176	H(2)	C(18)[5)]	3.165
H(2)	H(9)[5)]	3.417	H(2)	H(16)[5)]	2.895
H(2)	H(19)[5)]	3.451	H(3)	Cl(3)[11)]	3.557
H(3)	Cl(5)[15)]	3.231	H(3)	C(15)[11)]	3.442
H(3)	C(16)[11)]	3.381	H(3)	C(16)[5)]	3.422
H(3)	H(9)[11)]	2.885	H(3)	H(10)[11)]	2.787
H(3)	H(10)[5)]	3.369	H(4)	Cl(3)[11)]	3.370
H(4)	C(15)[11)]	3.218	H(4)	C(16)[11)]	3.483
H(4)	C(28)[11)]	3.505	H(4)	H(9)[11)]	2.472
H(4)	H(10)[11)]	3.027	H(4)	H(14)[11)]	3.117
H(4)	H(21)[10)]	3.108	H(4)	H(24)[11)]	3.025
H(5)	Cl(1)[1)]	3.155	H(5)	H(25)[11)]	3.188
H(6)	C(17)[13)]	3.409	H(6)	C(18)[13)]	3.238
H(6)	H(11)[13)]	2.886	H(6)	H(12)[13)]	2.520
H(6)	H(18)[13)]	3.058	H(6)	H(25)[11)]	3.295
H(7)	Cl(1)[16)]	3.429	H(7)	Cl(2)[12)]	3.590

H(7)	Cl(3)[16)]	3.086	H(7)	H(18)[13)]	3.189
H(8)	Cl(2)[12)]	3.150	H(8)	C(19)[12)]	3.087
H(8)	H(1)[12)]	3.112	H(8)	H(13)[12)]	3.007
H(8)	H(14)[12)]	3.502	H(8)	H(15)[12)]	2.389
H(8)	H(17)[10)]	3.005	H(9)	Cl(5)[11)]	3.378
H(9)	C(5)[3)]	3.341	H(9)	C(6)[3)]	3.145
H(9)	H(2)[12)]	3.417	H(9)	H(3)[3)]	2.885
H(9)	H(4)[3)]	2.472	H(10)	Cl(5)[17)]	3.154
H(10)	C(5)[3)]	2.976	H(10)	C(6)[3)]	3.119
H(10)	C(26)[5)]	3.570	H(10)	H(3)[3)]	2.787
H(10)	H(3)[12)]	3.369	H(10)	H(4)[3)]	3.027
H(10)	H(21)[5)]	2.840	H(11)	Cl(5)[17)]	3.554
H(11)	H(6)[14)]	2.886	H(12)	Cl(1)[11)]	3.406
H(12)	C(10)[14)]	3.430	H(12)	H(6)[14)]	2.520
H(12)	H(20)[5)]	3.122	H(13)	Cl(1)[1)]	3.204
H(13)	H(8)[5)]	3.007	H(14)	H(4)[3)]	3.117
H(14)	H(8)[5)]	3.502	H(15)	C(12)[5)]	3.183
H(15)	H(8)[5)]	2.389	H(16)	C(3)[12)]	3.079
H(16)	C(4)[12)]	3.173	H(16)	H(1)[12)]	2.711
H(16)	H(2)[12)]	2.895	H(17)	Cl(2)[11)]	3.503
H(17)	O(1)[10)]	2.758	H(17)	O(2)[10)]	3.362
H(17)	O(4)[10)]	2.887	H(17)	C(7)[10)]	3.293
H(17)	C(12)[10)]	3.130	H(17)	B(1)[10)]	3.221
H(17)	H(8)[10)]	3.005	H(18)	Cl(1)[4)]	3.487
H(18)	C(10)[14)]	3.532	H(18)	C(11)[14)]	3.596
H(18)	H(6)[14)]	3.058	H(18)	H(7)[14)]	3.189
H(19)	O(3)[12)]	3.594	H(19)	C(1)[12)]	3.514
H(19)	C(2)[12)]	3.154	H(19)	C(3)[12)]	2.909
H(19)	C(4)[12)]	3.063	H(19)	C(5)[12)]	3.429
H(19)	C(13)[12)]	3.585	H(19)	H(1)[12)]	3.216
H(19)	H(2)[12)]	3.451	H(19)	H(24)[4)]	3.136
H(20)	Cl(1)[4)]	3.351	H(20)	O(3)[12)]	3.320
H(20)	C(13)[12)]	2.930	H(20)	C(14)[12)]	3.394
H(20)	C(17)[12)]	3.383	H(20)	C(18)[12)]	2.900
H(20)	H(12)[12)]	3.122	H(20)	H(24)[4)]	3.312
H(21)	Cl(4)[18)]	3.451	H(21)	O(1)[10)]	2.933
H(21)	C(1)[10)]	2.905	H(21)	C(2)[10)]	3.590
H(21)	C(6)[10)]	3.025	H(21)	C(16)[12)]	3.400
H(21)	H(4)[10)]	3.108	H(21)	H(10)[12)]	2.840
H(22)	O(1)[10)]	3.128	H(22)	C(1)[10)]	3.576
H(22)	C(7)[10)]	3.281	H(22)	C(8)[10)]	3.267
H(22)	C(9)[10)]	3.172	H(22)	C(10)[10)]	3.189

H(22)	C(11)[10)]	3.214	H(22)	C(12)[10)]	3.280
H(23)	Cl(4)[18)]	3.543	H(24)	O(1)[3)]	3.259
H(24)	O(3)[3)]	2.461	H(24)	O(4)[3)]	3.244
H(24)	C(1)[3)]	3.139	H(24)	C(6)[3)]	3.087
H(24)	C(13)[3)]	3.497	H(24)	C(25)[4)]	3.567
H(24)	B(1)[3)]	3.145	H(24)	H(4)[3)]	3.025
H(24)	H(19)[4)]	3.136	H(24)	H(20)[4)]	3.312
H(25)	C(7)[3)]	3.096	H(25)	C(8)[3)]	2.905
H(25)	C(9)[3)]	2.737	H(25)	C(10)[3)]	2.822
H(25)	C(11)[3)]	3.038	H(25)	C(12)[3)]	3.151
H(25)	H(5)[3)]	3.188	H(25)	H(6)[3)]	3.295

Symmetry Operators:

(1)	-X+2,-Y+1,-Z	(2)	-X+1/2+2,Y+1/2,-Z+1/2
(3)	-X+1/2+1,Y+1/2,-Z+1/2	(4)	-X+2,-Y+1,-Z+1
(5)	X+1/2-1,-Y+1/2,Z+1/2-1	(6)	X-1,Y+1,Z-1
(7)	-X+1,-Y+1,-Z	(8)	X,Y+1,Z
(9)	X+1/2-1,-Y+1/2+1,Z+1/2-1	(10)	-X+2,-Y,-Z+1
(11)	-X+1/2+1,Y+1/2-1,-Z+1/2	(12)	X+1/2,-Y+1/2,Z+1/2
(13)	X+1/2,-Y+1/2,Z+1/2-1	(14)	X+1/2-1,-Y+1/2,Z+1/2
(15)	X,Y-1,Z	(16)	-X+1/2+2,Y+1/2-1,-Z+1/2
(17)	X+1/2,-Y+1/2+1,Z+1/2	(18)	X+1,Y-1,Z+1