# SYNTHESIS, BIOLOGICAL EVALUATION, AND RADIOIODINATION OF HALOGENATED *CLOSO*-CARBORANYL THYMIDINE ANALOGUES

*Rohit Tiwari[1], Antonio Toppino[1,2], Hitesh K. Agarwal[1], Tianyao Huo[3], Youngjoo Byun,[1,4] Judith Gallucci[5], Sherifa Hasabelnaby[1,6], Ahmed Khalil[1,7], Ayman Goudah[1,8], Robert A. Baiocchi[9], Michael V. Darby[1], Rolf. F. Barth[3], and Werner Tjarks[1]*

Division of Medicinal Chemistry & Pharmacognosy, 500 W. 12th Ave, The Ohio State University, Columbus, OH 43210; [2]Dipartimento di Chimica Generale e Chimica Organica, Università degli Studi di Torino, Torino, Italy; [3]Department of Pathology, The Ohio State University, Columbus, Ohio; [4] College of Pharmacy, Korea University, Chungnam, South Korea; [5]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [6]Division of Pharmaceutical Organic Chemistry, College of Pharmacy, Helwan University, Cairo, Egypt; [7]Chemistry Department, Faculty of Science, Zagazig University, Zagazig, Egypt, [8]Division of Pharmacology, College of Veterinary Medicine, Cairo University, Giza, Egypt, and [9]Division of Hematology and Oncology, Department of Internal Medicine, The Ohio State University, Columbus, Ohio.

*Corresponding author: Werner Tjarks, The Ohio State University College of Pharmacy, 500 w. 12th Ave, Columbus, OH 43210. E-mail: tjarks.1@osu.edu

**Supporting Information:** **Page No.**

**1) Addition general experimental information**

Silica gel 60 (0.063-0.200 mm) from Merck was used for gravity column chromatography whereas silica gel 60 (0.015-0.049 mm) from EM science was used for flash column chromatography. Reagent-grade solvents were used for column chromatography. Pre-coated glass-backed TLC plates with silica gel 60 F254 (0.25-mm layer thickness) from Dynamic Adsorbents (Norcross, GA) were used for TLC studies. General compound visualization for TLC was achieved by UV light. Carborane-containing compounds were selectively visualized by spraying the plate with a 0.06% $PdCl_2$/1% HCl solution and heating at 120 °C, which caused the slow (15-45 s) formation of a gray spot due to the reduction of Pd (II) to Pd(0).

Anhydrous solvents, such as DMF and $CH_2Cl_2$, were purchased from Acros Organics (Morris Plains, NJ), EMD (Gibbstown, NJ), or Sigma Aldrich (Milwaukee, WI). Other solvents were purchased from standard commercial suppliers. THF was distilled from sodium and benzophenone indicator under argon. Unless specified otherwise, all reactions were carried out under an argon atmosphere.

$Na^{125}I$ was obtained from PerkinElmer (Waltham, MA) as an alkaline (NaOH) solution (pH 8-11) with a specific activity of *c.a.* 17 Ci (629 GBq)/mg. Herrmann's catalyst (*trans*-di-*m*-acetatobis[2-(di-*o*-tolylphosphino)benzyl]dipalladium) (II) was purchased from Alfa Aesar Ltd. (Ward Hill, MA), BPA (98% pure) was purchased from Rysor Science Inc (Raleigh, NC). *o*-Carborane was purchased from Katchem, Ltd, Prague, Czech Republic. Decaborane was obtained from Boron Biologicals, Inc. Raleigh, NC. Decaborane is a highly toxic and explosive compound. It is advisable to read the MSDS carefully before usage. All other chemicals were purchased from commercial suppliers.

For all non-radioactive materials, (semi)-preparative HPLC purification was performed either with a Gemini 5μ C18 column (21.20 mm × 250 mm, 5 μm particle size), supplied by Phenomenex Inc. CA, USA or with a Supelco Discovery® HS C18 column (10 mm × 250 mm, 10 μm particle size) supplied by Sigma Aldrich (MO, USA) on a Hitachi HPLC system (L-2130) with a Windows-based data acquisition and Hitachi Diode array detector (L-2455). A LiChrocart® 250-4 HPLC cartridge packed

with LiChrospher® RP-18 stationary phase (4 mm × 250 mm, 5 μm particle size) supplied by EM Science, NJ, USA was used for analytical reversed-phase chromatography on a Hitachi HPLC system (L-2130) with a Windows-based data acquisition and Hitachi diode array detector (L-2455).

For all radioactive materials, semi-preparative HPLC purification was performed with a Supelco Discovery® HS C18 column (10 mm × 250 mm, 10 μm particle size). A Beckman Ultrasphere® column (4.6 mm × 250 mm, 5 μm particle size) supplied by Beckmann Coulter Inc., CA, USA, was used for analytical reversed-phase chromatography. A Beckmann HPLC system with a Windows-based data acquisition and Beckman System Gold UV detector module (166) and Radiomatic FLO-ONE detector series A-500 was used for data analysis.

**2) $^{13}$C NMR chemical shifts of the compounds described in the main article.**

**3-[5-(9-Iodo-*o*-carboran-1-yl)pentyl]thymidine** and **3-[5-(12-Iodo-*o*-carboran-1-yl)pentyl]thymidine (4a/4b, [N5-I]) [Strategy 1]**

$^{13}$C NMR ($CD_3COCD_3$) δ 13.4, 26.8, 27.7, 37.7, 37.9, 41.1, 41.3, 62.9, 64.4, 72.2, 78.3, 86.5, 88.7, 109.9, 135.6. 151.7, 163.8.

**3-[5-(8,9,10,12-Tetra-iodo-*o*-carboran-1-yl)pentyl]thymidine (5, N5-$I_4$)**

$^{13}$C NMR ($CD_3COCD_3$) δ.13.3, 25.7, 26.6, 27.5, 37.2, 41.0, 41.2, 63.1, 63.7, 72.1, 77.7, 86.4, 88.6, 109.8, 135.5, 151.6, 163.7.

**9-Iodo-*o*-carborane** (**7**)

$^{13}$C NMR ($CD_3COCD_3$) δ 53.3, 57.9.

**1-(*tert*-Butyldimethylsilyl)-9-iodo-*o*-carborane (8a) and 1-(*tert*-Butyldimethylsilyl)-12-iodo-*o*-carborane** (**8b**)

$^{13}$C-NMR ($CD_3COCD_3$) δ -4.43, 20.0, 20.1, 27.2, 27.2, 58.7, 60.6, 61.9, 63.0.

**1-(*tert*-Butyldimethylsilyl)-9-iodo-*o*-carborane (8a)**

$^{13}$C-NMR ($CD_3COCD_3$) δ -4.4, 20.1, 27.2, 58.70.

**1-(*tert*-Butyldimethylsilyl)-12-iodo-*o*-carborane (8b)**

$^{13}$C-NMR ($CD_3COCD_3$) δ -4.4, 20.0, 27.2, 61.9, 63.0.

**1-(*tert*-Butyldimethylsilyl)-2-[5-(tert-butyldimethylsilyloxy)pentyl]-9-iodo-*o*-carborane** and **1-(*tert*-Butyldimethylsilyl)-2-[5-(*tert*-butyldimethyl silyloxy)pentyl]-12-iodo-*o*-carborane** (**9a/9b**)

$^{13}$C NMR ($CD_3COCD_3$) δ -5.1, -2.2, 18.9, 21.0, 21.1, 26.1, 26.2, 26.4 (x2), 27.9, 30.8, 31.0, 33.0, 38.4(x2), 63.2, 63.3, 78.9, 79.5, 83.7.

**5-(9-Iodo-*o*-carboran-1-yl)pentan-1-ol** and **5-(12-Iodo-*o*-carboran-1-yl)pentan-1-ol (10a/10b)**

$^{13}$C-NMR ($CD_3COCD_3$) δ 26.0, 33.1, 37.9, 38.1, 59.6, 62.0, 64.4, 73.9, 78.3.

**5-(9-Iodo-*o*-carboran-1-yl)pentyl 4-Methylbenzenesulfonate** and **5-(12-Iodo-*o*-carboran-1-yl)pentyl 4-Methyl benzenesulfonate (11a/11b)**

$^{13}$C-NMR ($CD_3COCD_3$) δ 21.6, 25.3, 28.9, 29.2, 29.3, 37.6, 37.7, 59.5, 64.3, 71.1, 73.6, 78.0, 128.6, 130.9, 134.3, 145.8.

**3-[5-(9-Bromo-*o*-carboran-1-yl)pentyl]thymidine** and **3-[5-(12-Bromo-*o*-carboran-1-yl) pentyl]thymidine (12a/12b - N5-Br)**

$^{13}$C NMR ($CD_3COCD_3$) δ 13.4, 26.8, 27.8, 36.8, 37.8, 41.1, 41.2, 55.6, 62.7, 62.8, 72.1, 86.4, 88.7, 109.9, 135.6, 151.7, 163.8.

**3) Calculation of molecular surface area and volume of 3 (N5) and 4a/4b (N5-I)**

The structure of **N5** (**3**) was fully optimized at B3LYP/6-31G** using Gaussian® 03W (Gaussian Inc.). The structures of **N5-9I** (**4a**) and **N5-12I** (**4b**) were built using the optimized geometry of **N5** by replacement of the B9-H and B12-H with B9-I and B12-I, respectively, using HyperChem 7.51 (Hypercube Inc., Gainsville, FL). The geometries of the newly constructed B-I bonds of **4a** and **4b** were then selectively optimized using the steepest descent algorithm implemented in HyperChem until either a RMS gradient of 0.001 kcal/Å mol or a maximum cycle of 1020 was reached. Molecular surface areas and molecular volumes of **3**, **4a**, and **4b** were calculated by using compute tab and selecting the QSAR properties option implemented in HyperChem. Figure S1 was generated with PyMOL 1.3 (DeLano Scientific, LLC., Palo Alto, CA).

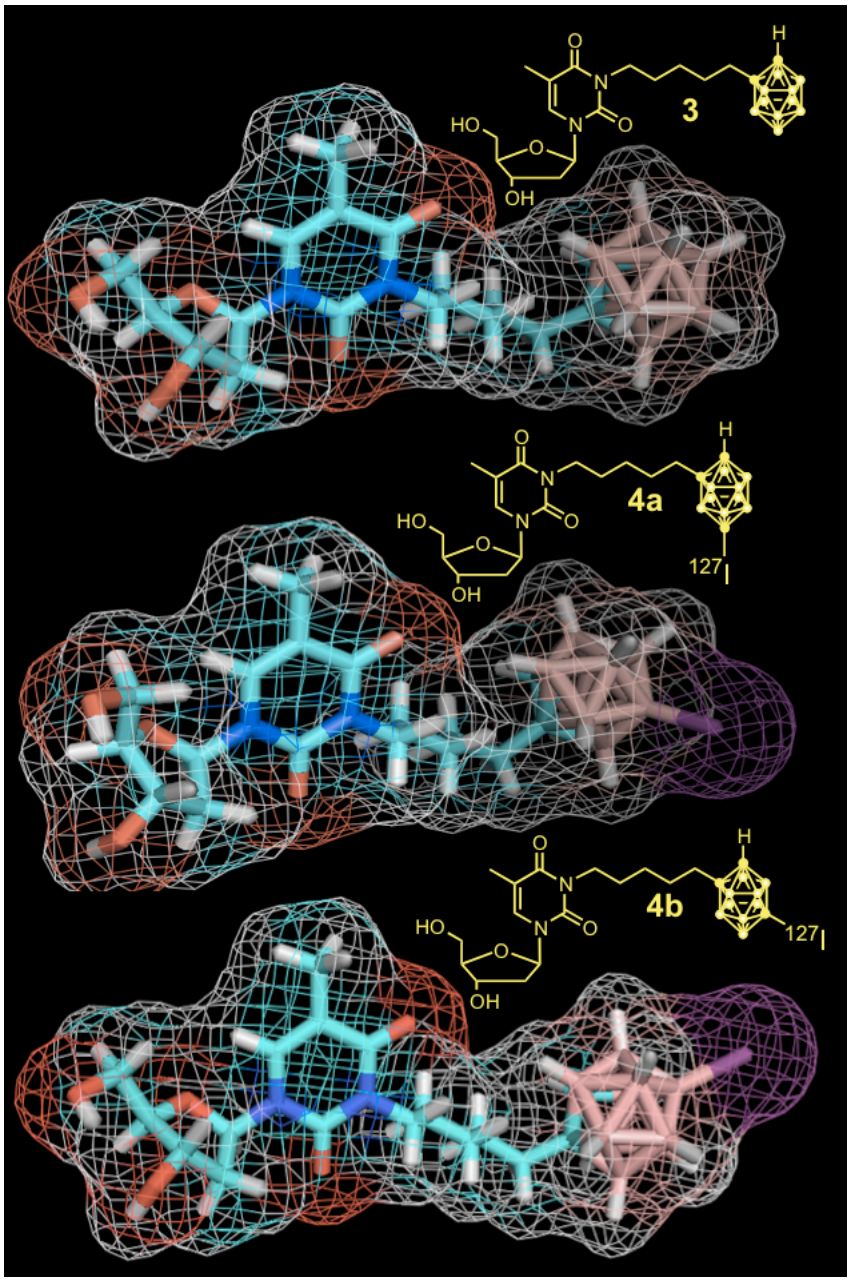
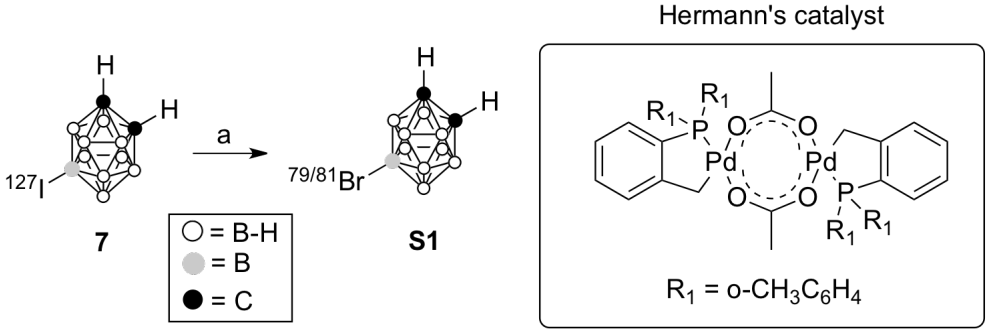


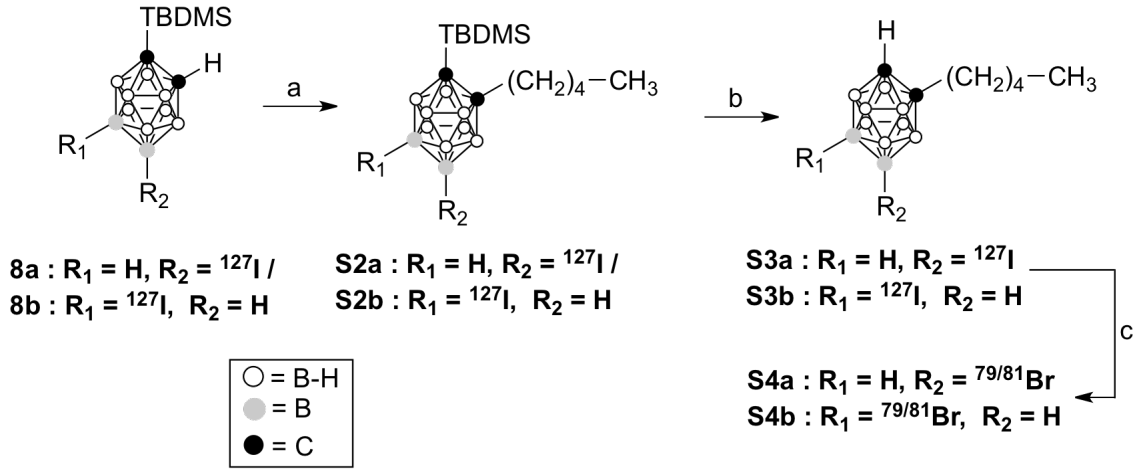

**Figure S1**: The 3D structures and molecular surfaces of **3**, **4a**, and **4b**

**4) Pilot halogen exchange reactions.**

**Results and Discussion.** Halogen/isotope exchange at the B-halo-*closo*-*o*-carboranes, which are linked to complex biomolecule such as thymidine, have not been explored in the past. Therefore, it was necessary to optimize the reaction conditions with surrogate B-iodo-*o*-carboranyl compounds before the final $^{127}I$ to $^{125}I$ isotope exchange reaction with **4a**/**4b** (main article, Scheme 3, reaction b). Of interest to us was the efficacy of the catalyzed halogen/isotope exchange[1-4] at B-iodo-*o*-carborane alone as compared to B-iodo-*o*-carborane substituted with a C-pentyl group and B-iodo-*o*-carborane in the presence of *n*-butanol or 3-butylthymidine.[5] Compound **7 (**Scheme S1) and 9-iodo-1-pentyl-*o*-carborane (**S3a**/**S3b**, Scheme S2**)** were subjected to halogen exchange using 10 equivalents of NaBr in presence of Herrmann's catalyst (10-50 mol %) in DMF at 110 ºC for 1 h. Complete exchange (100%) of iodine by bromine was observed in both reactions. In the case of **7**, complete halogen exchange was also observed when *n*-butanol or 3-butylthymidine were added to the reaction. Pilot reactions in the presence of *n*-butanol and 3-butylthymidine were chosen to simulate the potential interference of either the presence of hydroxyl functionalities or an entire N3-substituted thymidine scaffold on the outcome of the halogen/isotope exchange. Compounds **S3a**/**S3b** were synthesized in 66% yield by reacting **S2a**/**S2b** with *n*-BuLi, and subsequently, iodopentane followed by removal of the TBDMS protective group with TBAF (**Scheme S2**).




Scheme S1**: Reagents and condition:** NaBr, Herrmann´s catalyst, DMF, 110 º C, 1 h.




Scheme S2: **Reagents and condition:** a) *n*-BuLi, 1-iodopentane, THF, 66°C, 18 h; b) TBAF, THF, -78°C to 0°C , 30 min.

**Experimental Procedures** (general experimental procedures are described in the main article).

**9-Bromo-*o*-carborane (S1**). To a solution of **7** [main article] **(**100 mg, 0.37 mmol) in 3 mL dichloromethane was added a solution of NaBr (381 mg, 3.7 mmol) in 5 mL of water. The solvents were evaporated *in vacuo* and a solution of Herrmann's Catalyst (17 mg, 5 mol %) in 1 mL anhydrous DMF was added to the anhydrous residue. The reaction mixture was then stirred at 110 °C for 1 h. Following evaporated, the residue was added to water, and extracted with dichloromethane. The organic phase was dried over anhydrous $MgSO_4$, concentrated *in vacuo*, and the residue purified by silica gel column chromatography to afford **S1** (40 mg, 49 %). $R_f$ 0.38 (hexanes: ethyl acetate, 10:4). $^1$H-NMR ($CDCl_3$) δ 1.3-3.2 (m, 9H, BH), 3.64 (s, 1H, H-$C_{carborane}$). $^{13}$C NMR ($CD_3COCD_3$) δ 46.8, 53.2. $^{11}$B {$^1$H} NMR ($CDCl_3$) δ -13.7 (m, 6B, B3, B4, B5, B6, B7, B11), -8.00 (s, 2B, B8, B10), -1.7 (s, 1B, B12), -0.6 (s, 1B, B9-Br). $^{11}$B NMR ($CDCl_3$) -13.8 (m, 6B), -7.9 (d, 2B, $J$ = 154.1 Hz), -1.8 (d, 1B, $J$ = 152.1 Hz), -0.4 (s, 1B). MS (HR-EI) $C_2B_{10}H_{11}Br$ $(M)^+$ calcd 222.1047, found 222.1048.

**1-(*tert*-Butyldimethylsilyl)-9-iodo-2-pentyl-*o*-carborane** and **1-(*tert*-Butyldimethylsilyl)-12-iodo-2-pentyl-*o*-carborane (S2a/S2b)**. Compounds **S2a/S2b** were synthesized and purified in 55% yield (3.0 g) from 4.70 g (12.2 mmol) of **8a**/**8b** (main article) by adapting the procedure described for the synthesis

of **9a/9b** (main article) using 2.56 mL (19.6 mmol) of 1-iodopentane as a starting material. $R_f$ 0.69 (hexanes: ethyl acetate, 20:1). $^1$H NMR ($CD_3COCD_3$) δ 0.39 (s, 6H, -Si($CH_3$)$_2$ ), 0.43 (s, 6H, -Si($CH_3$)$_2$), 0.89 (m, 6H, -$CH_3$), 1.09 (s, 9H, -C($CH_3$)$_3$), 1.12 (s, 9H, -C($CH_3$)$_3$), 1.29-1.62 (m, 12H, -$CH_2$-$CH_2$-$CH_2$), 1.3-3.4 (m, 9H, BH), 2.20 (m, 2H, -$CH_2$-$C_{carborane}$), 2.32 (m, 2H, -$CH_2$-$C_{carborane}$). ). $^{13}$C NMR ($CD_3COCD_3$) δ -3.7, -2.4, 14.1, 14.2, 20.9, 21.0, 22.8, 27.7, 30.6, 30.8, 31.7, 38.1, 38.2, 71.7, 78.7, 79.4, 83.7. $^{11}$B{$^1$H} NMR ($CDCl_3$) δ -16.7 (s, 1B, B12-I/ B9-I), -15.0 (s, 1B, B9-I/ B12-I), -10.3 (m, 12 B), -6.0 (d,4B, B8, B10), -3.1(s, 1B, B12-H/B9-H), 1.5 (s,1B, B9-H/B12-H).$^{11}$B NMR ($CDCl_3$) δ. -16.8 (s, 1B), -15.0 (s, 1B), -10.4 (m, 8B), -5.9 (d, 4B, *J* = 141.1 Hz), -3.2 (d, 2B, *J* = 175.1Hz), 1.3 (d, 2B, *J* = 147.7 Hz). MS (HR-EI) $C_{13}H_{35}B_{10}ISi$ $(M)^+$ calcd 454.2556, found 454.2555.

**9-Iodo-1-pentyl-*o*-carborane** and **12-Iodo-1-pentyl-*o*-carborane (S3a/S3b)**. A stirred solution of **S2a**/**S2b** (1.61g, 3.54 mmol) in anhydrous THF (20 mL) was cooled to -78 ºC and a 1.0 M solution of TBAF in THF (4.25 mL, 4.25 mmol) was added dropwise. The mixture was allowed to stir for 30 min at 0 ºC followed by addition of 10 mL of water. The mixture was extracted 3 x 30 mL of diethyl ether, the combined organic layers were dried over anhydrous $MgSO_4$, and evaporated *in vacuo*. The residue was purified by silica gel column chromatography to furnish **S3a/S3b** (800 mg, 66 %) as a brownish oil. $R_f$ 0.52 (hexanes: ethyl acetate, 9:1). $^1$H NMR ($CD_3COCD_3$) δ 0.89 (m, 6H, -$CH_3$), 0.9-3.4 (m, 9H, BH), 1.29 (m, 8H, -$CH_2$-$CH_2$), 1.54 (m, 4H, -$CH_2$), 2.24 (m, 2H, -$CH_2$-$C_{carborane}$), 2.37 (m, 2H, $CH_2$-$C_{carborane}$), 4.86 (br, 1H, H-$C_{carborane}$), 5.06 (br, 1H, H-$C_{carborane}$). $^{13}$C NMR ($CD_3COCD_3$) δ 14.2, 22.9, 31.7, 37.9, 38.1, 59.6, 64.4, 73.9, 78.4. $^{11}$B{$^1$H}NMR ($CD_3COCD_3$) δ -17.9 (s, 1B, B12-I/B9-I), -16.3 (s,1B, B9-I/B12-I), -12.2—10.44 (m, 12B, B3, B4, B5, B6, B7, B11), -7.2 (d, 4B, B8, B10), -4.1 (s, 1B, B12-H/B9-H), -0.7 (s,1B, B9-H/B12-H) $^{11}$B NMR ($CD_3COCD_3$) δ -17.9, -16.3, -11.4 (m, 12B), -7.3 (d, 4B, *J* = 153.2 Hz) , -4.1 (d, 2B, *J* = 151.5 Hz), -0.8 (d, 2B, *J* = 149.7 Hz). MS (HR-EI) $C_7H_{21}B_{10}I$ $(M)^+$ calcd 340.1692, found 340.1689.

**9-Bromo-1-pentyl-*o*-carborane** and **12-Bromo-1-pentyl-*o*-carborane (S4a/S4b)**. Compounds **S4a/S4b** were synthesized and purified in 63% yield (54 mg) from 100 mg (0.29 mmol) of **S3a**/**S3b** by adapting the procedure described for the synthesis of **S1**. $R_f$ 0.52 (hexanes: ethyl acetate, 9:1). $^1$H NMR

($CD_3COCD_3$) δ 0.88 (m, 6H, $-CH_3$), 1.28 (m, 8H, $-CH_2-CH_2$), 1.56 (m, 4H, $-CH_2$), 2.35 (m, 4H,$-CH_2-C_{carborane}$), 4.83 (s, 2H, $H-C_{carborane}$). $^{13}C$ NMR ($CD_3COCD_3$) δ 14.7, 23.4, 32.3, 37.5, 38.6, 6.2, 63.3. $^{11}B\{^1H\}$ NMR ($CD_3COCD_3$) δ -11.8 (m, 12B, B3, B4, B5, B6, B7, B11), -8.1 (s, 2B, B8, B10), -4.9 (B12-H/B9-H), -1.4 and -0.4 (m, 4B, B12-Br/B9-Br and B9-H/B12-H); $^{11}B$ NMR ($CD_3COCD_3$) δ -12.2 (m, 12B), -8.1 (d, 1H, $J$ = 149.5Hz), -4.9 (m, 1B), -0.7 (m, 4B); MS (HR-EI) $C_7H_{21}B_{10}{}^{81}Br$ $(M)^+$ calcd 296.1767, found 293.1737.

**5) Radio TLC analysis of the isotope exchange reaction of 4a/4b with $Na^{125}I$**

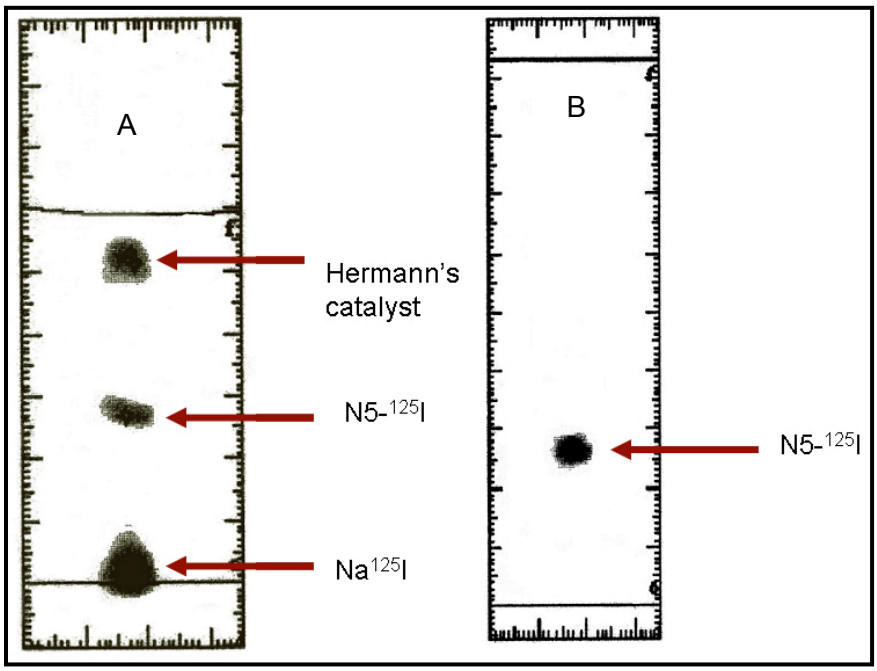



**Figure S2**: Radio TLC analysis of the isotope exchange reaction of **4a/4b** with $Na^{125}I$ in presence of Herrmann´s catalyst: A) Radio-TLC of the crude reaction mixture indicating that three $^{125}I$ containing species are present. B) Radio TLC of pure N5-$^{125}I$ (**13a/13b**) RadioTLC was visualized using AMBIS Imaging Hardware/Software (AMBIS Image Acquisition and Analysis, Version 4.0; AMBIS, San Diego, CA). $R_f$: 0.28 (dichloromethane: methanol, 10:1). See main article for general TLC conditions.

**6) Preliminary HPLC studies for the separation of 3CTAs substituted with different halogens**

**<u>Retention time for N5-I: 45.1 min; Retention time for N5-Br: 44.0 min</u>**

**N5-I** and **N5-Br** were analyzed using a Gemini 5µ C18 110A Column (250 mm x 4.6 mm) (Phenomenex Inc. CA) using a gradient solvent system on a Hitachi HPLC system (L-2130) with a Windows-based data acquisition and Hitachi Diode array detector (L-2455) at constant flow rate of 1 ml/min.

Table 1. HPLC method used for the analysis of the compounds.

| Time (minutes) | Water Concentration A (%) | Acetonitrile Concentration B (%) | Flow rate (mL/min) |
|---|---|---|---|
| 0.00 | 100.0 | 0.0 | 1.0 |
| 49.0 | 0.0 | 100.0 | 1.0 |
| 50.0 | 100.0 | 0.0 | 1.0 |
| 60.0 | 100.0 | 0.0 | 1.0 |

**7) Detailed crystal structure data for 8a and 8b**

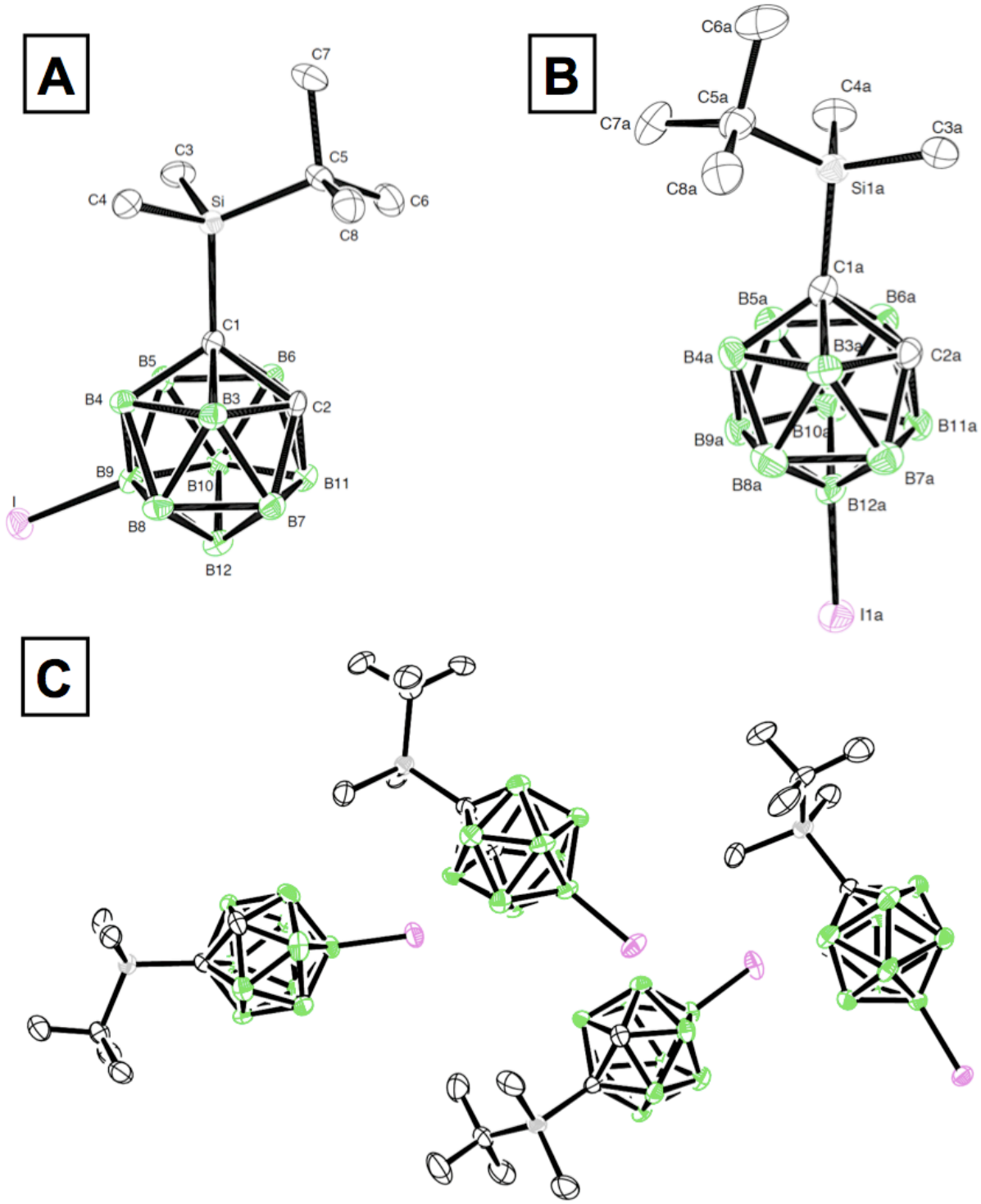



**Figure S2**: Crystal structure of **8a** (**A**), **8b** (**B**), and the four rotational isomers of **8b** (**C**) in the asymmetric unit. The Ortep plots were drawn with 50% probability displacement ellipsoids. The hydrogen atoms are omitted for clarity.

**X-ray crystallographic analysis of 8a.**

The data collection crystal was a clear, colorless rectangular plate. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated a monoclinic crystal system. All work was done at 150 K using an Oxford Cryosystems Cryostream Cooler. The data collection strategy was set up to measure a quadrant of reciprocal space with a redundancy factor of 4.7, which means that 90% of these reflections were measured at least 4.7 times. Phi and omega scans with a frame width of 1.0˚ were used. Data integration was carried out with Denzo,[6] and an absorption correction and merging of the data was done with Sortav.[7, 8] Merging the data and averaging the symmetry equivalent reflections (for the Laue group m) resulted in an Rint value of 0.040. The structure was solved in Cc by the direct methods procedure in SHELXS-97.[9] Full-matrix least-squares refinements based on $F^2$ were performed in SHELXL-97(4), as incorporated in the WinGX package.[10]

For each methyl group, the hydrogen atoms were added at calculated positions using a riding model with U(H) = 1.5*Ueq (bonded carbon atom). The torsion angle, which defines the orientation of the methyl group about the C-C or Si-C bond, was refined. The hydrogen atoms in the cluster were refined isotropically.

The final refinement cycle was based on 4013 intensities and 226variables and resulted in agreement factors of R1(F) = 0.032 and wR2($F^2$) = 0.044. For the subset of data with I > 2*sigma(I), the R1(F) value is 0.024 for 3573 reflections. The final difference electron density map contains maximum and minimum peak heights of 0.62 and -0.38 e/Å$^3$.Neutral atom scattering factors were used and include terms for anomalous dispersion.[11]

**X-ray crystallographic analysis of 8b.**

The data collection crystal was a colorless rod. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated an orthorhombic crystal system. All work was done at 150 K using an Oxford Cryosystems Cryostream Cooler. The data collection strategy was set up to measure a quadrant of reciprocal space with a redundancy factor of 4.4, which means that 90% of these reflections

were measured at least 4.4 times. Phi and omega scans with a frame width of 1.0˚ were used. Data integration was done with Denzo,[6] and an absorption correction and merging of the data was done with Sortav.[7, 8] Merging the data and averaging the symmetry equivalent reflections (for the Laue group mm2) resulted in an Rint value of 0.064. The structure was solved in the non-centrosymmetric space group $Pca2_1$by the direct methods procedure in SHELXS-97.[9] There are four independent molecules in the asymmetric unit (Z'=4) and these are labeled as A, B, C and D. Full-matrix least-squares refinements based on $F^2$ were performed in SHELXL-97,[9] as incorporated in the WinGX package.[10]

The location of the C2 atom in each of the four molecules was determined as follows. Initially all five atoms in the cluster which are bonded to atom C1 were treated as boron atoms and refined isotropically. The boron atom with the smallest Uiso value also has the shortest bond length with atom C1 in each molecule. These boron atoms were then relabeled as C2 atoms.

The four molecules are slightly different rotamers, as seen in the values of the torsion angle for C5-Si-C1-C2: -131.8(2)° for molecule A, -140.6(2)° for molecule B, 138.5(2)° for molecule C, and 142.1(2)° for molecule D. Molecule D is involved in an I···I interaction of 3.7032(3) Å with molecule C [I(1D)···I(1C)] and in a C-H···I interaction of 3.17(3) Å (H···I distance) with molecule B [I(1D)···H(2B)-C(2B)]. Molecule A is not involved in any intermolecular interactions.

For each methyl group, the hydrogen atoms were added at calculated positions using a riding model with U(H) = 1.5*Ueq (bonded carbon atom). The torsion angle, which defines the orientation of the methyl group about the C-C or Si-C bond, was refined. The remaining hydrogen atoms in each cluster were refined isotropically. The final refinement cycle was based on 16557 intensities, 1 restraint and 901 variables and resulted in agreement factors of R1(F) = 0.054 and $wR2(F^2)$ = 0.049. For the subset of data with I > 2*sigma(I), the R1(F) value is 0.030 for 13244 reflections. The final difference electron density map contains maximum and minimum peak heights of 0.54 and -0.51 e/$Å^3$.Neutral atom scattering factors were used and include terms for anomalous dispersion.[11]

Table 1. Crystallographic details for **8a**

| | |
|---|---|
| Formula | C8 H25 B10 I Si |
| Formula weight | 384.37 |
| Temperature | 150(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | monoclinic |
| Space group | Cc |
| Unit cell dimensions | a = 6.8264(1) Å |
| | b = 20.6488(3) Å |
| | c = 12.5390(2) Å |
| | β= 90.346(1)° |
| Volume | 1767.43(5) $Å^3$ |
| Z | 4 |
| Density (calculated) | 1.444 $Mg/m^3$ |
| Absorption coefficient | 1.859 $mm^{-1}$ |
| F(000) | 760 |
| Crystal size | 0.04 x 0.12 x 0.38 $mm^3$ |
| Theta range for data collection | 2.56 to 27.48° |
| Index ranges | -8<=h<=8, 0<=k<=26, -16<=l<=16 |
| Reflections collected | 17121 |
| Independent reflections | 4013 [R(int) = 0.040] |
| Completeness to theta = 27.48° | 99.9 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4013 / 2 / 226 |
| Goodness-of-fit on $F^2$ | 0.904 |
| Final R indices [I>2sigma(I)] | R1 = 0.0238, wR2 = 0.0421 |
| R indices (all data) | R1 = 0.0316, wR2 = 0.0440 |
| Absolute structure parameter | -0.050(13) |
| Largest diff. peak and hole | 0.616 and -0.378 e/$Å^3$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **8a**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 2766(4) | 3113(1) | 8003(2) | 16(1) |
| C(2) | 1911(4) | 2945(1) | 9212(2) | 16(1) |
| C(3) | 5697(5) | 4036(2) | 6996(3) | 26(1) |
| C(4) | 1379(5) | 4097(2) | 6358(2) | 24(1) |
| C(5) | 2691(4) | 4630(1) | 8549(2) | 20(1) |
| C(6) | 3921(6) | 4529(2) | 9563(3) | 29(1) |
| C(7) | 3314(5) | 5281(2) | 8047(3) | 27(1) |
| C(8) | 508(4) | 4681(1) | 8818(2) | 25(1) |
| B(3) | 372(5) | 2843(2) | 8153(3) | 19(1) |
| B(4) | 1906(4) | 2535(2) | 7135(2) | 17(1) |
| B(5) | 4352(4) | 2506(2) | 7638(2) | 17(1) |
| B(6) | 4348(5) | 2802(2) | 8968(2) | 18(1) |
| B(7) | 432(5) | 2286(2) | 9235(3) | 20(1) |
| B(8) | 420(5) | 1998(2) | 7905(3) | 20(1) |
| B(9) | 2906(4) | 1797(2) | 7599(2) | 19(1) |
| B(10) | 4421(4) | 1951(2) | 8728(2) | 19(1) |
| B(11) | 2871(5) | 2261(2) | 9739(2) | 21(1) |
| B(12) | 1999(5) | 1632(2) | 8895(3) | 21(1) |
| I | 3549(1) | 1042(1) | 6434(1) | 26(1) |
| Si | 3134(1) | 3991(1) | 7488(1) | 16(1) |

Table 3. Bond lengths [Å] and angles [°] for **8a**.

| | |
|---|---|
| C(1)-C(2) | 1.664(4) |
| C(1)-B(4) | 1.716(4) |
| C(1)-B(5) | 1.720(4) |
| C(1)-B(3) | 1.738(4) |
| C(1)-B(6) | 1.741(4) |
| C(1)-Si | 1.941(3) |
| C(2)-B(11) | 1.690(4) |
| C(2)-B(7) | 1.694(4) |
| C(2)-B(3) | 1.701(5) |
| C(2)-B(6) | 1.719(4) |
| C(2)-H(2) | 0.92(3) |
| C(3)-Si | 1.861(3) |
| C(3)-H(3A) | 0.9800 |
| C(3)-H(3B) | 0.9800 |
| C(3)-H(3C) | 0.9800 |
| C(4)-Si | 1.863(3) |
| C(4)-H(4A) | 0.9800 |
| C(4)-H(4B) | 0.9800 |
| C(4)-H(4C) | 0.9800 |
| C(5)-C(8) | 1.533(4) |
| C(5)-C(6) | 1.535(5) |
| C(5)-C(7) | 1.546(4) |
| C(5)-Si | 1.899(3) |
| C(6)-H(6A) | 0.9800 |
| C(6)-H(6B) | 0.9800 |
| C(6)-H(6C) | 0.9800 |
| C(7)-H(7A) | 0.9800 |
| C(7)-H(7B) | 0.9800 |
| C(7)-H(7C) | 0.9800 |
| C(8)-H(8A) | 0.9800 |
| C(8)-H(8B) | 0.9800 |
| C(8)-H(8C) | 0.9800 |
| B(3)-B(8) | 1.771(5) |
| B(3)-B(4) | 1.773(4) |
| B(3)-B(7) | 1.778(4) |
| B(3)-H(3) | 1.04(3) |
| B(4)-B(9) | 1.768(4) |

| | |
|---|---|
| B(4)-B(5) | 1.782(4) |
| B(4)-B(8) | 1.789(4) |
| B(4)-H(4) | 1.09(3) |
| B(5)-B(9) | 1.767(4) |
| B(5)-B(6) | 1.776(4) |
| B(5)-B(10) | 1.784(4) |
| B(5)-H(5) | 1.05(2) |
| B(6)-B(10) | 1.783(4) |
| B(6)-B(11) | 1.791(4) |
| B(6)-H(6) | 1.13(3) |
| B(7)-B(8) | 1.771(5) |
| B(7)-B(12) | 1.777(5) |
| B(7)-B(11) | 1.778(5) |
| B(7)-H(7) | 1.19(3) |
| B(8)-B(9) | 1.791(4) |
| B(8)-B(12) | 1.805(5) |
| B(8)-H(8) | 1.05(3) |
| B(9)-B(12) | 1.776(4) |
| B(9)-B(10) | 1.777(4) |
| B(9)-I | 2.182(3) |
| B(10)-B(11) | 1.776(4) |
| B(10)-B(12) | 1.793(4) |
| B(10)-H(10) | 1.07(3) |
| B(11)-B(12) | 1.776(5) |
| B(11)-H(11) | 1.07(2) |
| B(12)-H(12) | 1.10(2) |

| | |
|---|---|
| C(2)-C(1)-B(4) | 108.1(2) |
| C(2)-C(1)-B(5) | 108.3(2) |
| B(4)-C(1)-B(5) | 62.49(17) |
| C(2)-C(1)-B(3) | 59.93(16) |
| B(4)-C(1)-B(3) | 61.78(17) |
| B(5)-C(1)-B(3) | 112.9(2) |
| C(2)-C(1)-B(6) | 60.58(16) |
| B(4)-C(1)-B(6) | 113.1(2) |
| B(5)-C(1)-B(6) | 61.76(17) |
| B(3)-C(1)-B(6) | 112.7(2) |
| C(2)-C(1)-Si | 123.01(18) |
| B(4)-C(1)-Si | 118.91(17) |

| | |
|---|---|
| B(5)-C(1)-Si | 120.61(17) |
| B(3)-C(1)-Si | 117.38(18) |
| B(6)-C(1)-Si | 119.67(18) |
| C(1)-C(2)-B(11) | 113.2(2) |
| C(1)-C(2)-B(7) | 113.3(3) |
| B(11)-C(2)-B(7) | 63.39(19) |
| C(1)-C(2)-B(3) | 62.20(17) |
| B(11)-C(2)-B(3) | 116.0(2) |
| B(7)-C(2)-B(3) | 63.2(2) |
| C(1)-C(2)-B(6) | 61.91(16) |
| B(11)-C(2)-B(6) | 63.41(18) |
| B(7)-C(2)-B(6) | 116.3(2) |
| B(3)-C(2)-B(6) | 115.7(2) |
| C(1)-C(2)-H(2) | 117.1(17) |
| B(11)-C(2)-H(2) | 120.8(18) |
| B(7)-C(2)-H(2) | 118.1(17) |
| B(3)-C(2)-H(2) | 114.0(18) |
| B(6)-C(2)-H(2) | 117.9(17) |
| Si-C(3)-H(3A) | 109.5 |
| Si-C(3)-H(3B) | 109.5 |
| H(3A)-C(3)-H(3B) | 109.5 |
| Si-C(3)-H(3C) | 109.5 |
| H(3A)-C(3)-H(3C) | 109.5 |
| H(3B)-C(3)-H(3C) | 109.5 |
| Si-C(4)-H(4A) | 109.5 |
| Si-C(4)-H(4B) | 109.5 |
| H(4A)-C(4)-H(4B) | 109.5 |
| Si-C(4)-H(4C) | 109.5 |
| H(4A)-C(4)-H(4C) | 109.5 |
| H(4B)-C(4)-H(4C) | 109.5 |
| C(8)-C(5)-C(6) | 110.8(2) |
| C(8)-C(5)-C(7) | 107.5(2) |
| C(6)-C(5)-C(7) | 107.8(3) |
| C(8)-C(5)-Si | 111.18(18) |
| C(6)-C(5)-Si | 113.4(2) |
| C(7)-C(5)-Si | 105.92(19) |
| C(5)-C(6)-H(6A) | 109.5 |
| C(5)-C(6)-H(6B) | 109.5 |
| H(6A)-C(6)-H(6B) | 109.5 |

| | |
|---|---|
| C(5)-C(6)-H(6C) | 109.5 |
| H(6A)-C(6)-H(6C) | 109.5 |
| H(6B)-C(6)-H(6C) | 109.5 |
| C(5)-C(7)-H(7A) | 109.5 |
| C(5)-C(7)-H(7B) | 109.5 |
| H(7A)-C(7)-H(7B) | 109.5 |
| C(5)-C(7)-H(7C) | 109.5 |
| H(7A)-C(7)-H(7C) | 109.5 |
| H(7B)-C(7)-H(7C) | 109.5 |
| C(5)-C(8)-H(8A) | 109.5 |
| C(5)-C(8)-H(8B) | 109.5 |
| H(8A)-C(8)-H(8B) | 109.5 |
| C(5)-C(8)-H(8C) | 109.5 |
| H(8A)-C(8)-H(8C) | 109.5 |
| H(8B)-C(8)-H(8C) | 109.5 |
| C(2)-B(3)-C(1) | 57.87(17) |
| C(2)-B(3)-B(8) | 104.3(2) |
| C(1)-B(3)-B(8) | 106.2(2) |
| C(2)-B(3)-B(4) | 104.0(2) |
| C(1)-B(3)-B(4) | 58.48(17) |
| B(8)-B(3)-B(4) | 60.63(18) |
| C(2)-B(3)-B(7) | 58.22(18) |
| C(1)-B(3)-B(7) | 105.8(2) |
| B(8)-B(3)-B(7) | 59.84(19) |
| B(4)-B(3)-B(7) | 107.8(2) |
| C(2)-B(3)-H(3) | 116.2(15) |
| C(1)-B(3)-H(3) | 117.2(15) |
| B(8)-B(3)-H(3) | 131.5(16) |
| B(4)-B(3)-H(3) | 127.1(14) |
| B(7)-B(3)-H(3) | 121.9(15) |
| C(1)-B(4)-B(9) | 105.2(2) |
| C(1)-B(4)-B(3) | 59.74(17) |
| B(9)-B(4)-B(3) | 107.5(2) |
| C(1)-B(4)-B(5) | 58.87(17) |
| B(9)-B(4)-B(5) | 59.72(18) |
| B(3)-B(4)-B(5) | 108.3(2) |
| C(1)-B(4)-B(8) | 106.4(2) |
| B(9)-B(4)-B(8) | 60.48(17) |
| B(3)-B(4)-B(8) | 59.63(18) |

| | |
|---|---|
| B(5)-B(4)-B(8) | 108.8(2) |
| C(1)-B(4)-H(4) | 117.8(13) |
| B(9)-B(4)-H(4) | 129.1(13) |
| B(3)-B(4)-H(4) | 116.8(13) |
| B(5)-B(4)-H(4) | 122.2(13) |
| B(8)-B(4)-H(4) | 124.4(13) |
| C(1)-B(5)-B(9) | 105.0(2) |
| C(1)-B(5)-B(6) | 59.70(16) |
| B(9)-B(5)-B(6) | 107.9(2) |
| C(1)-B(5)-B(4) | 58.64(17) |
| B(9)-B(5)-B(4) | 59.74(17) |
| B(6)-B(5)-B(4) | 108.3(2) |
| C(1)-B(5)-B(10) | 106.2(2) |
| B(9)-B(5)-B(10) | 60.05(17) |
| B(6)-B(5)-B(10) | 60.12(17) |
| B(4)-B(5)-B(10) | 108.2(2) |
| C(1)-B(5)-H(5) | 118.3(13) |
| B(9)-B(5)-H(5) | 126.7(13) |
| B(6)-B(5)-H(5) | 119.8(13) |
| B(4)-B(5)-H(5) | 119.2(13) |
| B(10)-B(5)-H(5) | 126.6(13) |
| C(2)-B(6)-C(1) | 57.50(16) |
| C(2)-B(6)-B(5) | 103.4(2) |
| C(1)-B(6)-B(5) | 58.54(16) |
| C(2)-B(6)-B(10) | 103.1(2) |
| C(1)-B(6)-B(10) | 105.3(2) |
| B(5)-B(6)-B(10) | 60.16(17) |
| C(2)-B(6)-B(11) | 57.50(17) |
| C(1)-B(6)-B(11) | 104.9(2) |
| B(5)-B(6)-B(11) | 107.2(2) |
| B(10)-B(6)-B(11) | 59.56(18) |
| C(2)-B(6)-H(6) | 117.3(13) |
| C(1)-B(6)-H(6) | 115.6(12) |
| B(5)-B(6)-H(6) | 125.2(13) |
| B(10)-B(6)-H(6) | 133.2(13) |
| B(11)-B(6)-H(6) | 124.8(13) |
| C(2)-B(7)-B(8) | 104.6(2) |
| C(2)-B(7)-B(12) | 104.3(2) |
| B(8)-B(7)-B(12) | 61.19(19) |

| | |
|---|---|
| C(2)-B(7)-B(11) | 58.19(18) |
| B(8)-B(7)-B(11) | 108.9(2) |
| B(12)-B(7)-B(11) | 59.96(18) |
| C(2)-B(7)-B(3) | 58.60(18) |
| B(8)-B(7)-B(3) | 59.89(19) |
| B(12)-B(7)-B(3) | 108.6(2) |
| B(11)-B(7)-B(3) | 107.9(2) |
| C(2)-B(7)-H(7) | 120.7(15) |
| B(8)-B(7)-H(7) | 128.7(15) |
| B(12)-B(7)-H(7) | 121.8(15) |
| B(11)-B(7)-H(7) | 114.5(15) |
| B(3)-B(7)-H(7) | 125.2(15) |
| B(7)-B(8)-B(3) | 60.28(19) |
| B(7)-B(8)-B(4) | 107.5(2) |
| B(3)-B(8)-B(4) | 59.74(18) |
| B(7)-B(8)-B(9) | 106.3(2) |
| B(3)-B(8)-B(9) | 106.6(2) |
| B(4)-B(8)-B(9) | 59.16(17) |
| B(7)-B(8)-B(12) | 59.57(18) |
| B(3)-B(8)-B(12) | 107.7(2) |
| B(4)-B(8)-B(12) | 107.0(2) |
| B(9)-B(8)-B(12) | 59.17(17) |
| B(7)-B(8)-H(8) | 123.9(14) |
| B(3)-B(8)-H(8) | 121.3(15) |
| B(4)-B(8)-H(8) | 120.1(14) |
| B(9)-B(8)-H(8) | 122.3(14) |
| B(12)-B(8)-H(8) | 123.8(15) |
| B(5)-B(9)-B(4) | 60.54(17) |
| B(5)-B(9)-B(12) | 109.3(2) |
| B(4)-B(9)-B(12) | 109.3(2) |
| B(5)-B(9)-B(10) | 60.44(17) |
| B(4)-B(9)-B(10) | 109.2(2) |
| B(12)-B(9)-B(10) | 60.63(17) |
| B(5)-B(9)-B(8) | 109.3(2) |
| B(4)-B(9)-B(8) | 60.36(17) |
| B(12)-B(9)-B(8) | 60.80(18) |
| B(10)-B(9)-B(8) | 109.6(2) |
| B(5)-B(9)-I | 119.73(17) |
| B(4)-B(9)-I | 118.35(17) |

| | |
|---|---|
| B(12)-B(9)-I | 123.3(2) |
| B(10)-B(9)-I | 122.88(18) |
| B(8)-B(9)-I | 120.30(19) |
| B(11)-B(10)-B(9) | 106.7(2) |
| B(11)-B(10)-B(6) | 60.44(17) |
| B(9)-B(10)-B(6) | 107.1(2) |
| B(11)-B(10)-B(5) | 107.6(2) |
| B(9)-B(10)-B(5) | 59.51(17) |
| B(6)-B(10)-B(5) | 59.72(17) |
| B(11)-B(10)-B(12) | 59.68(18) |
| B(9)-B(10)-B(12) | 59.65(17) |
| B(6)-B(10)-B(12) | 108.4(2) |
| B(5)-B(10)-B(12) | 107.8(2) |
| B(11)-B(10)-H(10) | 121.0(13) |
| B(9)-B(10)-H(10) | 125.6(13) |
| B(6)-B(10)-H(10) | 118.0(13) |
| B(5)-B(10)-H(10) | 120.8(13) |
| B(12)-B(10)-H(10) | 124.6(14) |
| C(2)-B(11)-B(10) | 104.7(2) |
| C(2)-B(11)-B(12) | 104.5(2) |
| B(10)-B(11)-B(12) | 60.66(17) |
| C(2)-B(11)-B(7) | 58.42(19) |
| B(10)-B(11)-B(7) | 108.5(2) |
| B(12)-B(11)-B(7) | 59.99(19) |
| C(2)-B(11)-B(6) | 59.09(17) |
| B(10)-B(11)-B(6) | 60.00(17) |
| B(12)-B(11)-B(6) | 108.8(2) |
| B(7)-B(11)-B(6) | 108.6(2) |
| C(2)-B(11)-H(11) | 121.5(13) |
| B(10)-B(11)-H(11) | 123.1(13) |
| B(12)-B(11)-H(11) | 126.6(13) |
| B(7)-B(11)-H(11) | 122.8(13) |
| B(6)-B(11)-H(11) | 117.1(13) |
| B(9)-B(12)-B(11) | 106.7(2) |
| B(9)-B(12)-B(7) | 106.7(2) |
| B(11)-B(12)-B(7) | 60.05(19) |
| B(9)-B(12)-B(10) | 59.73(16) |
| B(11)-B(12)-B(10) | 59.66(18) |
| B(7)-B(12)-B(10) | 107.8(2) |

| | |
|---|---|
| B(9)-B(12)-B(8) | 60.03(17) |
| B(11)-B(12)-B(8) | 107.4(2) |
| B(7)-B(12)-B(8) | 59.24(18) |
| B(10)-B(12)-B(8) | 108.2(2) |
| B(9)-B(12)-H(12) | 123.7(14) |
| B(11)-B(12)-H(12) | 121.5(15) |
| B(7)-B(12)-H(12) | 121.1(14) |
| B(10)-B(12)-H(12) | 122.3(15) |
| B(8)-B(12)-H(12) | 121.8(15) |
| C(3)-Si-C(4) | 110.10(13) |
| C(3)-Si-C(5) | 110.57(14) |
| C(4)-Si-C(5) | 110.23(14) |
| C(3)-Si-C(1) | 106.34(13) |
| C(4)-Si-C(1) | 106.20(14) |
| C(5)-Si-C(1) | 113.25(11) |

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 15(1) | 18(2) | 14(1) | 0(1) | 2(1) | 1(1) |
| C(2) | 18(2) | 21(2) | 10(1) | -2(1) | 3(1) | 0(1) |
| C(3) | 22(2) | 23(2) | 33(2) | 3(2) | 8(2) | -3(1) |
| C(4) | 31(2) | 21(2) | 20(2) | 4(2) | -4(2) | -2(1) |
| C(5) | 23(2) | 14(1) | 24(1) | -2(1) | -2(1) | 1(1) |
| C(6) | 36(2) | 25(2) | 27(2) | -4(2) | -7(1) | -3(2) |
| C(7) | 30(2) | 16(2) | 36(2) | -2(2) | -4(2) | -5(1) |
| C(8) | 26(2) | 22(2) | 27(2) | -2(1) | 0(1) | 6(1) |
| B(3) | 15(2) | 20(2) | 21(2) | 1(1) | 3(2) | -1(1) |
| B(4) | 17(2) | 16(2) | 19(2) | 3(1) | -2(1) | -1(1) |
| B(5) | 15(2) | 20(2) | 15(1) | 0(1) | 1(1) | 1(1) |
| B(6) | 16(2) | 20(2) | 18(2) | 3(1) | -1(1) | 2(1) |
| B(7) | 19(2) | 21(2) | 19(2) | 1(1) | 1(1) | -1(1) |
| B(8) | 16(2) | 20(2) | 24(2) | 3(1) | 0(1) | -3(1) |
| B(9) | 18(2) | 23(2) | 15(1) | 1(1) | 2(1) | 1(1) |
| B(10) | 18(2) | 21(2) | 18(2) | 2(1) | -1(1) | 2(1) |
| B(11) | 25(2) | 23(2) | 16(2) | 2(1) | 3(1) | -2(2) |
| B(12) | 21(2) | 22(2) | 21(2) | 5(1) | 1(1) | -1(1) |
| I | 34(1) | 21(1) | 23(1) | -5(1) | 1(1) | 3(1) |
| Si | 16(1) | 16(1) | 16(1) | 1(1) | 0(1) | -1(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$) for **8a**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 1590(40) | 3290(13) | 9640(20) | 12(7)* |
| H(3A) | 5909 | 3697 | 6462 | 39 |
| H(3B) | 6608 | 3974 | 7594 | 39 |
| H(3C) | 5924 | 4462 | 6673 | 39 |
| H(4A) | 1207 | 4560 | 6212 | 36 |
| H(4B) | 113 | 3906 | 6546 | 36 |
| H(4C) | 1893 | 3882 | 5722 | 36 |
| H(6A) | 3833 | 4915 | 10015 | 44 |
| H(6B) | 5291 | 4455 | 9369 | 44 |
| H(6C) | 3425 | 4153 | 9954 | 44 |
| H(7A) | 2636 | 5339 | 7362 | 41 |
| H(7B) | 4732 | 5281 | 7932 | 41 |
| H(7C) | 2968 | 5637 | 8528 | 41 |
| H(8A) | 323 | 5010 | 9373 | 38 |
| H(8B) | 37 | 4262 | 9077 | 38 |
| H(8C) | -231 | 4805 | 8177 | 38 |
| H(3) | -740(40) | 3183(14) | 8070(20) | 18(7)* |
| H(4) | 1570(40) | 2685(12) | 6320(20) | 12(7)* |
| H(5) | 5510(30) | 2623(11) | 7130(19) | 6(6)* |
| H(6) | 5440(40) | 3157(12) | 9310(20) | 14(6)* |
| H(7) | -800(40) | 2233(15) | 9900(30) | 37(9)* |
| H(8) | -770(40) | 1762(13) | 7550(20) | 18(7)* |
| H(10) | 5740(40) | 1696(12) | 8926(18) | 10(6)* |
| H(11) | 3200(40) | 2223(12) | 10570(20) | 16(7)* |
| H(12) | 1730(40) | 1140(12) | 9200(20) | 20(7)* |

*Refined isotropically

Table 6. Torsion angles [°] for **8a**.

| | |
|---|---|
| B(4)-C(1)-C(2)-B(11) | 68.1(3) |
| B(5)-C(1)-C(2)-B(11) | 1.9(3) |
| B(3)-C(1)-C(2)-B(11) | 108.2(3) |
| B(6)-C(1)-C(2)-B(11) | -38.7(2) |
| Si-C(1)-C(2)-B(11) | -146.8(2) |
| B(4)-C(1)-C(2)-B(7) | -1.6(3) |
| B(5)-C(1)-C(2)-B(7) | -67.8(3) |
| B(3)-C(1)-C(2)-B(7) | 38.5(2) |
| B(6)-C(1)-C(2)-B(7) | -108.5(2) |
| Si-C(1)-C(2)-B(7) | 143.41(19) |
| B(4)-C(1)-C(2)-B(3) | -40.1(2) |
| B(5)-C(1)-C(2)-B(3) | -106.3(2) |
| B(6)-C(1)-C(2)-B(3) | -146.9(2) |
| Si-C(1)-C(2)-B(3) | 104.9(2) |
| B(4)-C(1)-C(2)-B(6) | 106.8(2) |
| B(5)-C(1)-C(2)-B(6) | 40.6(2) |
| B(3)-C(1)-C(2)-B(6) | 146.9(2) |
| Si-C(1)-C(2)-B(6) | -108.1(2) |
| B(11)-C(2)-B(3)-C(1) | -103.8(2) |
| B(7)-C(2)-B(3)-C(1) | -140.2(2) |
| B(6)-C(2)-B(3)-C(1) | -32.3(2) |
| C(1)-C(2)-B(3)-B(8) | 100.4(2) |
| B(11)-C(2)-B(3)-B(8) | -3.4(3) |
| B(7)-C(2)-B(3)-B(8) | -39.8(2) |
| B(6)-C(2)-B(3)-B(8) | 68.0(3) |
| C(1)-C(2)-B(3)-B(4) | 37.6(2) |
| B(11)-C(2)-B(3)-B(4) | -66.2(3) |
| B(7)-C(2)-B(3)-B(4) | -102.6(2) |
| B(6)-C(2)-B(3)-B(4) | 5.3(3) |
| C(1)-C(2)-B(3)-B(7) | 140.2(2) |
| B(11)-C(2)-B(3)-B(7) | 36.4(2) |
| B(6)-C(2)-B(3)-B(7) | 107.9(3) |
| B(4)-C(1)-B(3)-C(2) | 136.0(2) |
| B(5)-C(1)-B(3)-C(2) | 98.6(2) |
| B(6)-C(1)-B(3)-C(2) | 31.0(2) |
| Si-C(1)-B(3)-C(2) | -114.2(2) |
| C(2)-C(1)-B(3)-B(8) | -97.0(2) |

| | |
|---|---|
| B(4)-C(1)-B(3)-B(8) | 39.0(2) |
| B(5)-C(1)-B(3)-B(8) | 1.7(3) |
| B(6)-C(1)-B(3)-B(8) | -66.0(3) |
| Si-C(1)-B(3)-B(8) | 148.88(18) |
| C(2)-C(1)-B(3)-B(4) | -136.0(2) |
| B(5)-C(1)-B(3)-B(4) | -37.3(2) |
| B(6)-C(1)-B(3)-B(4) | -105.0(2) |
| Si-C(1)-B(3)-B(4) | 109.9(2) |
| C(2)-C(1)-B(3)-B(7) | -34.5(2) |
| B(4)-C(1)-B(3)-B(7) | 101.5(2) |
| B(5)-C(1)-B(3)-B(7) | 64.2(3) |
| B(6)-C(1)-B(3)-B(7) | -3.4(3) |
| Si-C(1)-B(3)-B(7) | -148.60(18) |
| C(2)-C(1)-B(4)-B(9) | -62.4(2) |
| B(5)-C(1)-B(4)-B(9) | 39.25(19) |
| B(3)-C(1)-B(4)-B(9) | -101.7(2) |
| B(6)-C(1)-B(4)-B(9) | 2.6(3) |
| Si-C(1)-B(4)-B(9) | 150.85(17) |
| C(2)-C(1)-B(4)-B(3) | 39.3(2) |
| B(5)-C(1)-B(4)-B(3) | 141.0(2) |
| B(6)-C(1)-B(4)-B(3) | 104.3(2) |
| Si-C(1)-B(4)-B(3) | -107.4(2) |
| C(2)-C(1)-B(4)-B(5) | -101.7(2) |
| B(3)-C(1)-B(4)-B(5) | -141.0(2) |
| B(6)-C(1)-B(4)-B(5) | -36.66(19) |
| Si-C(1)-B(4)-B(5) | 111.6(2) |
| C(2)-C(1)-B(4)-B(8) | 0.7(3) |
| B(5)-C(1)-B(4)-B(8) | 102.4(2) |
| B(3)-C(1)-B(4)-B(8) | -38.6(2) |
| B(6)-C(1)-B(4)-B(8) | 65.7(3) |
| Si-C(1)-B(4)-B(8) | -146.04(18) |
| C(2)-B(3)-B(4)-C(1) | -37.33(19) |
| B(8)-B(3)-B(4)-C(1) | -136.1(2) |
| B(7)-B(3)-B(4)-C(1) | -98.0(3) |
| C(2)-B(3)-B(4)-B(9) | 60.4(3) |
| C(1)-B(3)-B(4)-B(9) | 97.7(2) |
| B(8)-B(3)-B(4)-B(9) | -38.4(2) |
| B(7)-B(3)-B(4)-B(9) | -0.3(3) |
| C(2)-B(3)-B(4)-B(5) | -2.7(3) |

| | |
|---|---|
| C(1)-B(3)-B(4)-B(5) | 34.6(2) |
| B(8)-B(3)-B(4)-B(5) | -101.5(2) |
| B(7)-B(3)-B(4)-B(5) | -63.4(3) |
| C(2)-B(3)-B(4)-B(8) | 98.7(2) |
| C(1)-B(3)-B(4)-B(8) | 136.1(2) |
| B(7)-B(3)-B(4)-B(8) | 38.1(2) |
| C(2)-C(1)-B(5)-B(9) | 62.2(2) |
| B(4)-C(1)-B(5)-B(9) | -39.22(19) |
| B(3)-C(1)-B(5)-B(9) | -2.2(3) |
| B(6)-C(1)-B(5)-B(9) | 102.2(2) |
| Si-C(1)-B(5)-B(9) | -148.20(17) |
| C(2)-C(1)-B(5)-B(6) | -40.1(2) |
| B(4)-C(1)-B(5)-B(6) | -141.4(2) |
| B(3)-C(1)-B(5)-B(6) | -104.4(2) |
| Si-C(1)-B(5)-B(6) | 109.6(2) |
| C(2)-C(1)-B(5)-B(4) | 101.4(2) |
| B(3)-C(1)-B(5)-B(4) | 37.0(2) |
| B(6)-C(1)-B(5)-B(4) | 141.4(2) |
| Si-C(1)-B(5)-B(4) | -109.0(2) |
| C(2)-C(1)-B(5)-B(10) | -0.4(3) |
| B(4)-C(1)-B(5)-B(10) | -101.8(2) |
| B(3)-C(1)-B(5)-B(10) | -64.8(3) |
| B(6)-C(1)-B(5)-B(10) | 39.6(2) |
| Si-C(1)-B(5)-B(10) | 149.21(18) |
| B(9)-B(4)-B(5)-C(1) | -135.0(2) |
| B(3)-B(4)-B(5)-C(1) | -35.0(2) |
| B(8)-B(4)-B(5)-C(1) | -98.2(2) |
| C(1)-B(4)-B(5)-B(9) | 135.0(2) |
| B(3)-B(4)-B(5)-B(9) | 100.0(2) |
| B(8)-B(4)-B(5)-B(9) | 36.8(2) |
| C(1)-B(4)-B(5)-B(6) | 34.53(19) |
| B(9)-B(4)-B(5)-B(6) | -100.5(2) |
| B(3)-B(4)-B(5)-B(6) | -0.4(3) |
| B(8)-B(4)-B(5)-B(6) | -63.7(3) |
| C(1)-B(4)-B(5)-B(10) | 98.2(2) |
| B(9)-B(4)-B(5)-B(10) | -36.80(19) |
| B(3)-B(4)-B(5)-B(10) | 63.2(3) |
| B(8)-B(4)-B(5)-B(10) | 0.0(3) |
| B(11)-C(2)-B(6)-C(1) | 140.0(2) |

| | |
|---|---|
| B(7)-C(2)-B(6)-C(1) | 103.7(3) |
| B(3)-C(2)-B(6)-C(1) | 32.4(2) |
| C(1)-C(2)-B(6)-B(5) | -37.96(19) |
| B(11)-C(2)-B(6)-B(5) | 102.1(2) |
| B(7)-C(2)-B(6)-B(5) | 65.7(3) |
| B(3)-C(2)-B(6)-B(5) | -5.6(3) |
| C(1)-C(2)-B(6)-B(10) | -100.0(2) |
| B(11)-C(2)-B(6)-B(10) | 40.1(2) |
| B(7)-C(2)-B(6)-B(10) | 3.8(3) |
| B(3)-C(2)-B(6)-B(10) | -67.6(3) |
| C(1)-C(2)-B(6)-B(11) | -140.0(2) |
| B(7)-C(2)-B(6)-B(11) | -36.3(2) |
| B(3)-C(2)-B(6)-B(11) | -107.6(3) |
| B(4)-C(1)-B(6)-C(2) | -98.5(2) |
| B(5)-C(1)-B(6)-C(2) | -135.5(2) |
| B(3)-C(1)-B(6)-C(2) | -30.8(2) |
| Si-C(1)-B(6)-C(2) | 113.5(2) |
| C(2)-C(1)-B(6)-B(5) | 135.5(2) |
| B(4)-C(1)-B(6)-B(5) | 36.9(2) |
| B(3)-C(1)-B(6)-B(5) | 104.7(2) |
| Si-C(1)-B(6)-B(5) | -111.0(2) |
| C(2)-C(1)-B(6)-B(10) | 96.0(2) |
| B(4)-C(1)-B(6)-B(10) | -2.5(3) |
| B(5)-C(1)-B(6)-B(10) | -39.44(19) |
| B(3)-C(1)-B(6)-B(10) | 65.2(2) |
| Si-C(1)-B(6)-B(10) | -150.49(17) |
| C(2)-C(1)-B(6)-B(11) | 34.1(2) |
| B(4)-C(1)-B(6)-B(11) | -64.4(2) |
| B(5)-C(1)-B(6)-B(11) | -101.4(2) |
| B(3)-C(1)-B(6)-B(11) | 3.3(3) |
| Si-C(1)-B(6)-B(11) | 147.59(18) |
| C(1)-B(5)-B(6)-C(2) | 37.46(18) |
| B(9)-B(5)-B(6)-C(2) | -59.8(2) |
| B(4)-B(5)-B(6)-C(2) | 3.4(3) |
| B(10)-B(5)-B(6)-C(2) | -97.6(2) |
| B(9)-B(5)-B(6)-C(1) | -97.3(2) |
| B(4)-B(5)-B(6)-C(1) | -34.10(19) |
| B(10)-B(5)-B(6)-C(1) | -135.1(2) |
| C(1)-B(5)-B(6)-B(10) | 135.1(2) |

| | |
|---|---|
| B(9)-B(5)-B(6)-B(10) | 37.8(2) |
| B(4)-B(5)-B(6)-B(10) | 101.0(2) |
| C(1)-B(5)-B(6)-B(11) | 97.2(2) |
| B(9)-B(5)-B(6)-B(11) | -0.1(3) |
| B(4)-B(5)-B(6)-B(11) | 63.1(3) |
| B(10)-B(5)-B(6)-B(11) | -37.9(2) |
| C(1)-C(2)-B(7)-B(8) | 1.9(3) |
| B(11)-C(2)-B(7)-B(8) | -103.4(2) |
| B(3)-C(2)-B(7)-B(8) | 39.9(2) |
| B(6)-C(2)-B(7)-B(8) | -67.1(3) |
| C(1)-C(2)-B(7)-B(12) | 65.3(3) |
| B(11)-C(2)-B(7)-B(12) | -40.0(2) |
| B(3)-C(2)-B(7)-B(12) | 103.3(2) |
| B(6)-C(2)-B(7)-B(12) | -3.7(3) |
| C(1)-C(2)-B(7)-B(11) | 105.3(2) |
| B(3)-C(2)-B(7)-B(11) | 143.4(2) |
| B(6)-C(2)-B(7)-B(11) | 36.3(2) |
| C(1)-C(2)-B(7)-B(3) | -38.1(2) |
| B(11)-C(2)-B(7)-B(3) | -143.4(2) |
| B(6)-C(2)-B(7)-B(3) | -107.1(3) |
| C(1)-B(3)-B(7)-C(2) | 34.3(2) |
| B(8)-B(3)-B(7)-C(2) | 134.1(2) |
| B(4)-B(3)-B(7)-C(2) | 95.7(3) |
| C(2)-B(3)-B(7)-B(8) | -134.1(2) |
| C(1)-B(3)-B(7)-B(8) | -99.8(2) |
| B(4)-B(3)-B(7)-B(8) | -38.5(2) |
| C(2)-B(3)-B(7)-B(12) | -95.7(2) |
| C(1)-B(3)-B(7)-B(12) | -61.4(3) |
| B(8)-B(3)-B(7)-B(12) | 38.4(2) |
| B(4)-B(3)-B(7)-B(12) | 0.0(3) |
| C(2)-B(3)-B(7)-B(11) | -32.2(2) |
| C(1)-B(3)-B(7)-B(11) | 2.1(3) |
| B(8)-B(3)-B(7)-B(11) | 101.9(2) |
| B(4)-B(3)-B(7)-B(11) | 63.4(3) |
| C(2)-B(7)-B(8)-B(3) | -39.3(2) |
| B(12)-B(7)-B(8)-B(3) | -137.8(2) |
| B(11)-B(7)-B(8)-B(3) | -100.2(2) |
| C(2)-B(7)-B(8)-B(4) | -1.3(3) |
| B(12)-B(7)-B(8)-B(4) | -99.8(2) |

| | |
|---|---|
| B(11)-B(7)-B(8)-B(4) | -62.2(3) |
| B(3)-B(7)-B(8)-B(4) | 38.0(2) |
| C(2)-B(7)-B(8)-B(9) | 60.8(3) |
| B(12)-B(7)-B(8)-B(9) | -37.7(2) |
| B(11)-B(7)-B(8)-B(9) | -0.1(3) |
| B(3)-B(7)-B(8)-B(9) | 100.1(3) |
| C(2)-B(7)-B(8)-B(12) | 98.5(2) |
| B(11)-B(7)-B(8)-B(12) | 37.6(2) |
| B(3)-B(7)-B(8)-B(12) | 137.8(2) |
| C(2)-B(3)-B(8)-B(7) | 39.04(19) |
| C(1)-B(3)-B(8)-B(7) | 99.2(2) |
| B(4)-B(3)-B(8)-B(7) | 137.2(2) |
| C(2)-B(3)-B(8)-B(4) | -98.2(2) |
| C(1)-B(3)-B(8)-B(4) | -38.0(2) |
| B(7)-B(3)-B(8)-B(4) | -137.2(2) |
| C(2)-B(3)-B(8)-B(9) | -60.6(3) |
| C(1)-B(3)-B(8)-B(9) | -0.4(3) |
| B(4)-B(3)-B(8)-B(9) | 37.6(2) |
| B(7)-B(3)-B(8)-B(9) | -99.6(2) |
| C(2)-B(3)-B(8)-B(12) | 1.6(3) |
| C(1)-B(3)-B(8)-B(12) | 61.8(3) |
| B(4)-B(3)-B(8)-B(12) | 99.8(2) |
| B(7)-B(3)-B(8)-B(12) | -37.4(2) |
| C(1)-B(4)-B(8)-B(7) | 0.4(3) |
| B(9)-B(4)-B(8)-B(7) | 98.9(2) |
| B(3)-B(4)-B(8)-B(7) | -38.2(2) |
| B(5)-B(4)-B(8)-B(7) | 62.4(3) |
| C(1)-B(4)-B(8)-B(3) | 38.6(2) |
| B(9)-B(4)-B(8)-B(3) | 137.1(2) |
| B(5)-B(4)-B(8)-B(3) | 100.7(2) |
| C(1)-B(4)-B(8)-B(9) | -98.5(2) |
| B(3)-B(4)-B(8)-B(9) | -137.1(2) |
| B(5)-B(4)-B(8)-B(9) | -36.5(2) |
| C(1)-B(4)-B(8)-B(12) | -62.2(3) |
| B(9)-B(4)-B(8)-B(12) | 36.2(2) |
| B(3)-B(4)-B(8)-B(12) | -100.9(3) |
| B(5)-B(4)-B(8)-B(12) | -0.2(3) |
| C(1)-B(5)-B(9)-B(4) | 38.69(18) |
| B(6)-B(5)-B(9)-B(4) | 101.2(2) |

| | |
|---|---|
| B(10)-B(5)-B(9)-B(4) | 139.0(2) |
| C(1)-B(5)-B(9)-B(12) | -63.0(3) |
| B(6)-B(5)-B(9)-B(12) | -0.6(3) |
| B(4)-B(5)-B(9)-B(12) | -101.7(2) |
| B(10)-B(5)-B(9)-B(12) | 37.2(2) |
| C(1)-B(5)-B(9)-B(10) | -100.3(2) |
| B(6)-B(5)-B(9)-B(10) | -37.8(2) |
| B(4)-B(5)-B(9)-B(10) | -139.0(2) |
| C(1)-B(5)-B(9)-B(8) | 1.8(3) |
| B(6)-B(5)-B(9)-B(8) | 64.3(3) |
| B(4)-B(5)-B(9)-B(8) | -36.9(2) |
| B(10)-B(5)-B(9)-B(8) | 102.1(2) |
| C(1)-B(5)-B(9)-I | 146.48(18) |
| B(6)-B(5)-B(9)-I | -151.05(18) |
| B(4)-B(5)-B(9)-I | 107.8(2) |
| B(10)-B(5)-B(9)-I | -113.3(2) |
| C(1)-B(4)-B(9)-B(5) | -38.84(18) |
| B(3)-B(4)-B(9)-B(5) | -101.3(2) |
| B(8)-B(4)-B(9)-B(5) | -139.3(2) |
| C(1)-B(4)-B(9)-B(12) | 63.0(3) |
| B(3)-B(4)-B(9)-B(12) | 0.5(3) |
| B(5)-B(4)-B(9)-B(12) | 101.8(2) |
| B(8)-B(4)-B(9)-B(12) | -37.5(2) |
| C(1)-B(4)-B(9)-B(10) | -1.6(3) |
| B(3)-B(4)-B(9)-B(10) | -64.1(3) |
| B(5)-B(4)-B(9)-B(10) | 37.21(19) |
| B(8)-B(4)-B(9)-B(10) | -102.1(2) |
| C(1)-B(4)-B(9)-B(8) | 100.5(2) |
| B(3)-B(4)-B(9)-B(8) | 38.0(2) |
| B(5)-B(4)-B(9)-B(8) | 139.3(2) |
| C(1)-B(4)-B(9)-I | -148.87(17) |
| B(3)-B(4)-B(9)-I | 148.6(2) |
| B(5)-B(4)-B(9)-I | -110.0(2) |
| B(8)-B(4)-B(9)-I | 110.6(2) |
| B(7)-B(8)-B(9)-B(5) | -64.0(3) |
| B(3)-B(8)-B(9)-B(5) | -0.9(3) |
| B(4)-B(8)-B(9)-B(5) | 37.0(2) |
| B(12)-B(8)-B(9)-B(5) | -101.9(2) |
| B(7)-B(8)-B(9)-B(4) | -101.0(2) |

| | |
|---|---|
| B(3)-B(8)-B(9)-B(4) | -37.8(2) |
| B(12)-B(8)-B(9)-B(4) | -138.8(2) |
| B(7)-B(8)-B(9)-B(12) | 37.9(2) |
| B(3)-B(8)-B(9)-B(12) | 101.0(3) |
| B(4)-B(8)-B(9)-B(12) | 138.8(2) |
| B(7)-B(8)-B(9)-B(10) | 0.5(3) |
| B(3)-B(8)-B(9)-B(10) | 63.7(3) |
| B(4)-B(8)-B(9)-B(10) | 101.5(2) |
| B(12)-B(8)-B(9)-B(10) | -37.4(2) |
| B(7)-B(8)-B(9)-I | 151.57(18) |
| B(3)-B(8)-B(9)-I | -145.3(2) |
| B(4)-B(8)-B(9)-I | -107.5(2) |
| B(12)-B(8)-B(9)-I | 113.7(2) |
| B(5)-B(9)-B(10)-B(11) | 100.9(2) |
| B(4)-B(9)-B(10)-B(11) | 63.7(3) |
| B(12)-B(9)-B(10)-B(11) | -38.2(2) |
| B(8)-B(9)-B(10)-B(11) | -0.7(3) |
| I-B(9)-B(10)-B(11) | -150.89(19) |
| B(5)-B(9)-B(10)-B(6) | 37.44(19) |
| B(4)-B(9)-B(10)-B(6) | 0.2(3) |
| B(12)-B(9)-B(10)-B(6) | -101.6(2) |
| B(8)-B(9)-B(10)-B(6) | -64.2(3) |
| I-B(9)-B(10)-B(6) | 145.63(18) |
| B(4)-B(9)-B(10)-B(5) | -37.26(19) |
| B(12)-B(9)-B(10)-B(5) | -139.1(2) |
| B(8)-B(9)-B(10)-B(5) | -101.7(2) |
| I-B(9)-B(10)-B(5) | 108.2(2) |
| B(5)-B(9)-B(10)-B(12) | 139.1(2) |
| B(4)-B(9)-B(10)-B(12) | 101.8(2) |
| B(8)-B(9)-B(10)-B(12) | 37.4(2) |
| I-B(9)-B(10)-B(12) | -112.7(2) |
| C(2)-B(6)-B(10)-B(11) | -39.0(2) |
| C(1)-B(6)-B(10)-B(11) | -98.5(2) |
| B(5)-B(6)-B(10)-B(11) | -137.2(2) |
| C(2)-B(6)-B(10)-B(9) | 60.8(2) |
| C(1)-B(6)-B(10)-B(9) | 1.3(2) |
| B(5)-B(6)-B(10)-B(9) | -37.34(19) |
| B(11)-B(6)-B(10)-B(9) | 99.8(2) |
| C(2)-B(6)-B(10)-B(5) | 98.1(2) |

| | |
|---|---|
| C(1)-B(6)-B(10)-B(5) | 38.67(18) |
| B(11)-B(6)-B(10)-B(5) | 137.2(2) |
| C(2)-B(6)-B(10)-B(12) | -2.2(3) |
| C(1)-B(6)-B(10)-B(12) | -61.6(2) |
| B(5)-B(6)-B(10)-B(12) | -100.3(2) |
| B(11)-B(6)-B(10)-B(12) | 36.9(2) |
| C(1)-B(5)-B(10)-B(11) | -1.1(3) |
| B(9)-B(5)-B(10)-B(11) | -99.4(2) |
| B(6)-B(5)-B(10)-B(11) | 38.4(2) |
| B(4)-B(5)-B(10)-B(11) | -62.7(3) |
| C(1)-B(5)-B(10)-B(9) | 98.3(2) |
| B(6)-B(5)-B(10)-B(9) | 137.7(2) |
| B(4)-B(5)-B(10)-B(9) | 36.7(2) |
| C(1)-B(5)-B(10)-B(6) | -39.4(2) |
| B(9)-B(5)-B(10)-B(6) | -137.7(2) |
| B(4)-B(5)-B(10)-B(6) | -101.1(2) |
| C(1)-B(5)-B(10)-B(12) | 61.9(3) |
| B(9)-B(5)-B(10)-B(12) | -36.4(2) |
| B(6)-B(5)-B(10)-B(12) | 101.3(2) |
| B(4)-B(5)-B(10)-B(12) | 0.3(3) |
| C(1)-C(2)-B(11)-B(10) | -2.5(3) |
| B(7)-C(2)-B(11)-B(10) | 103.0(2) |
| B(3)-C(2)-B(11)-B(10) | 66.6(3) |
| B(6)-C(2)-B(11)-B(10) | -40.6(2) |
| C(1)-C(2)-B(11)-B(12) | -65.4(3) |
| B(7)-C(2)-B(11)-B(12) | 40.1(2) |
| B(3)-C(2)-B(11)-B(12) | 3.7(3) |
| B(6)-C(2)-B(11)-B(12) | -103.5(2) |
| C(1)-C(2)-B(11)-B(7) | -105.5(3) |
| B(3)-C(2)-B(11)-B(7) | -36.3(2) |
| B(6)-C(2)-B(11)-B(7) | -143.6(2) |
| C(1)-C(2)-B(11)-B(6) | 38.1(2) |
| B(7)-C(2)-B(11)-B(6) | 143.6(2) |
| B(3)-C(2)-B(11)-B(6) | 107.2(2) |
| B(9)-B(10)-B(11)-C(2) | -60.4(3) |
| B(6)-B(10)-B(11)-C(2) | 40.1(2) |
| B(5)-B(10)-B(11)-C(2) | 2.1(3) |
| B(12)-B(10)-B(11)-C(2) | -98.6(3) |
| B(9)-B(10)-B(11)-B(12) | 38.2(2) |

| | |
|---|---|
| B(6)-B(10)-B(11)-B(12) | 138.7(2) |
| B(5)-B(10)-B(11)-B(12) | 100.7(2) |
| B(9)-B(10)-B(11)-B(7) | 0.7(3) |
| B(6)-B(10)-B(11)-B(7) | 101.3(2) |
| B(5)-B(10)-B(11)-B(7) | 63.2(3) |
| B(12)-B(10)-B(11)-B(7) | -37.5(2) |
| B(9)-B(10)-B(11)-B(6) | -100.6(2) |
| B(5)-B(10)-B(11)-B(6) | -38.0(2) |
| B(12)-B(10)-B(11)-B(6) | -138.7(2) |
| B(8)-B(7)-B(11)-C(2) | 95.8(2) |
| B(12)-B(7)-B(11)-C(2) | 134.0(2) |
| B(3)-B(7)-B(11)-C(2) | 32.4(2) |
| C(2)-B(7)-B(11)-B(10) | -96.2(2) |
| B(8)-B(7)-B(11)-B(10) | -0.3(3) |
| B(12)-B(7)-B(11)-B(10) | 37.8(2) |
| B(3)-B(7)-B(11)-B(10) | -63.8(3) |
| C(2)-B(7)-B(11)-B(12) | -134.0(2) |
| B(8)-B(7)-B(11)-B(12) | -38.1(2) |
| B(3)-B(7)-B(11)-B(12) | -101.6(2) |
| C(2)-B(7)-B(11)-B(6) | -32.5(2) |
| B(8)-B(7)-B(11)-B(6) | 63.3(3) |
| B(12)-B(7)-B(11)-B(6) | 101.4(2) |
| B(3)-B(7)-B(11)-B(6) | -0.2(3) |
| C(1)-B(6)-B(11)-C(2) | -34.1(2) |
| B(5)-B(6)-B(11)-C(2) | -95.2(2) |
| B(10)-B(6)-B(11)-C(2) | -133.4(2) |
| C(2)-B(6)-B(11)-B(10) | 133.4(2) |
| C(1)-B(6)-B(11)-B(10) | 99.3(2) |
| B(5)-B(6)-B(11)-B(10) | 38.1(2) |
| C(2)-B(6)-B(11)-B(12) | 96.0(3) |
| C(1)-B(6)-B(11)-B(12) | 61.9(3) |
| B(5)-B(6)-B(11)-B(12) | 0.8(3) |
| B(10)-B(6)-B(11)-B(12) | -37.4(2) |
| C(2)-B(6)-B(11)-B(7) | 32.3(2) |
| C(1)-B(6)-B(11)-B(7) | -1.8(3) |
| B(5)-B(6)-B(11)-B(7) | -63.0(3) |
| B(10)-B(6)-B(11)-B(7) | -101.1(2) |
| B(5)-B(9)-B(12)-B(11) | 1.0(3) |
| B(4)-B(9)-B(12)-B(11) | -63.5(3) |

| | |
|---|---|
| B(10)-B(9)-B(12)-B(11) | 38.2(2) |
| B(8)-B(9)-B(12)-B(11) | -100.8(3) |
| I-B(9)-B(12)-B(11) | 150.2(2) |
| B(5)-B(9)-B(12)-B(7) | 64.0(3) |
| B(4)-B(9)-B(12)-B(7) | -0.5(3) |
| B(10)-B(9)-B(12)-B(7) | 101.2(2) |
| B(8)-B(9)-B(12)-B(7) | -37.8(2) |
| I-B(9)-B(12)-B(7) | -146.8(2) |
| B(5)-B(9)-B(12)-B(10) | -37.1(2) |
| B(4)-B(9)-B(12)-B(10) | -101.7(2) |
| B(8)-B(9)-B(12)-B(10) | -139.0(2) |
| I-B(9)-B(12)-B(10) | 112.1(2) |
| B(5)-B(9)-B(12)-B(8) | 101.9(2) |
| B(4)-B(9)-B(12)-B(8) | 37.3(2) |
| B(10)-B(9)-B(12)-B(8) | 139.0(2) |
| I-B(9)-B(12)-B(8) | -108.9(2) |
| C(2)-B(11)-B(12)-B(9) | 60.7(3) |
| B(10)-B(11)-B(12)-B(9) | -38.2(2) |
| B(7)-B(11)-B(12)-B(9) | 100.0(2) |
| B(6)-B(11)-B(12)-B(9) | -1.1(3) |
| C(2)-B(11)-B(12)-B(7) | -39.3(2) |
| B(10)-B(11)-B(12)-B(7) | -138.2(2) |
| B(6)-B(11)-B(12)-B(7) | -101.1(2) |
| C(2)-B(11)-B(12)-B(10) | 98.9(2) |
| B(7)-B(11)-B(12)-B(10) | 138.2(2) |
| B(6)-B(11)-B(12)-B(10) | 37.1(2) |
| C(2)-B(11)-B(12)-B(8) | -2.4(3) |
| B(10)-B(11)-B(12)-B(8) | -101.3(2) |
| B(7)-B(11)-B(12)-B(8) | 36.9(2) |
| B(6)-B(11)-B(12)-B(8) | -64.2(3) |
| C(2)-B(7)-B(12)-B(9) | -60.9(3) |
| B(8)-B(7)-B(12)-B(9) | 38.2(2) |
| B(11)-B(7)-B(12)-B(9) | -100.0(2) |
| B(3)-B(7)-B(12)-B(9) | 0.3(3) |
| C(2)-B(7)-B(12)-B(11) | 39.1(2) |
| B(8)-B(7)-B(12)-B(11) | 138.2(2) |
| B(3)-B(7)-B(12)-B(11) | 100.4(2) |
| C(2)-B(7)-B(12)-B(10) | 2.0(3) |
| B(8)-B(7)-B(12)-B(10) | 101.0(2) |

| | |
|---|---|
| B(11)-B(7)-B(12)-B(10) | -37.2(2) |
| B(3)-B(7)-B(12)-B(10) | 63.2(3) |
| C(2)-B(7)-B(12)-B(8) | -99.1(2) |
| B(11)-B(7)-B(12)-B(8) | -138.2(2) |
| B(3)-B(7)-B(12)-B(8) | -37.8(2) |
| B(11)-B(10)-B(12)-B(9) | 136.7(2) |
| B(6)-B(10)-B(12)-B(9) | 99.5(2) |
| B(5)-B(10)-B(12)-B(9) | 36.3(2) |
| B(9)-B(10)-B(12)-B(11) | -136.7(2) |
| B(6)-B(10)-B(12)-B(11) | -37.2(2) |
| B(5)-B(10)-B(12)-B(11) | -100.4(2) |
| B(11)-B(10)-B(12)-B(7) | 37.3(2) |
| B(9)-B(10)-B(12)-B(7) | -99.4(2) |
| B(6)-B(10)-B(12)-B(7) | 0.1(3) |
| B(5)-B(10)-B(12)-B(7) | -63.0(3) |
| B(11)-B(10)-B(12)-B(8) | 100.0(3) |
| B(9)-B(10)-B(12)-B(8) | -36.7(2) |
| B(6)-B(10)-B(12)-B(8) | 62.8(3) |
| B(5)-B(10)-B(12)-B(8) | -0.4(3) |
| B(7)-B(8)-B(12)-B(9) | -136.9(2) |
| B(3)-B(8)-B(12)-B(9) | -99.1(2) |
| B(4)-B(8)-B(12)-B(9) | -36.2(2) |
| B(7)-B(8)-B(12)-B(11) | -37.3(2) |
| B(3)-B(8)-B(12)-B(11) | 0.5(3) |
| B(4)-B(8)-B(12)-B(11) | 63.4(3) |
| B(9)-B(8)-B(12)-B(11) | 99.6(2) |
| B(3)-B(8)-B(12)-B(7) | 37.8(2) |
| B(4)-B(8)-B(12)-B(7) | 100.7(2) |
| B(9)-B(8)-B(12)-B(7) | 136.9(2) |
| B(7)-B(8)-B(12)-B(10) | -100.3(2) |
| B(3)-B(8)-B(12)-B(10) | -62.5(3) |
| B(4)-B(8)-B(12)-B(10) | 0.4(3) |
| B(9)-B(8)-B(12)-B(10) | 36.6(2) |
| C(8)-C(5)-Si-C(3) | 169.84(19) |
| C(6)-C(5)-Si-C(3) | -64.6(3) |
| C(7)-C(5)-Si-C(3) | 53.4(2) |
| C(8)-C(5)-Si-C(4) | 47.9(2) |
| C(6)-C(5)-Si-C(4) | 173.5(2) |
| C(7)-C(5)-Si-C(4) | -68.6(2) |

| | |
|---|---|
| C(8)-C(5)-Si-C(1) | -70.9(2) |
| C(6)-C(5)-Si-C(1) | 54.6(2) |
| C(7)-C(5)-Si-C(1) | 172.6(2) |
| C(2)-C(1)-Si-C(3) | 127.9(2) |
| B(4)-C(1)-Si-C(3) | -90.5(2) |
| B(5)-C(1)-Si-C(3) | -17.2(2) |
| B(3)-C(1)-Si-C(3) | -161.7(2) |
| B(6)-C(1)-Si-C(3) | 55.6(2) |
| C(2)-C(1)-Si-C(4) | -114.8(2) |
| B(4)-C(1)-Si-C(4) | 26.7(2) |
| B(5)-C(1)-Si-C(4) | 100.1(2) |
| B(3)-C(1)-Si-C(4) | -44.4(2) |
| B(6)-C(1)-Si-C(4) | 172.90(19) |
| C(2)-C(1)-Si-C(5) | 6.3(2) |
| B(4)-C(1)-Si-C(5) | 147.86(18) |
| B(5)-C(1)-Si-C(5) | -138.78(19) |
| B(3)-C(1)-Si-C(5) | 76.7(2) |
| B(6)-C(1)-Si-C(5) | -66.0(2) |

Table 1. Crystallographic details for **8b**

| | |
|---|---|
| Formula | C8 H25 B10 I Si |
| Formula weight | 384.37 |
| Temperature | 150(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | orthorhombic |
| Space group | $Pca2_1$ |
| Unit cell dimensions | a = 13.6530(1) Å |
| | b = 19.5285(1) Å |
| | c = 27.7225(2) Å |
| Volume | 7391.45(8) $Å^3$ |
| Z | 16 |
| Density (calculated) | 1.382 $Mg/m^3$ |
| Absorption coefficient | 1.778 $mm^{-1}$ |
| F(000) | 3040 |
| Crystal size | 0.19 x 0.19 x 0.27 $mm^3$ |
| Theta range for data collection | 2.09 to 27.48° |
| Index ranges | 0<=h<=17, 0<=k<=25, -35<=l<=35 |
| Reflections collected | 143725 |
| Independent reflections | 16557 [R(int) = 0.064] |
| Completeness to theta = 27.48° | 98.3 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 16557 / 1 / 901 |
| Goodness-of-fit on $F^2$ | 0.977 |
| Final R indices [I>2sigma(I)] | R1 = 0.0303, wR2 = 0.0460 |
| R indices (all data) | R1 = 0.0538, wR2 = 0.0489 |
| Absolute structure parameter | -0.042(7) |
| Largest diff. peak and hole | 0.536 and -0.506 e/$Å^3$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **8b**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| I(1A) | -602(1) | 962(1) | 4243(1) | 36(1) |
| Si(1A) | 1408(1) | -2401(1) | 3551(1) | 24(1) |
| C(1A) | 847(2) | -1507(2) | 3673(1) | 24(1) |
| C(2A) | 1366(2) | -1008(2) | 4088(1) | 24(1) |
| C(3A) | 2592(2) | -2418(2) | 3880(1) | 33(1) |
| C(4A) | 557(2) | -3048(2) | 3816(1) | 39(1) |
| C(5A) | 1591(2) | -2581(2) | 2883(1) | 30(1) |
| C(6A) | 2167(3) | -3273(2) | 2858(2) | 48(1) |
| C(7A) | 628(2) | -2679(2) | 2620(1) | 41(1) |
| C(8A) | 2210(2) | -2031(2) | 2632(1) | 36(1) |
| B(3A) | 1475(3) | -766(2) | 3505(1) | 27(1) |
| B(4A) | 313(3) | -978(2) | 3252(2) | 29(1) |
| B(5A) | -389(3) | -1384(2) | 3701(2) | 30(1) |
| B(6A) | 314(3) | -1425(2) | 4241(2) | 28(1) |
| B(7A) | 1265(3) | -162(2) | 3972(2) | 30(1) |
| B(8A) | 562(3) | -127(2) | 3433(2) | 32(1) |
| B(9A) | -599(3) | -516(2) | 3559(1) | 29(1) |
| B(10A) | -603(3) | -802(2) | 4178(2) | 31(1) |
| B(11A) | 546(3) | -564(2) | 4425(1) | 27(1) |
| B(12A) | -13(3) | -19(2) | 4012(1) | 27(1) |
| I(1B) | 2598(1) | -1619(1) | 5335(1) | 36(1) |
| Si(1B) | 1548(1) | -5132(1) | 6174(1) | 25(1) |
| C(1B) | 1831(2) | -4184(2) | 6016(1) | 23(1) |
| C(2B) | 1492(2) | -3898(2) | 5476(1) | 30(1) |
| C(3B) | 2699(2) | -5624(2) | 6072(1) | 38(1) |
| C(4B) | 564(2) | -5414(2) | 5750(1) | 33(1) |
| C(5B) | 1138(2) | -5248(2) | 6823(1) | 29(1) |
| C(6B) | 1961(2) | -5067(2) | 7182(1) | 42(1) |
| C(7B) | 206(3) | -4833(2) | 6938(1) | 40(1) |
| C(8B) | 883(3) | -6012(2) | 6882(1) | 40(1) |
| B(3B) | 879(3) | -3602(2) | 5961(2) | 33(1) |
| B(4B) | 1795(3) | -3500(2) | 6410(2) | 31(1) |
| B(5B) | 2912(3) | -3799(2) | 6161(2) | 29(1) |
| B(6B) | 2702(3) | -4076(2) | 5560(2) | 30(1) |

| | | | | |
|---|---|---|---|---|
| B(7B) | 1177(3) | -3059(2) | 5470(2) | 38(1) |
| B(8B) | 1405(3) | -2791(2) | 6068(2) | 33(1) |
| B(9B) | 2670(3) | -2907(2) | 6190(1) | 30(1) |
| B(10B) | 3226(3) | -3265(2) | 5670(2) | 30(1) |
| B(11B) | 2309(3) | -3357(2) | 5225(1) | 35(1) |
| B(12B) | 2294(3) | -2640(2) | 5614(1) | 28(1) |
| I(1C) | 3224(1) | 2857(1) | 4825(1) | 37(1) |
| Si(1C) | 328(1) | 532(1) | 6354(1) | 28(1) |
| C(1C) | 1168(2) | 1146(2) | 5999(1) | 24(1) |
| C(2C) | 935(2) | 1266(2) | 5416(1) | 27(1) |
| C(3C) | -335(3) | 18(2) | 5894(1) | 48(1) |
| C(4C) | -548(2) | 1079(2) | 6692(1) | 46(1) |
| C(5C) | 1031(2) | -38(2) | 6783(1) | 36(1) |
| C(6C) | 1765(3) | -511(2) | 6524(2) | 53(1) |
| C(7C) | 1550(3) | 368(2) | 7185(1) | 47(1) |
| C(8C) | 262(3) | -509(2) | 7028(2) | 63(1) |
| B(3C) | 617(3) | 1898(2) | 5802(2) | 29(1) |
| B(4C) | 1599(3) | 1901(2) | 6224(2) | 26(1) |
| B(5C) | 2406(2) | 1237(2) | 6075(1) | 25(1) |
| B(6C) | 1946(3) | 804(2) | 5564(1) | 26(1) |
| B(7C) | 1115(3) | 2077(2) | 5229(2) | 29(1) |
| B(8C) | 1584(3) | 2500(2) | 5743(2) | 32(1) |
| B(9C) | 2691(3) | 2090(2) | 5910(2) | 30(1) |
| B(10C) | 2908(3) | 1398(2) | 5500(1) | 27(1) |
| B(11C) | 1941(3) | 1395(2) | 5077(2) | 26(1) |
| B(12C) | 2395(2) | 2176(2) | 5294(2) | 25(1) |
| I(1D) | -608(1) | 5465(1) | 4587(1) | 29(1) |
| Si(1D) | 1712(1) | 2745(1) | 3140(1) | 27(1) |
| C(1D) | 1064(2) | 3501(2) | 3463(1) | 23(1) |
| C(2D) | 1053(2) | 3490(2) | 4062(1) | 27(1) |
| C(3D) | 1774(3) | 2027(2) | 3580(1) | 40(1) |
| C(4D) | 2962(2) | 3049(2) | 2986(1) | 38(1) |
| C(5D) | 1044(2) | 2474(2) | 2575(1) | 36(1) |
| C(6D) | -13(2) | 2250(2) | 2665(2) | 51(1) |
| C(7D) | 1597(3) | 1851(2) | 2371(2) | 49(1) |
| C(8D) | 1076(3) | 3044(2) | 2188(1) | 51(1) |
| B(3D) | 1821(3) | 4046(2) | 3787(1) | 28(1) |
| B(4D) | 1144(3) | 4340(2) | 3282(2) | 30(1) |
| B(5D) | 11(3) | 3899(2) | 3272(2) | 31(1) |

| | | | | |
|---|---|---|---|---|
| B(6D) | -18(3) | 3328(2) | 3765(2) | 33(1) |
| B(7D) | 1157(3) | 4269(2) | 4314(2) | 31(1) |
| B(8D) | 1189(3) | 4837(2) | 3819(1) | 27(1) |
| B(9D) | 64(3) | 4741(2) | 3501(1) | 27(1) |
| B(10D) | -652(3) | 4107(2) | 3799(2) | 29(1) |
| B(11D) | 18(3) | 3820(2) | 4304(2) | 31(1) |
| B(12D) | 70(3) | 4686(2) | 4138(1) | 26(1) |

Table 3. Bond lengths [Å] and angles [°] for **8b**.

| | |
|---|---|
| I(1A)-B(12A) | 2.175(4) |
| Si(1A)-C(3A) | 1.856(3) |
| Si(1A)-C(4A) | 1.866(3) |
| Si(1A)-C(5A) | 1.901(3) |
| Si(1A)-C(1A) | 1.937(3) |
| C(1A)-C(2A) | 1.667(4) |
| C(1A)-B(5A) | 1.706(4) |
| C(1A)-B(4A) | 1.720(5) |
| C(1A)-B(6A) | 1.742(5) |
| C(1A)-B(3A) | 1.745(5) |
| C(2A)-B(7A) | 1.688(5) |
| C(2A)-B(3A) | 1.690(5) |
| C(2A)-B(11A) | 1.696(5) |
| C(2A)-B(6A) | 1.704(5) |
| C(2A)-H(2A) | 0.93(3) |
| C(3A)-H(3A1) | 0.9800 |
| C(3A)-H(3A2) | 0.9800 |
| C(3A)-H(3A3) | 0.9800 |
| C(4A)-H(4A1) | 0.9800 |
| C(4A)-H(4A2) | 0.9800 |
| C(4A)-H(4A3) | 0.9800 |
| C(5A)-C(7A) | 1.518(4) |
| C(5A)-C(8A) | 1.535(5) |
| C(5A)-C(6A) | 1.565(5) |
| C(6A)-H(6A1) | 0.9800 |
| C(6A)-H(6A2) | 0.9800 |
| C(6A)-H(6A3) | 0.9800 |
| C(7A)-H(7A1) | 0.9800 |
| C(7A)-H(7A2) | 0.9800 |
| C(7A)-H(7A3) | 0.9800 |
| C(8A)-H(8A1) | 0.9800 |
| C(8A)-H(8A2) | 0.9800 |
| C(8A)-H(8A3) | 0.9800 |
| B(3A)-B(7A) | 1.774(6) |
| B(3A)-B(8A) | 1.774(5) |
| B(3A)-B(4A) | 1.784(5) |
| B(3A)-H(3A) | 1.02(3) |

| | |
|---|---|
| B(4A)-B(9A) | 1.757(5) |
| B(4A)-B(5A) | 1.761(6) |
| B(4A)-B(8A) | 1.769(6) |
| B(4A)-H(4A) | 1.05(3) |
| B(5A)-B(9A) | 1.763(6) |
| B(5A)-B(10A) | 1.767(6) |
| B(5A)-B(6A) | 1.778(6) |
| B(5A)-H(5A) | 1.07(4) |
| B(6A)-B(10A) | 1.754(5) |
| B(6A)-B(11A) | 1.785(5) |
| B(6A)-H(6A) | 1.09(3) |
| B(7A)-B(12A) | 1.772(5) |
| B(7A)-B(8A) | 1.777(6) |
| B(7A)-B(11A) | 1.779(6) |
| B(7A)-H(7A) | 1.14(3) |
| B(8A)-B(9A) | 1.792(6) |
| B(8A)-B(12A) | 1.798(5) |
| B(8A)-H(8A) | 1.13(4) |
| B(9A)-B(12A) | 1.776(5) |
| B(9A)-B(10A) | 1.805(6) |
| B(9A)-H(9A) | 1.08(3) |
| B(10A)-B(11A) | 1.773(5) |
| B(10A)-B(12A) | 1.788(5) |
| B(10A)-H(10A) | 1.11(3) |
| B(11A)-B(12A) | 1.741(5) |
| B(11A)-H(11A) | 1.07(4) |
| I(1B)-B(12B) | 2.178(4) |
| Si(1B)-C(3B) | 1.863(3) |
| Si(1B)-C(4B) | 1.868(3) |
| Si(1B)-C(5B) | 1.895(3) |
| Si(1B)-C(1B) | 1.943(3) |
| C(1B)-C(2B) | 1.664(4) |
| C(1B)-B(5B) | 1.703(5) |
| C(1B)-B(4B) | 1.726(5) |
| C(1B)-B(3B) | 1.733(5) |
| C(1B)-B(6B) | 1.748(5) |
| C(2B)-B(11B) | 1.686(5) |
| C(2B)-B(3B) | 1.686(5) |
| C(2B)-B(7B) | 1.692(6) |

| | |
|---|---|
| C(2B)-B(6B) | 1.704(5) |
| C(2B)-H(2B) | 0.87(3) |
| C(3B)-H(3B1) | 0.9800 |
| C(3B)-H(3B2) | 0.9800 |
| C(3B)-H(3B3) | 0.9800 |
| C(4B)-H(4B1) | 0.9800 |
| C(4B)-H(4B2) | 0.9800 |
| C(4B)-H(4B3) | 0.9800 |
| C(5B)-C(8B) | 1.542(5) |
| C(5B)-C(7B) | 1.543(5) |
| C(5B)-C(6B) | 1.543(5) |
| C(6B)-H(6B1) | 0.9800 |
| C(6B)-H(6B2) | 0.9800 |
| C(6B)-H(6B3) | 0.9800 |
| C(7B)-H(7B1) | 0.9800 |
| C(7B)-H(7B2) | 0.9800 |
| C(7B)-H(7B3) | 0.9800 |
| C(8B)-H(8B1) | 0.9800 |
| C(8B)-H(8B2) | 0.9800 |
| C(8B)-H(8B3) | 0.9800 |
| B(3B)-B(8B) | 1.763(6) |
| B(3B)-B(7B) | 1.771(6) |
| B(3B)-B(4B) | 1.775(6) |
| B(3B)-H(3B) | 1.01(3) |
| B(4B)-B(8B) | 1.759(6) |
| B(4B)-B(9B) | 1.773(6) |
| B(4B)-B(5B) | 1.773(6) |
| B(4B)-H(4B) | 1.03(3) |
| B(5B)-B(10B) | 1.768(6) |
| B(5B)-B(6B) | 1.774(6) |
| B(5B)-B(9B) | 1.775(6) |
| B(5B)-H(5B) | 0.99(3) |
| B(6B)-B(10B) | 1.765(5) |
| B(6B)-B(11B) | 1.767(6) |
| B(6B)-H(6B) | 1.03(3) |
| B(7B)-B(8B) | 1.766(6) |
| B(7B)-B(12B) | 1.777(5) |
| B(7B)-B(11B) | 1.785(6) |
| B(7B)-H(7B) | 1.02(3) |

| | |
|---|---|
| B(8B)-B(9B) | 1.775(6) |
| B(8B)-B(12B) | 1.775(6) |
| B(8B)-H(8B) | 1.01(4) |
| B(9B)-B(12B) | 1.757(5) |
| B(9B)-B(10B) | 1.771(6) |
| B(9B)-H(9B) | 1.10(3) |
| B(10B)-B(11B) | 1.766(6) |
| B(10B)-B(12B) | 1.770(5) |
| B(10B)-H(10B) | 1.12(3) |
| B(11B)-B(12B) | 1.767(6) |
| B(11B)-H(11B) | 0.99(4) |
| I(1C)-B(12C) | 2.177(4) |
| Si(1C)-C(4C) | 1.858(4) |
| Si(1C)-C(3C) | 1.858(4) |
| Si(1C)-C(5C) | 1.892(4) |
| Si(1C)-C(1C) | 1.930(3) |
| C(1C)-C(2C) | 1.664(4) |
| C(1C)-B(4C) | 1.705(5) |
| C(1C)-B(5C) | 1.712(4) |
| C(1C)-B(3C) | 1.738(5) |
| C(1C)-B(6C) | 1.739(5) |
| C(2C)-B(11C) | 1.683(5) |
| C(2C)-B(7C) | 1.683(5) |
| C(2C)-B(3C) | 1.692(5) |
| C(2C)-B(6C) | 1.699(5) |
| C(2C)-H(2C) | 0.87(3) |
| C(3C)-H(3C1) | 0.9800 |
| C(3C)-H(3C2) | 0.9800 |
| C(3C)-H(3C3) | 0.9800 |
| C(4C)-H(4C1) | 0.9800 |
| C(4C)-H(4C2) | 0.9800 |
| C(4C)-H(4C3) | 0.9800 |
| C(5C)-C(6C) | 1.539(5) |
| C(5C)-C(7C) | 1.540(5) |
| C(5C)-C(8C) | 1.551(5) |
| C(6C)-H(6C1) | 0.9800 |
| C(6C)-H(6C2) | 0.9800 |
| C(6C)-H(6C3) | 0.9800 |
| C(7C)-H(7C1) | 0.9800 |

| | |
|---|---|
| C(7C)-H(7C2) | 0.9800 |
| C(7C)-H(7C3) | 0.9800 |
| C(8C)-H(8C1) | 0.9800 |
| C(8C)-H(8C2) | 0.9800 |
| C(8C)-H(8C3) | 0.9800 |
| B(3C)-B(7C) | 1.762(6) |
| B(3C)-B(8C) | 1.776(6) |
| B(3C)-B(4C) | 1.779(5) |
| B(3C)-H(3C) | 1.07(3) |
| B(4C)-B(5C) | 1.750(5) |
| B(4C)-B(9C) | 1.766(5) |
| B(4C)-B(8C) | 1.775(6) |
| B(4C)-H(4C) | 1.06(3) |
| B(5C)-B(10C) | 1.763(5) |
| B(5C)-B(6C) | 1.765(5) |
| B(5C)-B(9C) | 1.770(6) |
| B(5C)-H(5C) | 1.04(3) |
| B(6C)-B(10C) | 1.761(5) |
| B(6C)-B(11C) | 1.777(6) |
| B(6C)-H(6C) | 1.04(3) |
| B(7C)-B(12C) | 1.767(5) |
| B(7C)-B(8C) | 1.766(6) |
| B(7C)-B(11C) | 1.795(5) |
| B(7C)-H(7C) | 1.03(3) |
| B(8C)-B(9C) | 1.772(5) |
| B(8C)-B(12C) | 1.782(6) |
| B(8C)-H(8C) | 0.99(3) |
| B(9C)-B(12C) | 1.762(6) |
| B(9C)-B(10C) | 1.789(6) |
| B(9C)-H(9C) | 1.10(3) |
| B(10C)-B(11C) | 1.765(5) |
| B(10C)-B(12C) | 1.767(5) |
| B(10C)-H(10C) | 1.03(3) |
| B(11C)-B(12C) | 1.753(5) |
| B(11C)-H(11C) | 1.06(3) |
| I(1D)-B(12D) | 2.175(4) |
| Si(1D)-C(4D) | 1.857(3) |
| Si(1D)-C(3D) | 1.860(4) |
| Si(1D)-C(5D) | 1.890(4) |

| | |
|---|---|
| Si(1D)-C(1D) | 1.940(3) |
| C(1D)-C(2D) | 1.661(4) |
| C(1D)-B(4D) | 1.716(5) |
| C(1D)-B(5D) | 1.717(5) |
| C(1D)-B(6D) | 1.731(5) |
| C(1D)-B(3D) | 1.735(5) |
| C(2D)-B(7D) | 1.680(5) |
| C(2D)-B(3D) | 1.691(5) |
| C(2D)-B(11D) | 1.693(5) |
| C(2D)-B(6D) | 1.709(5) |
| C(2D)-H(2D) | 0.84(3) |
| C(3D)-H(3D1) | 0.9800 |
| C(3D)-H(3D2) | 0.9800 |
| C(3D)-H(3D3) | 0.9800 |
| C(4D)-H(4D1) | 0.9800 |
| C(4D)-H(4D2) | 0.9800 |
| C(4D)-H(4D3) | 0.9800 |
| C(5D)-C(6D) | 1.529(5) |
| C(5D)-C(7D) | 1.540(5) |
| C(5D)-C(8D) | 1.546(5) |
| C(6D)-H(6D1) | 0.9800 |
| C(6D)-H(6D2) | 0.9800 |
| C(6D)-H(6D3) | 0.9800 |
| C(7D)-H(7D1) | 0.9800 |
| C(7D)-H(7D2) | 0.9800 |
| C(7D)-H(7D3) | 0.9800 |
| C(8D)-H(8D1) | 0.9800 |
| C(8D)-H(8D2) | 0.9800 |
| C(8D)-H(8D3) | 0.9800 |
| B(3D)-B(8D) | 1.771(5) |
| B(3D)-B(4D) | 1.773(6) |
| B(3D)-B(7D) | 1.772(5) |
| B(3D)-H(3D) | 1.07(2) |
| B(4D)-B(5D) | 1.770(6) |
| B(4D)-B(9D) | 1.777(6) |
| B(4D)-B(8D) | 1.778(6) |
| B(4D)-H(4D) | 1.17(3) |
| B(5D)-B(6D) | 1.763(6) |
| B(5D)-B(9D) | 1.764(6) |

| | |
|---|---|
| B(5D)-B(10D) | 1.766(6) |
| B(5D)-H(5D) | 1.05(3) |
| B(6D)-B(10D) | 1.754(5) |
| B(6D)-B(11D) | 1.778(6) |
| B(6D)-H(6D) | 1.05(3) |
| B(7D)-B(12D) | 1.761(5) |
| B(7D)-B(8D) | 1.765(6) |
| B(7D)-B(11D) | 1.786(5) |
| B(7D)-H(7D) | 1.13(3) |
| B(8D)-B(9D) | 1.781(5) |
| B(8D)-B(12D) | 1.789(5) |
| B(8D)-H(8D) | 1.12(3) |
| B(9D)-B(12D) | 1.769(5) |
| B(9D)-B(10D) | 1.781(6) |
| B(9D)-H(9D) | 1.07(3) |
| B(10D)-B(11D) | 1.763(6) |
| B(10D)-B(12D) | 1.769(5) |
| B(10D)-H(10D) | 1.06(3) |
| B(11D)-B(12D) | 1.753(5) |
| B(11D)-H(11D) | 1.04(3) |

| | |
|---|---|
| C(3A)-Si(1A)-C(4A) | 109.67(17) |
| C(3A)-Si(1A)-C(5A) | 111.15(15) |
| C(4A)-Si(1A)-C(5A) | 109.89(16) |
| C(3A)-Si(1A)-C(1A) | 105.99(14) |
| C(4A)-Si(1A)-C(1A) | 107.17(15) |
| C(5A)-Si(1A)-C(1A) | 112.82(14) |
| C(2A)-C(1A)-B(5A) | 107.8(2) |
| C(2A)-C(1A)-B(4A) | 107.3(3) |
| B(5A)-C(1A)-B(4A) | 61.9(2) |
| C(2A)-C(1A)-B(6A) | 59.92(19) |
| B(5A)-C(1A)-B(6A) | 62.1(2) |
| B(4A)-C(1A)-B(6A) | 112.4(3) |
| C(2A)-C(1A)-B(3A) | 59.3(2) |
| B(5A)-C(1A)-B(3A) | 112.5(3) |
| B(4A)-C(1A)-B(3A) | 62.0(2) |
| B(6A)-C(1A)-B(3A) | 111.7(3) |
| C(2A)-C(1A)-Si(1A) | 118.6(2) |
| B(5A)-C(1A)-Si(1A) | 121.8(2) |

| | |
|---|---|
| B(4A)-C(1A)-Si(1A) | 126.3(2) |
| B(6A)-C(1A)-Si(1A) | 113.9(2) |
| B(3A)-C(1A)-Si(1A) | 120.5(2) |
| C(1A)-C(2A)-B(7A) | 113.9(3) |
| C(1A)-C(2A)-B(3A) | 62.6(2) |
| B(7A)-C(2A)-B(3A) | 63.3(2) |
| C(1A)-C(2A)-B(11A) | 113.5(2) |
| B(7A)-C(2A)-B(11A) | 63.4(2) |
| B(3A)-C(2A)-B(11A) | 116.3(3) |
| C(1A)-C(2A)-B(6A) | 62.2(2) |
| B(7A)-C(2A)-B(6A) | 116.5(3) |
| B(3A)-C(2A)-B(6A) | 116.4(3) |
| B(11A)-C(2A)-B(6A) | 63.3(2) |
| C(1A)-C(2A)-H(2A) | 117.1(17) |
| B(7A)-C(2A)-H(2A) | 118.0(16) |
| B(3A)-C(2A)-H(2A) | 114.4(17) |
| B(11A)-C(2A)-H(2A) | 120.0(17) |
| B(6A)-C(2A)-H(2A) | 117.1(16) |
| Si(1A)-C(3A)-H(3A1) | 109.5 |
| Si(1A)-C(3A)-H(3A2) | 109.5 |
| H(3A1)-C(3A)-H(3A2) | 109.5 |
| Si(1A)-C(3A)-H(3A3) | 109.5 |
| H(3A1)-C(3A)-H(3A3) | 109.5 |
| H(3A2)-C(3A)-H(3A3) | 109.5 |
| Si(1A)-C(4A)-H(4A1) | 109.5 |
| Si(1A)-C(4A)-H(4A2) | 109.5 |
| H(4A1)-C(4A)-H(4A2) | 109.5 |
| Si(1A)-C(4A)-H(4A3) | 109.5 |
| H(4A1)-C(4A)-H(4A3) | 109.5 |
| H(4A2)-C(4A)-H(4A3) | 109.5 |
| C(7A)-C(5A)-C(8A) | 110.3(3) |
| C(7A)-C(5A)-C(6A) | 107.8(3) |
| C(8A)-C(5A)-C(6A) | 107.9(3) |
| C(7A)-C(5A)-Si(1A) | 112.3(2) |
| C(8A)-C(5A)-Si(1A) | 112.7(2) |
| C(6A)-C(5A)-Si(1A) | 105.6(2) |
| C(5A)-C(6A)-H(6A1) | 109.5 |
| C(5A)-C(6A)-H(6A2) | 109.5 |
| H(6A1)-C(6A)-H(6A2) | 109.5 |

| | |
|---|---|
| C(5A)-C(6A)-H(6A3) | 109.5 |
| H(6A1)-C(6A)-H(6A3) | 109.5 |
| H(6A2)-C(6A)-H(6A3) | 109.5 |
| C(5A)-C(7A)-H(7A1) | 109.5 |
| C(5A)-C(7A)-H(7A2) | 109.5 |
| H(7A1)-C(7A)-H(7A2) | 109.5 |
| C(5A)-C(7A)-H(7A3) | 109.5 |
| H(7A1)-C(7A)-H(7A3) | 109.5 |
| H(7A2)-C(7A)-H(7A3) | 109.5 |
| C(5A)-C(8A)-H(8A1) | 109.5 |
| C(5A)-C(8A)-H(8A2) | 109.5 |
| H(8A1)-C(8A)-H(8A2) | 109.5 |
| C(5A)-C(8A)-H(8A3) | 109.5 |
| H(8A1)-C(8A)-H(8A3) | 109.5 |
| H(8A2)-C(8A)-H(8A3) | 109.5 |
| C(2A)-B(3A)-C(1A) | 58.03(19) |
| C(2A)-B(3A)-B(7A) | 58.3(2) |
| C(1A)-B(3A)-B(7A) | 106.1(3) |
| C(2A)-B(3A)-B(8A) | 104.0(3) |
| C(1A)-B(3A)-B(8A) | 105.5(3) |
| B(7A)-B(3A)-B(8A) | 60.1(2) |
| C(2A)-B(3A)-B(4A) | 103.5(3) |
| C(1A)-B(3A)-B(4A) | 58.3(2) |
| B(7A)-B(3A)-B(4A) | 107.3(3) |
| B(8A)-B(3A)-B(4A) | 59.6(2) |
| C(2A)-B(3A)-H(3A) | 115.4(16) |
| C(1A)-B(3A)-H(3A) | 116.6(16) |
| B(7A)-B(3A)-H(3A) | 121.6(16) |
| B(8A)-B(3A)-H(3A) | 133.0(16) |
| B(4A)-B(3A)-H(3A) | 128.3(16) |
| C(1A)-B(4A)-B(9A) | 106.2(3) |
| C(1A)-B(4A)-B(5A) | 58.7(2) |
| B(9A)-B(4A)-B(5A) | 60.2(2) |
| C(1A)-B(4A)-B(8A) | 106.8(3) |
| B(9A)-B(4A)-B(8A) | 61.1(2) |
| B(5A)-B(4A)-B(8A) | 109.1(3) |
| C(1A)-B(4A)-B(3A) | 59.7(2) |
| B(9A)-B(4A)-B(3A) | 108.7(3) |
| B(5A)-B(4A)-B(3A) | 108.1(3) |

| | |
|---|---|
| B(8A)-B(4A)-B(3A) | 59.9(2) |
| C(1A)-B(4A)-H(4A) | 115.3(15) |
| B(9A)-B(4A)-H(4A) | 129.5(14) |
| B(5A)-B(4A)-H(4A) | 120.9(15) |
| B(8A)-B(4A)-H(4A) | 126.0(16) |
| B(3A)-B(4A)-H(4A) | 116.3(14) |
| C(1A)-B(5A)-B(4A) | 59.5(2) |
| C(1A)-B(5A)-B(9A) | 106.6(3) |
| B(4A)-B(5A)-B(9A) | 59.8(2) |
| C(1A)-B(5A)-B(10A) | 106.8(3) |
| B(4A)-B(5A)-B(10A) | 109.3(3) |
| B(9A)-B(5A)-B(10A) | 61.5(2) |
| C(1A)-B(5A)-B(6A) | 59.95(19) |
| B(4A)-B(5A)-B(6A) | 108.8(3) |
| B(9A)-B(5A)-B(6A) | 108.6(3) |
| B(10A)-B(5A)-B(6A) | 59.3(2) |
| C(1A)-B(5A)-H(5A) | 117(2) |
| B(4A)-B(5A)-H(5A) | 122(2) |
| B(9A)-B(5A)-H(5A) | 128(2) |
| B(10A)-B(5A)-H(5A) | 124(2) |
| B(6A)-B(5A)-H(5A) | 117(2) |
| C(2A)-B(6A)-C(1A) | 57.86(18) |
| C(2A)-B(6A)-B(10A) | 104.2(3) |
| C(1A)-B(6A)-B(10A) | 105.8(3) |
| C(2A)-B(6A)-B(5A) | 103.0(3) |
| C(1A)-B(6A)-B(5A) | 58.0(2) |
| B(10A)-B(6A)-B(5A) | 60.0(2) |
| C(2A)-B(6A)-B(11A) | 58.1(2) |
| C(1A)-B(6A)-B(11A) | 105.8(3) |
| B(10A)-B(6A)-B(11A) | 60.1(2) |
| B(5A)-B(6A)-B(11A) | 107.1(3) |
| C(2A)-B(6A)-H(6A) | 120.2(14) |
| C(1A)-B(6A)-H(6A) | 119.1(16) |
| B(10A)-B(6A)-H(6A) | 128.4(15) |
| B(5A)-B(6A)-H(6A) | 125.4(15) |
| B(11A)-B(6A)-H(6A) | 123.0(16) |
| C(2A)-B(7A)-B(12A) | 102.8(3) |
| C(2A)-B(7A)-B(3A) | 58.4(2) |
| B(12A)-B(7A)-B(3A) | 108.0(3) |

| | |
|---|---|
| C(2A)-B(7A)-B(8A) | 104.0(3) |
| B(12A)-B(7A)-B(8A) | 60.9(2) |
| B(3A)-B(7A)-B(8A) | 60.0(2) |
| C(2A)-B(7A)-B(11A) | 58.5(2) |
| B(12A)-B(7A)-B(11A) | 58.7(2) |
| B(3A)-B(7A)-B(11A) | 108.1(3) |
| B(8A)-B(7A)-B(11A) | 108.2(3) |
| C(2A)-B(7A)-H(7A) | 119.7(17) |
| B(12A)-B(7A)-H(7A) | 127.4(17) |
| B(3A)-B(7A)-H(7A) | 119.7(17) |
| B(8A)-B(7A)-H(7A) | 127.2(18) |
| B(11A)-B(7A)-H(7A) | 119.0(18) |
| B(4A)-B(8A)-B(3A) | 60.5(2) |
| B(4A)-B(8A)-B(7A) | 107.9(3) |
| B(3A)-B(8A)-B(7A) | 59.9(2) |
| B(4A)-B(8A)-B(9A) | 59.1(2) |
| B(3A)-B(8A)-B(9A) | 107.5(3) |
| B(7A)-B(8A)-B(9A) | 107.3(3) |
| B(4A)-B(8A)-B(12A) | 106.2(3) |
| B(3A)-B(8A)-B(12A) | 106.8(3) |
| B(7A)-B(8A)-B(12A) | 59.4(2) |
| B(9A)-B(8A)-B(12A) | 59.3(2) |
| B(4A)-B(8A)-H(8A) | 123.0(19) |
| B(3A)-B(8A)-H(8A) | 121.8(16) |
| B(7A)-B(8A)-H(8A) | 121.0(18) |
| B(9A)-B(8A)-H(8A) | 122.8(16) |
| B(12A)-B(8A)-H(8A) | 122.5(18) |
| B(4A)-B(9A)-B(5A) | 60.0(2) |
| B(4A)-B(9A)-B(12A) | 107.7(3) |
| B(5A)-B(9A)-B(12A) | 107.1(3) |
| B(4A)-B(9A)-B(8A) | 59.8(2) |
| B(5A)-B(9A)-B(8A) | 107.9(3) |
| B(12A)-B(9A)-B(8A) | 60.5(2) |
| B(4A)-B(9A)-B(10A) | 107.7(3) |
| B(5A)-B(9A)-B(10A) | 59.4(2) |
| B(12A)-B(9A)-B(10A) | 59.9(2) |
| B(8A)-B(9A)-B(10A) | 108.6(3) |
| B(4A)-B(9A)-H(9A) | 122.5(18) |
| B(5A)-B(9A)-H(9A) | 121.3(18) |

| | |
|---|---|
| B(12A)-B(9A)-H(9A) | 122.2(18) |
| B(8A)-B(9A)-H(9A) | 122.6(17) |
| B(10A)-B(9A)-H(9A) | 120.6(17) |
| B(6A)-B(10A)-B(5A) | 60.7(2) |
| B(6A)-B(10A)-B(11A) | 60.8(2) |
| B(5A)-B(10A)-B(11A) | 108.1(3) |
| B(6A)-B(10A)-B(12A) | 107.3(3) |
| B(5A)-B(10A)-B(12A) | 106.4(3) |
| B(11A)-B(10A)-B(12A) | 58.5(2) |
| B(6A)-B(10A)-B(9A) | 107.8(3) |
| B(5A)-B(10A)-B(9A) | 59.2(2) |
| B(11A)-B(10A)-B(9A) | 106.5(3) |
| B(12A)-B(10A)-B(9A) | 59.2(2) |
| B(6A)-B(10A)-H(10A) | 119.7(17) |
| B(5A)-B(10A)-H(10A) | 122.9(17) |
| B(11A)-B(10A)-H(10A) | 120.3(17) |
| B(12A)-B(10A)-H(10A) | 123.3(17) |
| B(9A)-B(10A)-H(10A) | 124.5(16) |
| C(2A)-B(11A)-B(12A) | 103.8(3) |
| C(2A)-B(11A)-B(10A) | 103.7(3) |
| B(12A)-B(11A)-B(10A) | 61.2(2) |
| C(2A)-B(11A)-B(7A) | 58.1(2) |
| B(12A)-B(11A)-B(7A) | 60.4(2) |
| B(10A)-B(11A)-B(7A) | 109.3(3) |
| C(2A)-B(11A)-B(6A) | 58.54(19) |
| B(12A)-B(11A)-B(6A) | 108.0(3) |
| B(10A)-B(11A)-B(6A) | 59.1(2) |
| B(7A)-B(11A)-B(6A) | 108.1(3) |
| C(2A)-B(11A)-H(11A) | 114.8(18) |
| B(12A)-B(11A)-H(11A) | 131.0(18) |
| B(10A)-B(11A)-H(11A) | 130.3(17) |
| B(7A)-B(11A)-H(11A) | 117.2(18) |
| B(6A)-B(11A)-H(11A) | 117.3(19) |
| B(11A)-B(12A)-B(7A) | 60.8(2) |
| B(11A)-B(12A)-B(9A) | 109.2(3) |
| B(7A)-B(12A)-B(9A) | 108.3(3) |
| B(11A)-B(12A)-B(10A) | 60.3(2) |
| B(7A)-B(12A)-B(10A) | 109.0(3) |
| B(9A)-B(12A)-B(10A) | 60.8(2) |

| | |
|---|---|
| B(11A)-B(12A)-B(8A) | 108.9(3) |
| B(7A)-B(12A)-B(8A) | 59.7(2) |
| B(9A)-B(12A)-B(8A) | 60.2(2) |
| B(10A)-B(12A)-B(8A) | 109.1(3) |
| B(11A)-B(12A)-I(1A) | 120.4(2) |
| B(7A)-B(12A)-I(1A) | 121.4(2) |
| B(9A)-B(12A)-I(1A) | 121.6(2) |
| B(10A)-B(12A)-I(1A) | 120.8(2) |
| B(8A)-B(12A)-I(1A) | 121.8(2) |
| C(3B)-Si(1B)-C(4B) | 111.02(16) |
| C(3B)-Si(1B)-C(5B) | 109.40(16) |
| C(4B)-Si(1B)-C(5B) | 110.46(15) |
| C(3B)-Si(1B)-C(1B) | 106.81(14) |
| C(4B)-Si(1B)-C(1B) | 106.35(14) |
| C(5B)-Si(1B)-C(1B) | 112.74(14) |
| C(2B)-C(1B)-B(5B) | 107.8(2) |
| C(2B)-C(1B)-B(4B) | 107.6(3) |
| B(5B)-C(1B)-B(4B) | 62.3(2) |
| C(2B)-C(1B)-B(3B) | 59.5(2) |
| B(5B)-C(1B)-B(3B) | 112.4(3) |
| B(4B)-C(1B)-B(3B) | 61.8(2) |
| C(2B)-C(1B)-B(6B) | 59.9(2) |
| B(5B)-C(1B)-B(6B) | 61.9(2) |
| B(4B)-C(1B)-B(6B) | 112.6(2) |
| B(3B)-C(1B)-B(6B) | 111.6(3) |
| C(2B)-C(1B)-Si(1B) | 117.9(2) |
| B(5B)-C(1B)-Si(1B) | 122.6(2) |
| B(4B)-C(1B)-Si(1B) | 126.1(2) |
| B(3B)-C(1B)-Si(1B) | 119.7(2) |
| B(6B)-C(1B)-Si(1B) | 114.4(2) |
| C(1B)-C(2B)-B(11B) | 113.4(3) |
| C(1B)-C(2B)-B(3B) | 62.3(2) |
| B(11B)-C(2B)-B(3B) | 116.2(3) |
| C(1B)-C(2B)-B(7B) | 113.8(3) |
| B(11B)-C(2B)-B(7B) | 63.8(2) |
| B(3B)-C(2B)-B(7B) | 63.2(2) |
| C(1B)-C(2B)-B(6B) | 62.5(2) |
| B(11B)-C(2B)-B(6B) | 62.8(2) |
| B(3B)-C(2B)-B(6B) | 116.2(3) |

| | |
|---|---|
| B(7B)-C(2B)-B(6B) | 116.4(3) |
| C(1B)-C(2B)-H(2B) | 116.1(18) |
| B(11B)-C(2B)-H(2B) | 123.4(19) |
| B(3B)-C(2B)-H(2B) | 109.9(18) |
| B(7B)-C(2B)-H(2B) | 115.6(18) |
| B(6B)-C(2B)-H(2B) | 121.4(18) |
| Si(1B)-C(3B)-H(3B1) | 109.5 |
| Si(1B)-C(3B)-H(3B2) | 109.5 |
| H(3B1)-C(3B)-H(3B2) | 109.5 |
| Si(1B)-C(3B)-H(3B3) | 109.5 |
| H(3B1)-C(3B)-H(3B3) | 109.5 |
| H(3B2)-C(3B)-H(3B3) | 109.5 |
| Si(1B)-C(4B)-H(4B1) | 109.5 |
| Si(1B)-C(4B)-H(4B2) | 109.5 |
| H(4B1)-C(4B)-H(4B2) | 109.5 |
| Si(1B)-C(4B)-H(4B3) | 109.5 |
| H(4B1)-C(4B)-H(4B3) | 109.5 |
| H(4B2)-C(4B)-H(4B3) | 109.5 |
| C(8B)-C(5B)-C(7B) | 107.4(3) |
| C(8B)-C(5B)-C(6B) | 108.4(3) |
| C(7B)-C(5B)-C(6B) | 110.3(3) |
| C(8B)-C(5B)-Si(1B) | 106.5(2) |
| C(7B)-C(5B)-Si(1B) | 112.2(2) |
| C(6B)-C(5B)-Si(1B) | 111.7(2) |
| C(5B)-C(6B)-H(6B1) | 109.5 |
| C(5B)-C(6B)-H(6B2) | 109.5 |
| H(6B1)-C(6B)-H(6B2) | 109.5 |
| C(5B)-C(6B)-H(6B3) | 109.5 |
| H(6B1)-C(6B)-H(6B3) | 109.5 |
| H(6B2)-C(6B)-H(6B3) | 109.5 |
| C(5B)-C(7B)-H(7B1) | 109.5 |
| C(5B)-C(7B)-H(7B2) | 109.5 |
| H(7B1)-C(7B)-H(7B2) | 109.5 |
| C(5B)-C(7B)-H(7B3) | 109.5 |
| H(7B1)-C(7B)-H(7B3) | 109.5 |
| H(7B2)-C(7B)-H(7B3) | 109.5 |
| C(5B)-C(8B)-H(8B1) | 109.5 |
| C(5B)-C(8B)-H(8B2) | 109.5 |
| H(8B1)-C(8B)-H(8B2) | 109.5 |

| | |
|---|---|
| C(5B)-C(8B)-H(8B3) | 109.5 |
| H(8B1)-C(8B)-H(8B3) | 109.5 |
| H(8B2)-C(8B)-H(8B3) | 109.5 |
| C(2B)-B(3B)-C(1B) | 58.2(2) |
| C(2B)-B(3B)-B(8B) | 103.9(3) |
| C(1B)-B(3B)-B(8B) | 105.6(3) |
| C(2B)-B(3B)-B(7B) | 58.6(2) |
| C(1B)-B(3B)-B(7B) | 106.7(3) |
| B(8B)-B(3B)-B(7B) | 60.0(2) |
| C(2B)-B(3B)-B(4B) | 104.4(3) |
| C(1B)-B(3B)-B(4B) | 58.9(2) |
| B(8B)-B(3B)-B(4B) | 59.6(2) |
| B(7B)-B(3B)-B(4B) | 108.1(3) |
| C(2B)-B(3B)-H(3B) | 120.1(19) |
| C(1B)-B(3B)-H(3B) | 120.0(19) |
| B(8B)-B(3B)-H(3B) | 128.1(19) |
| B(7B)-B(3B)-H(3B) | 121.3(19) |
| B(4B)-B(3B)-H(3B) | 125.3(19) |
| C(1B)-B(4B)-B(8B) | 106.0(3) |
| C(1B)-B(4B)-B(9B) | 105.5(3) |
| B(8B)-B(4B)-B(9B) | 60.3(2) |
| C(1B)-B(4B)-B(5B) | 58.2(2) |
| B(8B)-B(4B)-B(5B) | 108.0(3) |
| B(9B)-B(4B)-B(5B) | 60.1(2) |
| C(1B)-B(4B)-B(3B) | 59.3(2) |
| B(8B)-B(4B)-B(3B) | 59.8(2) |
| B(9B)-B(4B)-B(3B) | 107.8(3) |
| B(5B)-B(4B)-B(3B) | 107.2(3) |
| C(1B)-B(4B)-H(4B) | 122.3(17) |
| B(8B)-B(4B)-H(4B) | 123.8(16) |
| B(9B)-B(4B)-H(4B) | 122.7(16) |
| B(5B)-B(4B)-H(4B) | 120.5(16) |
| B(3B)-B(4B)-H(4B) | 122.3(16) |
| C(1B)-B(5B)-B(10B) | 106.8(3) |
| C(1B)-B(5B)-B(4B) | 59.5(2) |
| B(10B)-B(5B)-B(4B) | 108.3(3) |
| C(1B)-B(5B)-B(6B) | 60.3(2) |
| B(10B)-B(5B)-B(6B) | 59.8(2) |
| B(4B)-B(5B)-B(6B) | 109.1(3) |

| | |
|---|---|
| C(1B)-B(5B)-B(9B) | 106.4(3) |
| B(10B)-B(5B)-B(9B) | 60.0(2) |
| B(4B)-B(5B)-B(9B) | 59.9(2) |
| B(6B)-B(5B)-B(9B) | 108.1(3) |
| C(1B)-B(5B)-H(5B) | 121.2(18) |
| B(10B)-B(5B)-H(5B) | 122.7(18) |
| B(4B)-B(5B)-H(5B) | 121.8(18) |
| B(6B)-B(5B)-H(5B) | 119.4(19) |
| B(9B)-B(5B)-H(5B) | 124.3(19) |
| C(2B)-B(6B)-C(1B) | 57.62(18) |
| C(2B)-B(6B)-B(10B) | 103.5(3) |
| C(1B)-B(6B)-B(10B) | 105.0(3) |
| C(2B)-B(6B)-B(11B) | 58.1(2) |
| C(1B)-B(6B)-B(11B) | 105.6(3) |
| B(10B)-B(6B)-B(11B) | 60.0(2) |
| C(2B)-B(6B)-B(5B) | 102.9(3) |
| C(1B)-B(6B)-B(5B) | 57.8(2) |
| B(10B)-B(6B)-B(5B) | 60.0(2) |
| B(11B)-B(6B)-B(5B) | 107.5(3) |
| C(2B)-B(6B)-H(6B) | 119.8(15) |
| C(1B)-B(6B)-H(6B) | 116.4(16) |
| B(10B)-B(6B)-H(6B) | 131.2(15) |
| B(11B)-B(6B)-H(6B) | 125.5(17) |
| B(5B)-B(6B)-H(6B) | 123.6(16) |
| C(2B)-B(7B)-B(8B) | 103.5(3) |
| C(2B)-B(7B)-B(3B) | 58.2(2) |
| B(8B)-B(7B)-B(3B) | 59.8(2) |
| C(2B)-B(7B)-B(12B) | 103.1(3) |
| B(8B)-B(7B)-B(12B) | 60.1(2) |
| B(3B)-B(7B)-B(12B) | 107.5(3) |
| C(2B)-B(7B)-B(11B) | 57.9(2) |
| B(8B)-B(7B)-B(11B) | 107.5(3) |
| B(3B)-B(7B)-B(11B) | 107.2(3) |
| B(12B)-B(7B)-B(11B) | 59.5(2) |
| C(2B)-B(7B)-H(7B) | 122.5(19) |
| B(8B)-B(7B)-H(7B) | 122.3(19) |
| B(3B)-B(7B)-H(7B) | 116.2(18) |
| B(12B)-B(7B)-H(7B) | 128.3(18) |
| B(11B)-B(7B)-H(7B) | 125.2(19) |

| | |
|---|---|
| B(4B)-B(8B)-B(3B) | 60.5(2) |
| B(4B)-B(8B)-B(7B) | 109.0(3) |
| B(3B)-B(8B)-B(7B) | 60.3(2) |
| B(4B)-B(8B)-B(9B) | 60.2(2) |
| B(3B)-B(8B)-B(9B) | 108.3(3) |
| B(7B)-B(8B)-B(9B) | 108.2(3) |
| B(4B)-B(8B)-B(12B) | 107.9(3) |
| B(3B)-B(8B)-B(12B) | 108.0(3) |
| B(7B)-B(8B)-B(12B) | 60.2(2) |
| B(9B)-B(8B)-B(12B) | 59.3(2) |
| B(4B)-B(8B)-H(8B) | 121(2) |
| B(3B)-B(8B)-H(8B) | 120(2) |
| B(7B)-B(8B)-H(8B) | 121(2) |
| B(9B)-B(8B)-H(8B) | 123(2) |
| B(12B)-B(8B)-H(8B) | 123(2) |
| B(12B)-B(9B)-B(10B) | 60.2(2) |
| B(12B)-B(9B)-B(4B) | 108.1(3) |
| B(10B)-B(9B)-B(4B) | 108.2(3) |
| B(12B)-B(9B)-B(8B) | 60.3(2) |
| B(10B)-B(9B)-B(8B) | 108.2(3) |
| B(4B)-B(9B)-B(8B) | 59.5(2) |
| B(12B)-B(9B)-B(5B) | 107.8(3) |
| B(10B)-B(9B)-B(5B) | 59.8(2) |
| B(4B)-B(9B)-B(5B) | 60.0(2) |
| B(8B)-B(9B)-B(5B) | 107.3(3) |
| B(12B)-B(9B)-H(9B) | 123.2(16) |
| B(10B)-B(9B)-H(9B) | 123.4(15) |
| B(4B)-B(9B)-H(9B) | 119.5(15) |
| B(8B)-B(9B)-H(9B) | 121.0(15) |
| B(5B)-B(9B)-H(9B) | 121.6(15) |
| B(6B)-B(10B)-B(11B) | 60.1(2) |
| B(6B)-B(10B)-B(5B) | 60.3(2) |
| B(11B)-B(10B)-B(5B) | 107.8(3) |
| B(6B)-B(10B)-B(12B) | 108.2(3) |
| B(11B)-B(10B)-B(12B) | 59.9(2) |
| B(5B)-B(10B)-B(12B) | 107.5(3) |
| B(6B)-B(10B)-B(9B) | 108.7(3) |
| B(11B)-B(10B)-B(9B) | 107.7(3) |
| B(5B)-B(10B)-B(9B) | 60.2(2) |

B(12B)-B(10B)-B(9B) 59.5(2)
B(6B)-B(10B)-H(10B) 118.7(16)
B(11B)-B(10B)-H(10B) 117.6(16)
B(5B)-B(10B)-H(10B) 124.6(16)
B(12B)-B(10B)-H(10B) 121.7(16)
B(9B)-B(10B)-H(10B) 125.8(16)
C(2B)-B(11B)-B(12B) 103.8(3)
C(2B)-B(11B)-B(10B) 104.2(3)
B(12B)-B(11B)-B(10B) 60.1(2)
C(2B)-B(11B)-B(6B) 59.1(2)
B(12B)-B(11B)-B(6B) 108.3(3)
B(10B)-B(11B)-B(6B) 59.9(2)
C(2B)-B(11B)-B(7B) 58.3(2)
B(12B)-B(11B)-B(7B) 60.0(2)
B(10B)-B(11B)-B(7B) 108.3(3)
B(6B)-B(11B)-B(7B) 108.8(3)
C(2B)-B(11B)-H(11B) 118(2)
B(12B)-B(11B)-H(11B) 127(2)
B(10B)-B(11B)-H(11B) 128.6(19)
B(6B)-B(11B)-H(11B) 120(2)
B(7B)-B(11B)-H(11B) 117.7(19)
B(9B)-B(12B)-B(11B) 108.4(3)
B(9B)-B(12B)-B(10B) 60.3(2)
B(11B)-B(12B)-B(10B) 59.9(2)
B(9B)-B(12B)-B(8B) 60.3(2)
B(11B)-B(12B)-B(8B) 107.9(3)
B(10B)-B(12B)-B(8B) 108.3(3)
B(9B)-B(12B)-B(7B) 108.5(3)
B(11B)-B(12B)-B(7B) 60.5(2)
B(10B)-B(12B)-B(7B) 108.6(3)
B(8B)-B(12B)-B(7B) 59.6(2)
B(9B)-B(12B)-I(1B) 122.6(2)
B(11B)-B(12B)-I(1B) 120.5(2)
B(10B)-B(12B)-I(1B) 121.7(2)
B(8B)-B(12B)-I(1B) 122.4(2)
B(7B)-B(12B)-I(1B) 120.4(2)
C(4C)-Si(1C)-C(3C) 110.16(18)
C(4C)-Si(1C)-C(5C) 110.28(17)
C(3C)-Si(1C)-C(5C) 111.17(18)

| | |
|---|---|
| C(4C)-Si(1C)-C(1C) | 106.41(16) |
| C(3C)-Si(1C)-C(1C) | 106.01(15) |
| C(5C)-Si(1C)-C(1C) | 112.63(14) |
| C(2C)-C(1C)-B(4C) | 107.5(3) |
| C(2C)-C(1C)-B(5C) | 107.1(2) |
| B(4C)-C(1C)-B(5C) | 61.6(2) |
| C(2C)-C(1C)-B(3C) | 59.6(2) |
| B(4C)-C(1C)-B(3C) | 62.2(2) |
| B(5C)-C(1C)-B(3C) | 112.2(3) |
| C(2C)-C(1C)-B(6C) | 59.9(2) |
| B(4C)-C(1C)-B(6C) | 112.1(2) |
| B(5C)-C(1C)-B(6C) | 61.5(2) |
| B(3C)-C(1C)-B(6C) | 111.8(3) |
| C(2C)-C(1C)-Si(1C) | 117.9(2) |
| B(4C)-C(1C)-Si(1C) | 123.8(2) |
| B(5C)-C(1C)-Si(1C) | 126.1(2) |
| B(3C)-C(1C)-Si(1C) | 115.3(2) |
| B(6C)-C(1C)-Si(1C) | 118.5(2) |
| C(1C)-C(2C)-B(11C) | 114.0(3) |
| C(1C)-C(2C)-B(7C) | 113.7(3) |
| B(11C)-C(2C)-B(7C) | 64.4(2) |
| C(1C)-C(2C)-B(3C) | 62.4(2) |
| B(11C)-C(2C)-B(3C) | 117.0(3) |
| B(7C)-C(2C)-B(3C) | 62.9(2) |
| C(1C)-C(2C)-B(6C) | 62.3(2) |
| B(11C)-C(2C)-B(6C) | 63.4(2) |
| B(7C)-C(2C)-B(6C) | 117.0(3) |
| B(3C)-C(2C)-B(6C) | 116.2(3) |
| C(1C)-C(2C)-H(2C) | 116(2) |
| B(11C)-C(2C)-H(2C) | 121(2) |
| B(7C)-C(2C)-H(2C) | 118(2) |
| B(3C)-C(2C)-H(2C) | 113(2) |
| B(6C)-C(2C)-H(2C) | 117.3(19) |
| Si(1C)-C(3C)-H(3C1) | 109.5 |
| Si(1C)-C(3C)-H(3C2) | 109.5 |
| H(3C1)-C(3C)-H(3C2) | 109.5 |
| Si(1C)-C(3C)-H(3C3) | 109.5 |
| H(3C1)-C(3C)-H(3C3) | 109.5 |
| H(3C2)-C(3C)-H(3C3) | 109.5 |

| | |
|---|---|
| Si(1C)-C(4C)-H(4C1) | 109.5 |
| Si(1C)-C(4C)-H(4C2) | 109.5 |
| H(4C1)-C(4C)-H(4C2) | 109.5 |
| Si(1C)-C(4C)-H(4C3) | 109.5 |
| H(4C1)-C(4C)-H(4C3) | 109.5 |
| H(4C2)-C(4C)-H(4C3) | 109.5 |
| C(6C)-C(5C)-C(7C) | 110.2(3) |
| C(6C)-C(5C)-C(8C) | 106.8(3) |
| C(7C)-C(5C)-C(8C) | 107.4(3) |
| C(6C)-C(5C)-Si(1C) | 112.9(3) |
| C(7C)-C(5C)-Si(1C) | 112.7(3) |
| C(8C)-C(5C)-Si(1C) | 106.3(3) |
| C(5C)-C(6C)-H(6C1) | 109.5 |
| C(5C)-C(6C)-H(6C2) | 109.5 |
| H(6C1)-C(6C)-H(6C2) | 109.5 |
| C(5C)-C(6C)-H(6C3) | 109.5 |
| H(6C1)-C(6C)-H(6C3) | 109.5 |
| H(6C2)-C(6C)-H(6C3) | 109.5 |
| C(5C)-C(7C)-H(7C1) | 109.5 |
| C(5C)-C(7C)-H(7C2) | 109.5 |
| H(7C1)-C(7C)-H(7C2) | 109.5 |
| C(5C)-C(7C)-H(7C3) | 109.5 |
| H(7C1)-C(7C)-H(7C3) | 109.5 |
| H(7C2)-C(7C)-H(7C3) | 109.5 |
| C(5C)-C(8C)-H(8C1) | 109.5 |
| C(5C)-C(8C)-H(8C2) | 109.5 |
| H(8C1)-C(8C)-H(8C2) | 109.5 |
| C(5C)-C(8C)-H(8C3) | 109.5 |
| H(8C1)-C(8C)-H(8C3) | 109.5 |
| H(8C2)-C(8C)-H(8C3) | 109.5 |
| C(2C)-B(3C)-C(1C) | 58.03(19) |
| C(2C)-B(3C)-B(7C) | 58.3(2) |
| C(1C)-B(3C)-B(7C) | 106.4(3) |
| C(2C)-B(3C)-B(8C) | 103.5(3) |
| C(1C)-B(3C)-B(8C) | 105.5(3) |
| B(7C)-B(3C)-B(8C) | 59.9(2) |
| C(2C)-B(3C)-B(4C) | 103.0(3) |
| C(1C)-B(3C)-B(4C) | 58.0(2) |
| B(7C)-B(3C)-B(4C) | 107.5(3) |

| | |
|---|---|
| B(8C)-B(3C)-B(4C) | 59.9(2) |
| C(2C)-B(3C)-H(3C) | 118.5(15) |
| C(1C)-B(3C)-H(3C) | 119.3(15) |
| B(7C)-B(3C)-H(3C) | 120.9(15) |
| B(8C)-B(3C)-H(3C) | 129.8(15) |
| B(4C)-B(3C)-H(3C) | 127.5(15) |
| C(1C)-B(4C)-B(5C) | 59.4(2) |
| C(1C)-B(4C)-B(9C) | 106.9(3) |
| B(5C)-B(4C)-B(9C) | 60.5(2) |
| C(1C)-B(4C)-B(8C) | 106.9(3) |
| B(5C)-B(4C)-B(8C) | 108.5(3) |
| B(9C)-B(4C)-B(8C) | 60.1(2) |
| C(1C)-B(4C)-B(3C) | 59.8(2) |
| B(5C)-B(4C)-B(3C) | 108.5(3) |
| B(9C)-B(4C)-B(3C) | 108.2(3) |
| B(8C)-B(4C)-B(3C) | 59.9(2) |
| C(1C)-B(4C)-H(4C) | 120.0(16) |
| B(5C)-B(4C)-H(4C) | 124.3(16) |
| B(9C)-B(4C)-H(4C) | 126.5(16) |
| B(8C)-B(4C)-H(4C) | 121.5(17) |
| B(3C)-B(4C)-H(4C) | 116.5(16) |
| C(1C)-B(5C)-B(4C) | 58.98(19) |
| C(1C)-B(5C)-B(10C) | 106.9(3) |
| B(4C)-B(5C)-B(10C) | 109.0(3) |
| C(1C)-B(5C)-B(6C) | 60.0(2) |
| B(4C)-B(5C)-B(6C) | 108.7(3) |
| B(10C)-B(5C)-B(6C) | 59.9(2) |
| C(1C)-B(5C)-B(9C) | 106.4(3) |
| B(4C)-B(5C)-B(9C) | 60.2(2) |
| B(10C)-B(5C)-B(9C) | 60.8(2) |
| B(6C)-B(5C)-B(9C) | 108.8(3) |
| C(1C)-B(5C)-H(5C) | 118.6(17) |
| B(4C)-B(5C)-H(5C) | 121.1(18) |
| B(10C)-B(5C)-H(5C) | 124.2(18) |
| B(6C)-B(5C)-H(5C) | 118.2(18) |
| B(9C)-B(5C)-H(5C) | 126.2(18) |
| C(2C)-B(6C)-C(1C) | 57.88(19) |
| C(2C)-B(6C)-B(10C) | 103.4(3) |
| C(1C)-B(6C)-B(10C) | 105.8(3) |

| | |
|---|---|
| C(2C)-B(6C)-B(5C) | 103.3(3) |
| C(1C)-B(6C)-B(5C) | 58.5(2) |
| B(10C)-B(6C)-B(5C) | 60.0(2) |
| C(2C)-B(6C)-B(11C) | 57.9(2) |
| C(1C)-B(6C)-B(11C) | 106.0(3) |
| B(10C)-B(6C)-B(11C) | 59.9(2) |
| B(5C)-B(6C)-B(11C) | 107.5(3) |
| C(2C)-B(6C)-H(6C) | 123.1(15) |
| C(1C)-B(6C)-H(6C) | 118.9(15) |
| B(10C)-B(6C)-H(6C) | 127.2(14) |
| B(5C)-B(6C)-H(6C) | 122.5(15) |
| B(11C)-B(6C)-H(6C) | 124.7(15) |
| C(2C)-B(7C)-B(3C) | 58.8(2) |
| C(2C)-B(7C)-B(12C) | 102.5(3) |
| B(3C)-B(7C)-B(12C) | 108.2(3) |
| C(2C)-B(7C)-B(8C) | 104.3(3) |
| B(3C)-B(7C)-B(8C) | 60.4(2) |
| B(12C)-B(7C)-B(8C) | 60.6(2) |
| C(2C)-B(7C)-B(11C) | 57.8(2) |
| B(3C)-B(7C)-B(11C) | 108.0(3) |
| B(12C)-B(7C)-B(11C) | 59.0(2) |
| B(8C)-B(7C)-B(11C) | 108.1(3) |
| C(2C)-B(7C)-H(7C) | 117.2(16) |
| B(3C)-B(7C)-H(7C) | 116.0(16) |
| B(12C)-B(7C)-H(7C) | 131.2(16) |
| B(8C)-B(7C)-H(7C) | 127.4(17) |
| B(11C)-B(7C)-H(7C) | 120.7(17) |
| B(7C)-B(8C)-B(9C) | 107.9(3) |
| B(7C)-B(8C)-B(3C) | 59.7(2) |
| B(9C)-B(8C)-B(3C) | 108.1(3) |
| B(7C)-B(8C)-B(4C) | 107.5(3) |
| B(9C)-B(8C)-B(4C) | 59.7(2) |
| B(3C)-B(8C)-B(4C) | 60.1(2) |
| B(7C)-B(8C)-B(12C) | 59.7(2) |
| B(9C)-B(8C)-B(12C) | 59.4(2) |
| B(3C)-B(8C)-B(12C) | 106.9(3) |
| B(4C)-B(8C)-B(12C) | 106.4(3) |
| B(7C)-B(8C)-H(8C) | 121(2) |
| B(9C)-B(8C)-H(8C) | 123.6(19) |

| | |
|---|---|
| B(3C)-B(8C)-H(8C) | 119.3(19) |
| B(4C)-B(8C)-H(8C) | 121(2) |
| B(12C)-B(8C)-H(8C) | 125(2) |
| B(12C)-B(9C)-B(4C) | 107.7(3) |
| B(12C)-B(9C)-B(5C) | 106.9(3) |
| B(4C)-B(9C)-B(5C) | 59.3(2) |
| B(12C)-B(9C)-B(8C) | 60.5(2) |
| B(4C)-B(9C)-B(8C) | 60.2(2) |
| B(5C)-B(9C)-B(8C) | 107.8(3) |
| B(12C)-B(9C)-B(10C) | 59.7(2) |
| B(4C)-B(9C)-B(10C) | 107.2(3) |
| B(5C)-B(9C)-B(10C) | 59.4(2) |
| B(8C)-B(9C)-B(10C) | 108.5(3) |
| B(12C)-B(9C)-H(9C) | 123.2(17) |
| B(4C)-B(9C)-H(9C) | 123.1(16) |
| B(5C)-B(9C)-H(9C) | 119.5(16) |
| B(8C)-B(9C)-H(9C) | 124.8(16) |
| B(10C)-B(9C)-H(9C) | 119.0(16) |
| B(6C)-B(10C)-B(5C) | 60.1(2) |
| B(6C)-B(10C)-B(11C) | 60.5(2) |
| B(5C)-B(10C)-B(11C) | 108.0(3) |
| B(6C)-B(10C)-B(12C) | 107.7(3) |
| B(5C)-B(10C)-B(12C) | 106.9(3) |
| B(11C)-B(10C)-B(12C) | 59.5(2) |
| B(6C)-B(10C)-B(9C) | 108.0(3) |
| B(5C)-B(10C)-B(9C) | 59.8(2) |
| B(11C)-B(10C)-B(9C) | 107.5(3) |
| B(12C)-B(10C)-B(9C) | 59.4(2) |
| B(6C)-B(10C)-H(10C) | 122.1(15) |
| B(5C)-B(10C)-H(10C) | 123.0(17) |
| B(11C)-B(10C)-H(10C) | 121.1(17) |
| B(12C)-B(10C)-H(10C) | 121.5(16) |
| B(9C)-B(10C)-H(10C) | 121.9(16) |
| C(2C)-B(11C)-B(12C) | 103.1(3) |
| C(2C)-B(11C)-B(10C) | 103.9(3) |
| B(12C)-B(11C)-B(10C) | 60.3(2) |
| C(2C)-B(11C)-B(6C) | 58.8(2) |
| B(12C)-B(11C)-B(6C) | 107.6(3) |
| B(10C)-B(11C)-B(6C) | 59.6(2) |

| | |
|---|---|
| C(2C)-B(11C)-B(7C) | 57.8(2) |
| B(12C)-B(11C)-B(7C) | 59.7(2) |
| B(10C)-B(11C)-B(7C) | 108.1(3) |
| B(6C)-B(11C)-B(7C) | 107.7(3) |
| C(2C)-B(11C)-H(11C) | 120.6(15) |
| B(12C)-B(11C)-H(11C) | 126.8(16) |
| B(10C)-B(11C)-H(11C) | 126.7(15) |
| B(6C)-B(11C)-H(11C) | 120.1(16) |
| B(7C)-B(11C)-H(11C) | 119.5(15) |
| B(11C)-B(12C)-B(9C) | 109.3(3) |
| B(11C)-B(12C)-B(7C) | 61.3(2) |
| B(9C)-B(12C)-B(7C) | 108.4(3) |
| B(11C)-B(12C)-B(10C) | 60.2(2) |
| B(9C)-B(12C)-B(10C) | 60.9(2) |
| B(7C)-B(12C)-B(10C) | 109.3(2) |
| B(11C)-B(12C)-B(8C) | 109.3(3) |
| B(9C)-B(12C)-B(8C) | 60.0(2) |
| B(7C)-B(12C)-B(8C) | 59.7(2) |
| B(10C)-B(12C)-B(8C) | 109.1(3) |
| B(11C)-B(12C)-I(1C) | 120.7(3) |
| B(9C)-B(12C)-I(1C) | 121.1(2) |
| B(7C)-B(12C)-I(1C) | 121.4(2) |
| B(10C)-B(12C)-I(1C) | 120.8(2) |
| B(8C)-B(12C)-I(1C) | 121.5(2) |
| C(4D)-Si(1D)-C(3D) | 110.53(17) |
| C(4D)-Si(1D)-C(5D) | 109.97(16) |
| C(3D)-Si(1D)-C(5D) | 110.78(17) |
| C(4D)-Si(1D)-C(1D) | 106.34(15) |
| C(3D)-Si(1D)-C(1D) | 107.05(15) |
| C(5D)-Si(1D)-C(1D) | 112.06(14) |
| C(2D)-C(1D)-B(4D) | 107.8(3) |
| C(2D)-C(1D)-B(5D) | 107.8(2) |
| B(4D)-C(1D)-B(5D) | 62.1(2) |
| C(2D)-C(1D)-B(6D) | 60.5(2) |
| B(4D)-C(1D)-B(6D) | 112.5(3) |
| B(5D)-C(1D)-B(6D) | 61.5(2) |
| C(2D)-C(1D)-B(3D) | 59.7(2) |
| B(4D)-C(1D)-B(3D) | 61.8(2) |
| B(5D)-C(1D)-B(3D) | 112.4(3) |

| | |
|---|---|
| B(6D)-C(1D)-B(3D) | 112.2(3) |
| C(2D)-C(1D)-Si(1D) | 117.0(2) |
| B(4D)-C(1D)-Si(1D) | 124.3(2) |
| B(5D)-C(1D)-Si(1D) | 125.8(2) |
| B(6D)-C(1D)-Si(1D) | 117.6(2) |
| B(3D)-C(1D)-Si(1D) | 115.8(2) |
| C(1D)-C(2D)-B(7D) | 113.7(3) |
| C(1D)-C(2D)-B(3D) | 62.3(2) |
| B(7D)-C(2D)-B(3D) | 63.4(2) |
| C(1D)-C(2D)-B(11D) | 113.4(3) |
| B(7D)-C(2D)-B(11D) | 63.9(2) |
| B(3D)-C(2D)-B(11D) | 116.8(3) |
| C(1D)-C(2D)-B(6D) | 61.8(2) |
| B(7D)-C(2D)-B(6D) | 116.1(3) |
| B(3D)-C(2D)-B(6D) | 115.6(3) |
| B(11D)-C(2D)-B(6D) | 63.0(2) |
| C(1D)-C(2D)-H(2D) | 117(2) |
| B(7D)-C(2D)-H(2D) | 121(2) |
| B(3D)-C(2D)-H(2D) | 119(2) |
| B(11D)-C(2D)-H(2D) | 117(2) |
| B(6D)-C(2D)-H(2D) | 113(2) |
| Si(1D)-C(3D)-H(3D1) | 109.5 |
| Si(1D)-C(3D)-H(3D2) | 109.5 |
| H(3D1)-C(3D)-H(3D2) | 109.5 |
| Si(1D)-C(3D)-H(3D3) | 109.5 |
| H(3D1)-C(3D)-H(3D3) | 109.5 |
| H(3D2)-C(3D)-H(3D3) | 109.5 |
| Si(1D)-C(4D)-H(4D1) | 109.5 |
| Si(1D)-C(4D)-H(4D2) | 109.5 |
| H(4D1)-C(4D)-H(4D2) | 109.5 |
| Si(1D)-C(4D)-H(4D3) | 109.5 |
| H(4D1)-C(4D)-H(4D3) | 109.5 |
| H(4D2)-C(4D)-H(4D3) | 109.5 |
| C(6D)-C(5D)-C(7D) | 107.3(3) |
| C(6D)-C(5D)-C(8D) | 110.3(3) |
| C(7D)-C(5D)-C(8D) | 107.5(3) |
| C(6D)-C(5D)-Si(1D) | 113.5(2) |
| C(7D)-C(5D)-Si(1D) | 106.8(2) |
| C(8D)-C(5D)-Si(1D) | 111.1(3) |

| | |
|---|---|
| C(5D)-C(6D)-H(6D1) | 109.5 |
| C(5D)-C(6D)-H(6D2) | 109.5 |
| H(6D1)-C(6D)-H(6D2) | 109.5 |
| C(5D)-C(6D)-H(6D3) | 109.5 |
| H(6D1)-C(6D)-H(6D3) | 109.5 |
| H(6D2)-C(6D)-H(6D3) | 109.5 |
| C(5D)-C(7D)-H(7D1) | 109.5 |
| C(5D)-C(7D)-H(7D2) | 109.5 |
| H(7D1)-C(7D)-H(7D2) | 109.5 |
| C(5D)-C(7D)-H(7D3) | 109.5 |
| H(7D1)-C(7D)-H(7D3) | 109.5 |
| H(7D2)-C(7D)-H(7D3) | 109.5 |
| C(5D)-C(8D)-H(8D1) | 109.5 |
| C(5D)-C(8D)-H(8D2) | 109.5 |
| H(8D1)-C(8D)-H(8D2) | 109.5 |
| C(5D)-C(8D)-H(8D3) | 109.5 |
| H(8D1)-C(8D)-H(8D3) | 109.5 |
| H(8D2)-C(8D)-H(8D3) | 109.5 |
| C(2D)-B(3D)-C(1D) | 58.00(19) |
| C(2D)-B(3D)-B(8D) | 103.7(3) |
| C(1D)-B(3D)-B(8D) | 105.7(2) |
| C(2D)-B(3D)-B(4D) | 103.9(3) |
| C(1D)-B(3D)-B(4D) | 58.6(2) |
| B(8D)-B(3D)-B(4D) | 60.2(2) |
| C(2D)-B(3D)-B(7D) | 58.0(2) |
| C(1D)-B(3D)-B(7D) | 105.9(3) |
| B(8D)-B(3D)-B(7D) | 59.8(2) |
| B(4D)-B(3D)-B(7D) | 107.7(3) |
| C(2D)-B(3D)-H(3D) | 120.9(15) |
| C(1D)-B(3D)-H(3D) | 120.5(14) |
| B(8D)-B(3D)-H(3D) | 127.4(15) |
| B(4D)-B(3D)-H(3D) | 125.1(15) |
| B(7D)-B(3D)-H(3D) | 121.9(15) |
| C(1D)-B(4D)-B(5D) | 59.0(2) |
| C(1D)-B(4D)-B(3D) | 59.6(2) |
| B(5D)-B(4D)-B(3D) | 108.1(3) |
| C(1D)-B(4D)-B(9D) | 105.6(3) |
| B(5D)-B(4D)-B(9D) | 59.7(2) |
| B(3D)-B(4D)-B(9D) | 107.8(3) |

| | |
|---|---|
| C(1D)-B(4D)-B(8D) | 106.2(3) |
| B(5D)-B(4D)-B(8D) | 108.0(3) |
| B(3D)-B(4D)-B(8D) | 59.8(2) |
| B(9D)-B(4D)-B(8D) | 60.1(2) |
| C(1D)-B(4D)-H(4D) | 120.7(15) |
| B(5D)-B(4D)-H(4D) | 122.9(15) |
| B(3D)-B(4D)-H(4D) | 118.4(15) |
| B(9D)-B(4D)-H(4D) | 126.0(15) |
| B(8D)-B(4D)-H(4D) | 122.9(16) |
| C(1D)-B(5D)-B(6D) | 59.7(2) |
| C(1D)-B(5D)-B(9D) | 106.1(3) |
| B(6D)-B(5D)-B(9D) | 108.2(3) |
| C(1D)-B(5D)-B(10D) | 106.2(3) |
| B(6D)-B(5D)-B(10D) | 59.6(2) |
| B(9D)-B(5D)-B(10D) | 60.6(2) |
| C(1D)-B(5D)-B(4D) | 58.9(2) |
| B(6D)-B(5D)-B(4D) | 108.4(3) |
| B(9D)-B(5D)-B(4D) | 60.4(2) |
| B(10D)-B(5D)-B(4D) | 108.9(3) |
| C(1D)-B(5D)-H(5D) | 119.0(17) |
| B(6D)-B(5D)-H(5D) | 119.9(18) |
| B(9D)-B(5D)-H(5D) | 125.5(18) |
| B(10D)-B(5D)-H(5D) | 125.4(16) |
| B(4D)-B(5D)-H(5D) | 119.7(17) |
| C(2D)-B(6D)-C(1D) | 57.74(19) |
| C(2D)-B(6D)-B(10D) | 103.6(3) |
| C(1D)-B(6D)-B(10D) | 106.1(3) |
| C(2D)-B(6D)-B(5D) | 103.7(3) |
| C(1D)-B(6D)-B(5D) | 58.8(2) |
| B(10D)-B(6D)-B(5D) | 60.3(2) |
| C(2D)-B(6D)-B(11D) | 58.0(2) |
| C(1D)-B(6D)-B(11D) | 106.1(3) |
| B(10D)-B(6D)-B(11D) | 59.9(2) |
| B(5D)-B(6D)-B(11D) | 107.9(3) |
| C(2D)-B(6D)-H(6D) | 119.7(16) |
| C(1D)-B(6D)-H(6D) | 117.0(16) |
| B(10D)-B(6D)-H(6D) | 130.2(16) |
| B(5D)-B(6D)-H(6D) | 124.0(17) |
| B(11D)-B(6D)-H(6D) | 124.1(17) |

| | |
|---|---|
| C(2D)-B(7D)-B(12D) | 103.4(3) |
| C(2D)-B(7D)-B(8D) | 104.4(3) |
| B(12D)-B(7D)-B(8D) | 61.0(2) |
| C(2D)-B(7D)-B(3D) | 58.6(2) |
| B(12D)-B(7D)-B(3D) | 108.4(3) |
| B(8D)-B(7D)-B(3D) | 60.1(2) |
| C(2D)-B(7D)-B(11D) | 58.4(2) |
| B(12D)-B(7D)-B(11D) | 59.2(2) |
| B(8D)-B(7D)-B(11D) | 108.5(3) |
| B(3D)-B(7D)-B(11D) | 108.2(3) |
| C(2D)-B(7D)-H(7D) | 125.9(17) |
| B(12D)-B(7D)-H(7D) | 124.1(17) |
| B(8D)-B(7D)-H(7D) | 119.7(17) |
| B(3D)-B(7D)-H(7D) | 118.4(16) |
| B(11D)-B(7D)-H(7D) | 124.5(17) |
| B(7D)-B(8D)-B(3D) | 60.2(2) |
| B(7D)-B(8D)-B(4D) | 107.9(3) |
| B(3D)-B(8D)-B(4D) | 60.0(2) |
| B(7D)-B(8D)-B(9D) | 107.3(3) |
| B(3D)-B(8D)-B(9D) | 107.7(3) |
| B(4D)-B(8D)-B(9D) | 59.9(2) |
| B(7D)-B(8D)-B(12D) | 59.4(2) |
| B(3D)-B(8D)-B(12D) | 107.2(3) |
| B(4D)-B(8D)-B(12D) | 107.1(3) |
| B(9D)-B(8D)-B(12D) | 59.4(2) |
| B(7D)-B(8D)-H(8D) | 118.0(17) |
| B(3D)-B(8D)-H(8D) | 117.4(16) |
| B(4D)-B(8D)-H(8D) | 123.0(17) |
| B(9D)-B(8D)-H(8D) | 127.2(16) |
| B(12D)-B(8D)-H(8D) | 124.4(16) |
| B(5D)-B(9D)-B(12D) | 107.6(3) |
| B(5D)-B(9D)-B(4D) | 60.0(2) |
| B(12D)-B(9D)-B(4D) | 108.0(3) |
| B(5D)-B(9D)-B(8D) | 108.1(3) |
| B(12D)-B(9D)-B(8D) | 60.5(2) |
| B(4D)-B(9D)-B(8D) | 60.0(2) |
| B(5D)-B(9D)-B(10D) | 59.8(2) |
| B(12D)-B(9D)-B(10D) | 59.8(2) |
| B(4D)-B(9D)-B(10D) | 107.9(3) |

| | |
|---|---|
| B(8D)-B(9D)-B(10D) | 108.5(3) |
| B(5D)-B(9D)-H(9D) | 121.0(15) |
| B(12D)-B(9D)-H(9D) | 123.8(15) |
| B(4D)-B(9D)-H(9D) | 119.4(15) |
| B(8D)-B(9D)-H(9D) | 120.7(14) |
| B(10D)-B(9D)-H(9D) | 123.5(14) |
| B(6D)-B(10D)-B(11D) | 60.7(2) |
| B(6D)-B(10D)-B(5D) | 60.1(2) |
| B(11D)-B(10D)-B(5D) | 108.4(3) |
| B(6D)-B(10D)-B(12D) | 107.9(3) |
| B(11D)-B(10D)-B(12D) | 59.5(2) |
| B(5D)-B(10D)-B(12D) | 107.4(3) |
| B(6D)-B(10D)-B(9D) | 107.9(3) |
| B(11D)-B(10D)-B(9D) | 107.7(3) |
| B(5D)-B(10D)-B(9D) | 59.6(2) |
| B(12D)-B(10D)-B(9D) | 59.8(2) |
| B(6D)-B(10D)-H(10D) | 126.4(16) |
| B(11D)-B(10D)-H(10D) | 123.2(16) |
| B(5D)-B(10D)-H(10D) | 122.8(16) |
| B(12D)-B(10D)-H(10D) | 118.4(16) |
| B(9D)-B(10D)-H(10D) | 117.8(16) |
| C(2D)-B(11D)-B(12D) | 103.3(3) |
| C(2D)-B(11D)-B(10D) | 103.9(3) |
| B(12D)-B(11D)-B(10D) | 60.4(2) |
| C(2D)-B(11D)-B(6D) | 58.9(2) |
| B(12D)-B(11D)-B(6D) | 107.6(3) |
| B(10D)-B(11D)-B(6D) | 59.4(2) |
| C(2D)-B(11D)-B(7D) | 57.7(2) |
| B(12D)-B(11D)-B(7D) | 59.7(2) |
| B(10D)-B(11D)-B(7D) | 108.0(3) |
| B(6D)-B(11D)-B(7D) | 107.6(3) |
| C(2D)-B(11D)-H(11D) | 116.7(15) |
| B(12D)-B(11D)-H(11D) | 129.5(16) |
| B(10D)-B(11D)-H(11D) | 129.7(15) |
| B(6D)-B(11D)-H(11D) | 118.8(16) |
| B(7D)-B(11D)-H(11D) | 118.2(15) |
| B(11D)-B(12D)-B(7D) | 61.1(2) |
| B(11D)-B(12D)-B(10D) | 60.1(2) |
| B(7D)-B(12D)-B(10D) | 108.8(3) |

| | |
|---|---|
| B(11D)-B(12D)-B(9D) | 108.7(3) |
| B(7D)-B(12D)-B(9D) | 108.0(3) |
| B(10D)-B(12D)-B(9D) | 60.4(2) |
| B(11D)-B(12D)-B(8D) | 108.9(3) |
| B(7D)-B(12D)-B(8D) | 59.6(2) |
| B(10D)-B(12D)-B(8D) | 108.6(3) |
| B(9D)-B(12D)-B(8D) | 60.1(2) |
| B(11D)-B(12D)-I(1D) | 120.5(2) |
| B(7D)-B(12D)-I(1D) | 121.6(2) |
| B(10D)-B(12D)-I(1D) | 120.9(2) |
| B(9D)-B(12D)-I(1D) | 121.8(2) |
| B(8D)-B(12D)-I(1D) | 122.1(2) |

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| I(1A) | 35(1) | 32(1) | 41(1) | -11(1) | -5(1) | 12(1) |
| Si(1A) | 21(1) | 24(1) | 27(1) | -2(1) | 1(1) | 1(1) |
| C(1A) | 24(2) | 27(2) | 21(2) | -2(1) | -1(1) | -2(1) |
| C(2A) | 18(2) | 28(2) | 26(2) | -5(2) | -5(1) | 2(2) |
| C(3A) | 33(2) | 28(2) | 38(2) | -4(2) | -3(2) | 8(2) |
| C(4A) | 40(2) | 29(2) | 47(2) | 0(2) | 8(2) | -1(2) |
| C(5A) | 30(2) | 32(2) | 28(2) | -7(2) | 4(2) | 3(2) |
| C(6A) | 57(3) | 37(2) | 50(2) | -14(2) | 17(2) | 8(2) |
| C(7A) | 45(2) | 44(2) | 34(2) | -14(2) | -6(2) | -12(2) |
| C(8A) | 34(2) | 46(2) | 28(2) | -3(2) | 9(2) | 4(2) |
| B(3A) | 30(2) | 22(2) | 28(2) | -2(2) | 3(2) | 0(2) |
| B(4A) | 30(2) | 34(2) | 24(2) | -3(2) | -5(2) | 11(2) |
| B(5A) | 19(2) | 33(2) | 36(3) | -2(2) | 1(2) | -2(2) |
| B(6A) | 29(2) | 33(2) | 22(2) | -1(2) | 7(2) | 3(2) |
| B(7A) | 25(2) | 29(2) | 36(2) | -4(2) | 2(2) | 3(2) |
| B(8A) | 41(2) | 30(2) | 25(2) | 3(2) | 8(2) | 10(2) |
| B(9A) | 26(2) | 37(2) | 25(2) | -8(2) | -5(2) | 9(2) |
| B(10A) | 24(2) | 32(2) | 38(3) | 0(2) | 0(2) | 7(2) |
| B(11A) | 32(2) | 29(2) | 21(2) | -4(2) | -2(2) | 8(2) |
| B(12A) | 29(2) | 27(2) | 24(2) | -7(2) | -2(2) | 4(2) |
| I(1B) | 47(1) | 28(1) | 32(1) | 8(1) | -6(1) | -8(1) |
| Si(1B) | 25(1) | 23(1) | 27(1) | 0(1) | -2(1) | -1(1) |
| C(1B) | 21(2) | 29(2) | 19(2) | 2(1) | -4(1) | -2(1) |
| C(2B) | 36(2) | 29(2) | 24(2) | 6(2) | -12(2) | -14(2) |
| C(3B) | 33(2) | 25(2) | 56(3) | 0(2) | 1(2) | -2(2) |
| C(4B) | 36(2) | 31(2) | 32(2) | -3(2) | -2(2) | -10(2) |
| C(5B) | 30(2) | 32(2) | 26(2) | 7(2) | -5(2) | 1(2) |
| C(6B) | 50(2) | 47(3) | 28(2) | 7(2) | -9(2) | -10(2) |
| C(7B) | 42(2) | 44(2) | 34(2) | 7(2) | 9(2) | 0(2) |
| C(8B) | 46(2) | 41(2) | 35(2) | 9(2) | -2(2) | -5(2) |
| B(3B) | 21(2) | 34(2) | 43(3) | 7(2) | 1(2) | -1(2) |
| B(4B) | 45(2) | 26(2) | 20(2) | -4(2) | 6(2) | 3(2) |
| B(5B) | 27(2) | 22(2) | 39(3) | 3(2) | -10(2) | -4(2) |
| B(6B) | 35(2) | 20(2) | 35(2) | -1(2) | 14(2) | -1(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B(7B) | 31(2) | 34(2) | 49(3) | 9(2) | -15(2) | -5(2) |
| B(8B) | 36(2) | 28(2) | 36(3) | 1(2) | 11(2) | 6(2) |
| B(9B) | 39(2) | 27(2) | 23(2) | 1(2) | -6(2) | -2(2) |
| B(10B) | 32(2) | 24(2) | 35(2) | -2(2) | 2(2) | 0(2) |
| B(11B) | 45(2) | 38(2) | 21(3) | 3(2) | 1(2) | -8(2) |
| B(12B) | 33(2) | 25(2) | 25(2) | 5(2) | -6(2) | -3(2) |
| I(1C) | 31(1) | 34(1) | 47(1) | 18(1) | -3(1) | -7(1) |
| Si(1C) | 29(1) | 29(1) | 26(1) | -3(1) | 6(1) | -6(1) |
| C(1C) | 27(2) | 24(2) | 21(2) | -4(1) | -2(1) | 4(1) |
| C(2C) | 27(2) | 26(2) | 28(2) | 1(2) | -6(2) | -6(2) |
| C(3C) | 54(2) | 53(3) | 37(2) | -5(2) | 7(2) | -34(2) |
| C(4C) | 35(2) | 55(3) | 48(3) | 5(2) | 15(2) | 3(2) |
| C(5C) | 38(2) | 31(2) | 38(2) | 7(2) | 13(2) | -3(2) |
| C(6C) | 56(2) | 38(2) | 64(3) | 12(2) | 12(2) | 9(2) |
| C(7C) | 48(2) | 60(3) | 34(2) | 12(2) | -4(2) | 5(2) |
| C(8C) | 59(3) | 60(3) | 68(3) | 31(3) | 19(2) | -2(2) |
| B(3C) | 29(2) | 23(2) | 36(2) | -1(2) | 1(2) | 3(2) |
| B(4C) | 28(2) | 22(2) | 29(2) | -9(2) | -2(2) | -2(2) |
| B(5C) | 21(2) | 32(2) | 23(2) | -1(2) | -3(2) | -3(2) |
| B(6C) | 31(2) | 26(2) | 23(2) | -1(2) | 7(2) | -5(2) |
| B(7C) | 25(2) | 26(2) | 35(3) | 7(2) | -5(2) | -1(2) |
| B(8C) | 32(2) | 23(2) | 40(3) | -4(2) | -1(2) | 0(2) |
| B(9C) | 28(2) | 30(2) | 33(2) | -2(2) | -5(2) | -4(2) |
| B(10C) | 23(2) | 27(2) | 32(2) | 7(2) | 4(2) | 1(2) |
| B(11C) | 26(2) | 29(2) | 22(2) | -7(2) | 2(2) | -3(2) |
| B(12C) | 25(2) | 22(2) | 27(2) | 5(2) | -3(2) | -1(2) |
| I(1D) | 32(1) | 27(1) | 28(1) | -4(1) | 0(1) | 7(1) |
| Si(1D) | 21(1) | 26(1) | 34(1) | -4(1) | 4(1) | 2(1) |
| C(1D) | 21(2) | 23(2) | 26(2) | -1(1) | 0(1) | 1(1) |
| C(2D) | 31(2) | 30(2) | 20(2) | 6(2) | 3(1) | 8(2) |
| C(3D) | 45(2) | 26(2) | 49(3) | 1(2) | 8(2) | 9(2) |
| C(4D) | 26(2) | 39(2) | 49(2) | -4(2) | 5(2) | 4(2) |
| C(5D) | 32(2) | 33(2) | 41(2) | -13(2) | 4(2) | 5(2) |
| C(6D) | 33(2) | 44(2) | 75(3) | -31(2) | -4(2) | -2(2) |
| C(7D) | 49(2) | 44(3) | 53(3) | -22(2) | 11(2) | 7(2) |
| C(8D) | 62(3) | 56(3) | 36(2) | -8(2) | -9(2) | 14(2) |
| B(3D) | 24(2) | 31(2) | 29(2) | -4(2) | -1(2) | -1(2) |
| B(4D) | 34(2) | 27(2) | 30(2) | 2(2) | -1(2) | 0(2) |
| B(5D) | 27(2) | 32(2) | 35(2) | -10(2) | -9(2) | 4(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B(6D) | 22(2) | 25(2) | 50(3) | -9(2) | 10(2) | -4(2) |
| B(7D) | 25(2) | 38(2) | 30(2) | -6(2) | -2(2) | 2(2) |
| B(8D) | 28(2) | 23(2) | 31(2) | 0(2) | -1(2) | -6(2) |
| B(9D) | 32(2) | 23(2) | 26(2) | 1(2) | -4(2) | 5(2) |
| B(10D) | 19(2) | 23(2) | 44(3) | -7(2) | -1(2) | 2(2) |
| B(11D) | 34(2) | 27(2) | 32(2) | 5(2) | 13(2) | 3(2) |
| B(12D) | 30(2) | 25(2) | 22(2) | 1(2) | 1(2) | 5(2) |

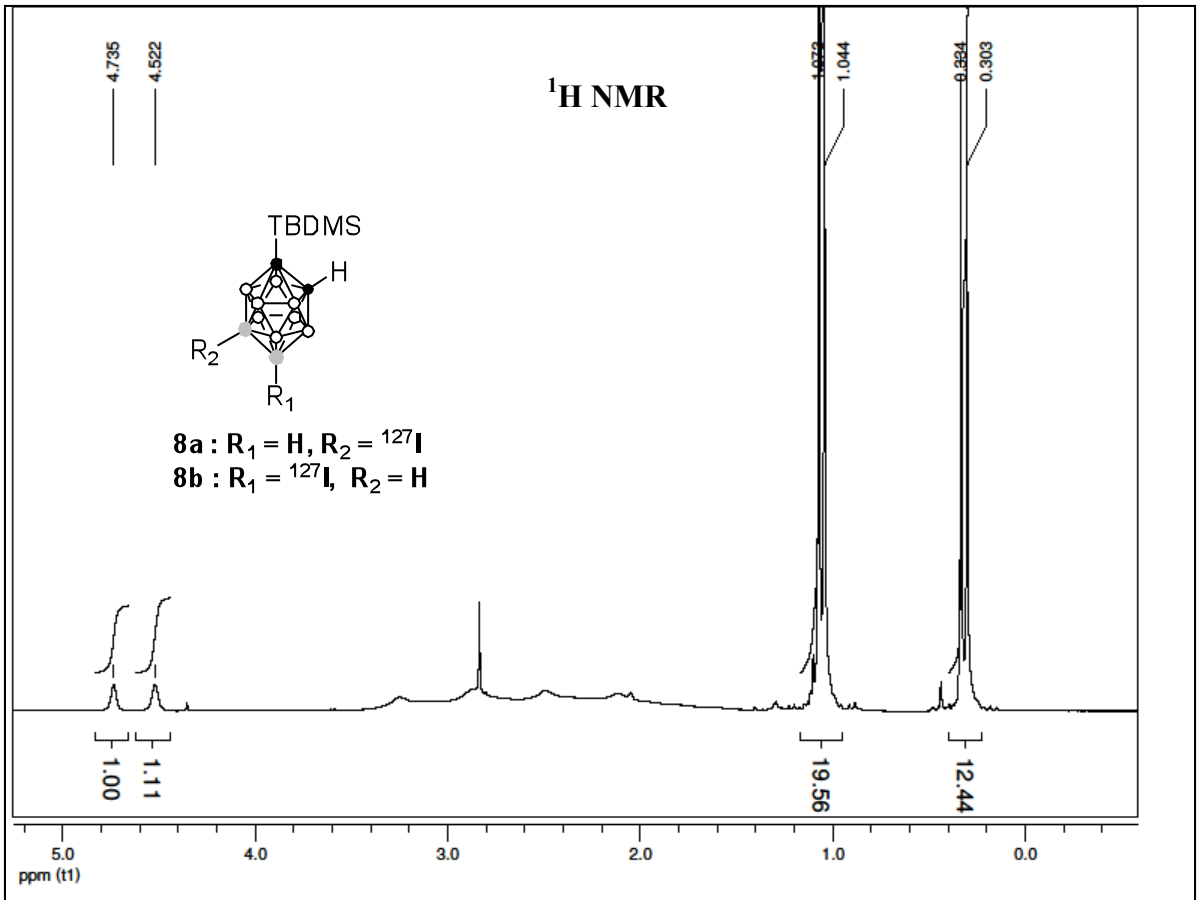
Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for **8b**.

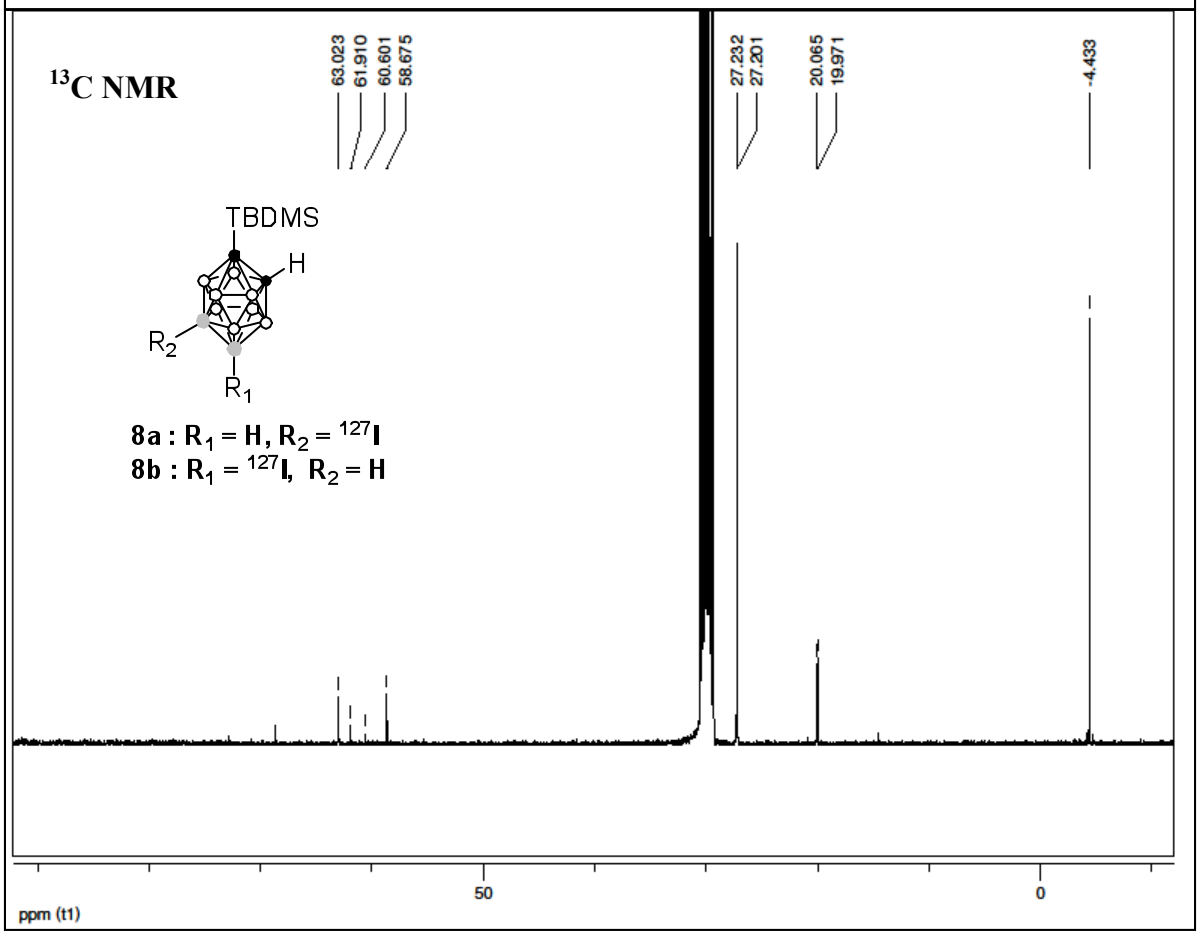
| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 1942(19) | -1164(13) | 4227(10) | 12(7)* |
| H(3A1) | 2480 | -2308 | 4221 | 49 |
| H(3A2) | 3038 | -2080 | 3739 | 49 |
| H(3A3) | 2883 | -2875 | 3854 | 49 |
| H(4A1) | 769 | -3508 | 3723 | 58 |
| H(4A2) | -108 | -2966 | 3696 | 58 |
| H(4A3) | 563 | -3008 | 4169 | 58 |
| H(6A1) | 2220 | -3420 | 2522 | 72 |
| H(6A2) | 1819 | -3622 | 3045 | 72 |
| H(6A3) | 2825 | -3208 | 2993 | 72 |
| H(7A1) | 230 | -2264 | 2650 | 62 |
| H(7A2) | 273 | -3067 | 2761 | 62 |
| H(7A3) | 757 | -2771 | 2278 | 62 |
| H(8A1) | 2378 | -2185 | 2306 | 54 |
| H(8A2) | 2812 | -1952 | 2816 | 54 |
| H(8A3) | 1836 | -1603 | 2612 | 54 |
| H(3A) | 2150(20) | -832(14) | 3358(10) | 18(8)* |
| H(4A) | 318(18) | -1163(14) | 2894(11) | 20(8)* |
| H(5A) | -840(30) | -1813(19) | 3623(13) | 61(12)* |
| H(6A) | 338(19) | -1858(15) | 4488(11) | 27(8)* |
| H(7A) | 1880(20) | 201(18) | 4085(13) | 48(11)* |
| H(8A) | 650(20) | 308(18) | 3169(14) | 48(10)* |
| H(9A) | -1270(20) | -353(16) | 3387(12) | 43(10)* |
| H(10A) | -1260(20) | -825(16) | 4411(11) | 43(10)* |
| H(11A) | 760(20) | -484(17) | 4793(14) | 49(10)* |
| H(2B) | 1116(19) | -4168(13) | 5308(10) | 12(7)* |
| H(3B1) | 2637 | -6080 | 6216 | 57 |
| H(3B2) | 3249 | -5381 | 6222 | 57 |
| H(3B3) | 2816 | -5668 | 5725 | 57 |
| H(4B1) | 819 | -5413 | 5420 | 49 |
| H(4B2) | 7 | -5099 | 5773 | 49 |
| H(4B3) | 351 | -5877 | 5836 | 49 |
| H(6B1) | 1747 | -5175 | 7511 | 62 |

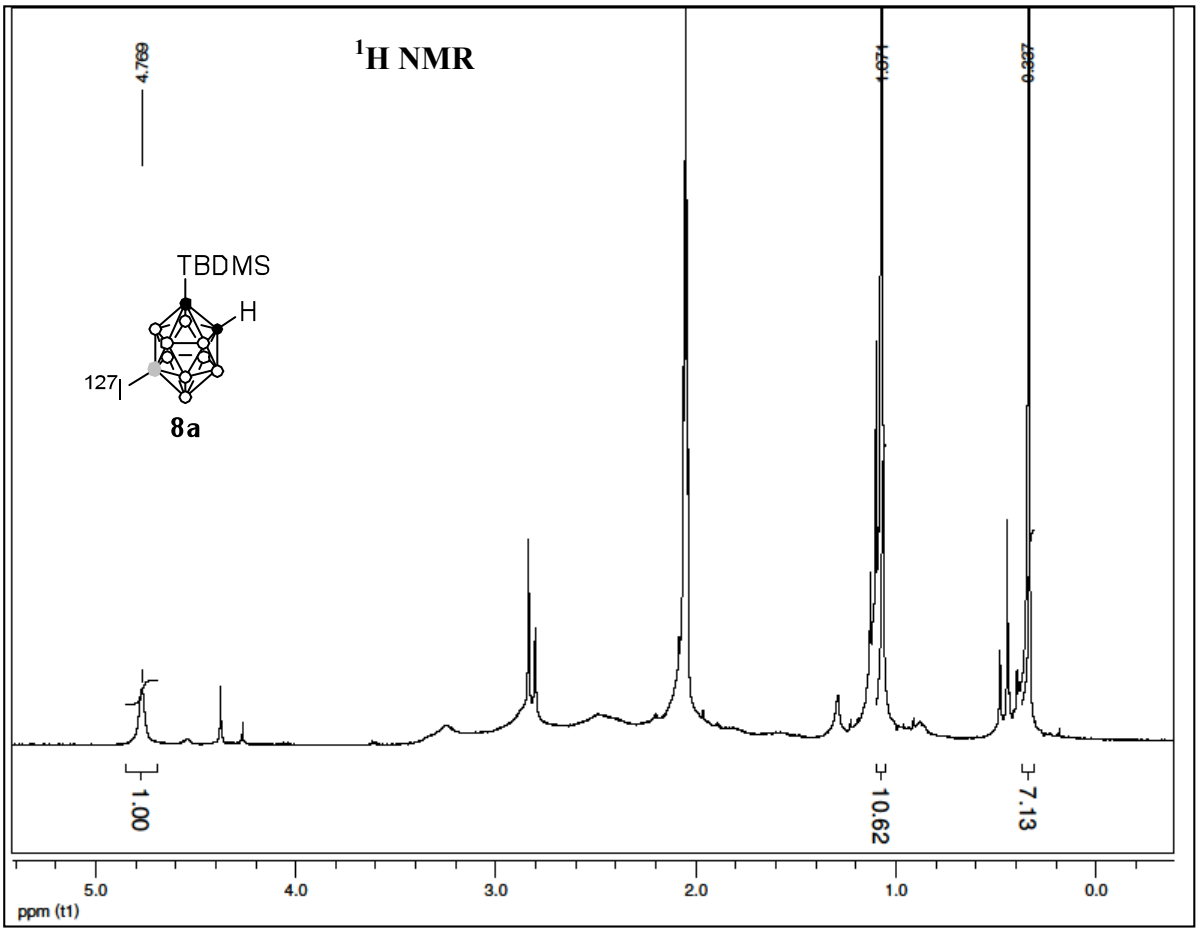
| | | | | |
|---|---|---|---|---|
| H(6B2) | 2112 | -4578 | 7159 | 62 |
| H(6B3) | 2549 | -5334 | 7105 | 62 |
| H(7B1) | -313 | -4955 | 6710 | 60 |
| H(7B2) | 349 | -4342 | 6912 | 60 |
| H(7B3) | -11 | -4937 | 7267 | 60 |
| H(8B1) | 693 | -6101 | 7217 | 61 |
| H(8B2) | 1455 | -6291 | 6800 | 61 |
| H(8B3) | 337 | -6130 | 6668 | 61 |
| H(3B) | 180(20) | -3753(17) | 6022(12) | 41(9)* |
| H(4B) | 1649(19) | -3560(15) | 6773(11) | 23(8)* |
| H(5B) | 3410(20) | -4037(16) | 6360(11) | 34(9)* |
| H(6B) | 2997(18) | -4516(15) | 5417(10) | 21(7)* |
| H(7B) | 600(20) | -2877(17) | 5273(12) | 41(10)* |
| H(8B) | 1000(30) | -2410(20) | 6221(13) | 55(11)* |
| H(9B) | 3060(20) | -2573(15) | 6443(11) | 27(8)* |
| H(10B) | 3990(20) | -3166(15) | 5545(11) | 34(9)* |
| H(11B) | 2380(20) | -3356(17) | 4869(15) | 54(11)* |
| H(2C) | 437(19) | 1043(15) | 5303(12) | 24(9)* |
| H(3C1) | -785 | -299 | 6055 | 72 |
| H(3C2) | 138 | -243 | 5701 | 72 |
| H(3C3) | -708 | 324 | 5682 | 72 |
| H(4C1) | -983 | 1314 | 6465 | 69 |
| H(4C2) | -184 | 1419 | 6881 | 69 |
| H(4C3) | -938 | 793 | 6910 | 69 |
| H(6C1) | 2031 | -842 | 6755 | 79 |
| H(6C2) | 2299 | -235 | 6390 | 79 |
| H(6C3) | 1430 | -755 | 6263 | 79 |
| H(7C1) | 1874 | 49 | 7406 | 71 |
| H(7C2) | 1068 | 641 | 7362 | 71 |
| H(7C3) | 2040 | 673 | 7041 | 71 |
| H(8C1) | -53 | -796 | 6784 | 94 |
| H(8C2) | -233 | -226 | 7189 | 94 |
| H(8C3) | 588 | -801 | 7267 | 94 |
| H(3C) | -150(20) | 1981(13) | 5874(10) | 17(7)* |
| H(4C) | 1430(20) | 2048(15) | 6581(11) | 26(8)* |
| H(5C) | 2750(20) | 950(16) | 6341(12) | 38(10)* |
| H(6C) | 1986(18) | 276(15) | 5527(10) | 17(8)* |
| H(7C) | 636(19) | 2268(15) | 4977(11) | 27(8)* |
| H(8C) | 1450(20) | 2993(17) | 5801(12) | 38(10)* |

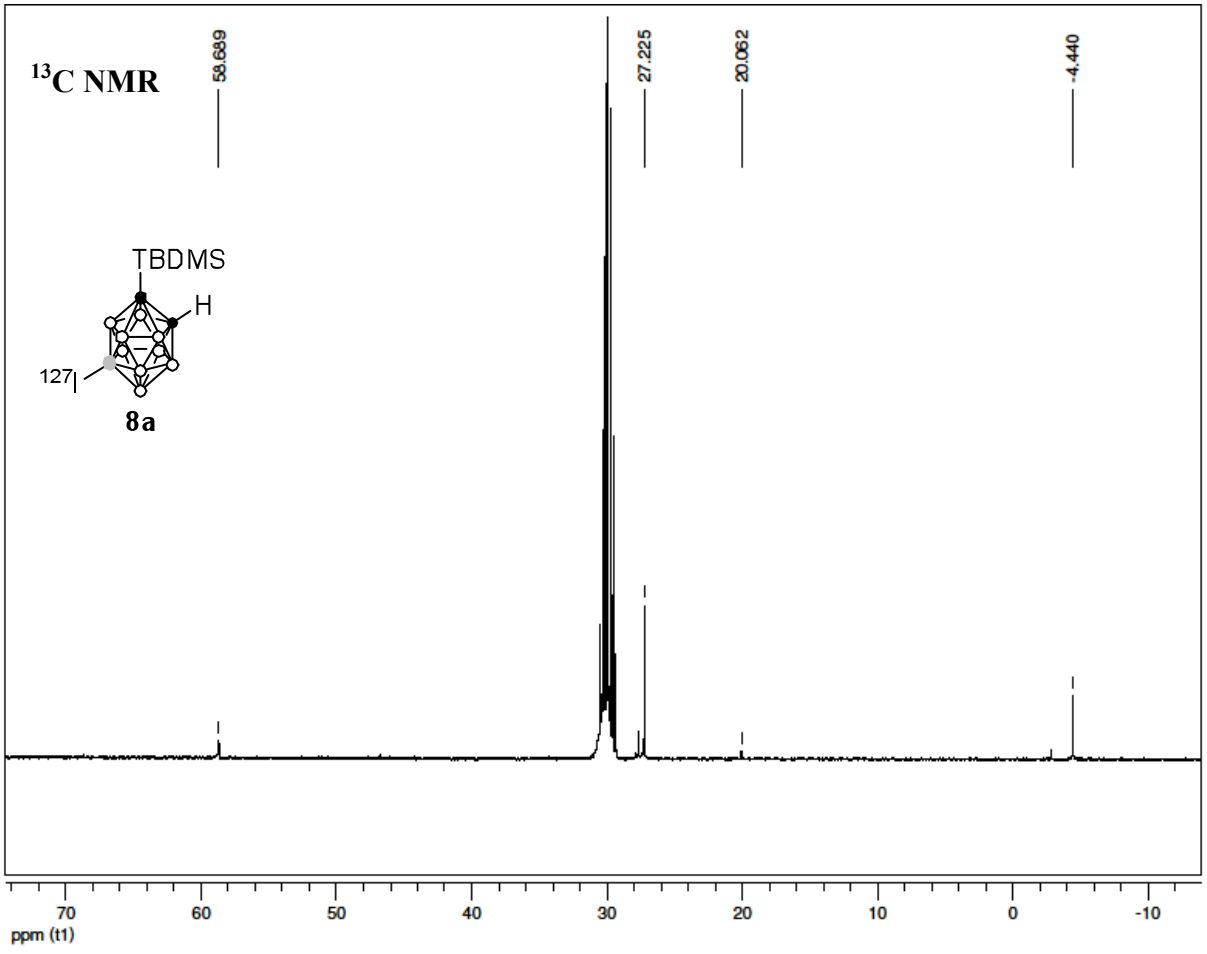
| | | | | |
|---|---|---|---|---|
| H(9C) | 3320(20) | 2346(16) | 6077(11) | 31(9)* |
| H(10C) | 3604(19) | 1251(14) | 5403(11) | 21(8)* |
| H(11C) | 1972(19) | 1214(15) | 4716(11) | 23(8)* |
| H(2D) | 1290(20) | 3141(15) | 4197(11) | 19(8)* |
| H(3D1) | 2068 | 1625 | 3424 | 60 |
| H(3D2) | 1111 | 1913 | 3690 | 60 |
| H(3D3) | 2175 | 2163 | 3857 | 60 |
| H(4D1) | 3286 | 2710 | 2780 | 57 |
| H(4D2) | 3342 | 3112 | 3283 | 57 |
| H(4D3) | 2916 | 3486 | 2814 | 57 |
| H(6D1) | -309 | 2100 | 2361 | 76 |
| H(6D2) | -388 | 2635 | 2796 | 76 |
| H(6D3) | -20 | 1870 | 2897 | 76 |
| H(7D1) | 1559 | 1471 | 2602 | 73 |
| H(7D2) | 2285 | 1973 | 2318 | 73 |
| H(7D3) | 1300 | 1712 | 2065 | 73 |
| H(8D1) | 721 | 2892 | 1900 | 77 |
| H(8D2) | 1758 | 3142 | 2103 | 77 |
| H(8D3) | 768 | 3460 | 2316 | 77 |
| H(3D) | 2593(18) | 3967(13) | 3793(9) | 13(7)* |
| H(4D) | 1570(20) | 4488(16) | 2932(12) | 40(10)* |
| H(5D) | -300(20) | 3754(16) | 2940(12) | 35(9)* |
| H(6D) | -280(20) | 2826(16) | 3745(11) | 26(8)* |
| H(7D) | 1580(20) | 4395(17) | 4652(12) | 47(10)* |
| H(8D) | 1640(20) | 5314(17) | 3853(12) | 40(10)* |
| H(9D) | -245(18) | 5162(15) | 3304(10) | 17(7)* |
| H(10D) | -1430(20) | 4172(14) | 3802(10) | 24(8)* |
| H(11D) | -230(18) | 3599(14) | 4623(11) | 22(8)* |

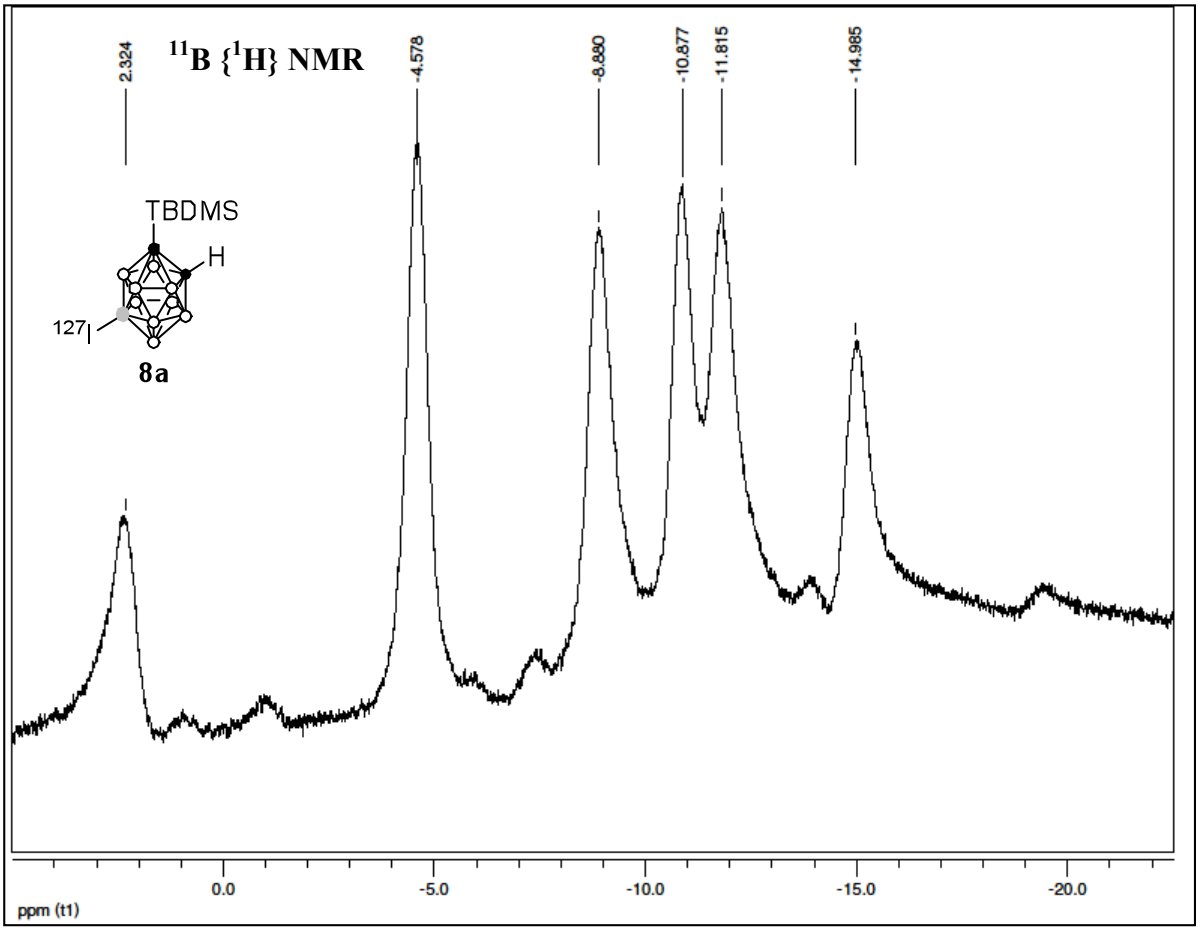
8) Spectroscopic data ($^{1}$H, $^{13}$C, $^{11}$B{$^{1}$H} and $^{11}$B NMR spectra of **8a/8b, 8a**, **8b**, **9a/9b**, **10a/10b**, **11a/11b**, **12a/12b**, **4a/4b**, **5, S3a/S3b, S4a/S4b**

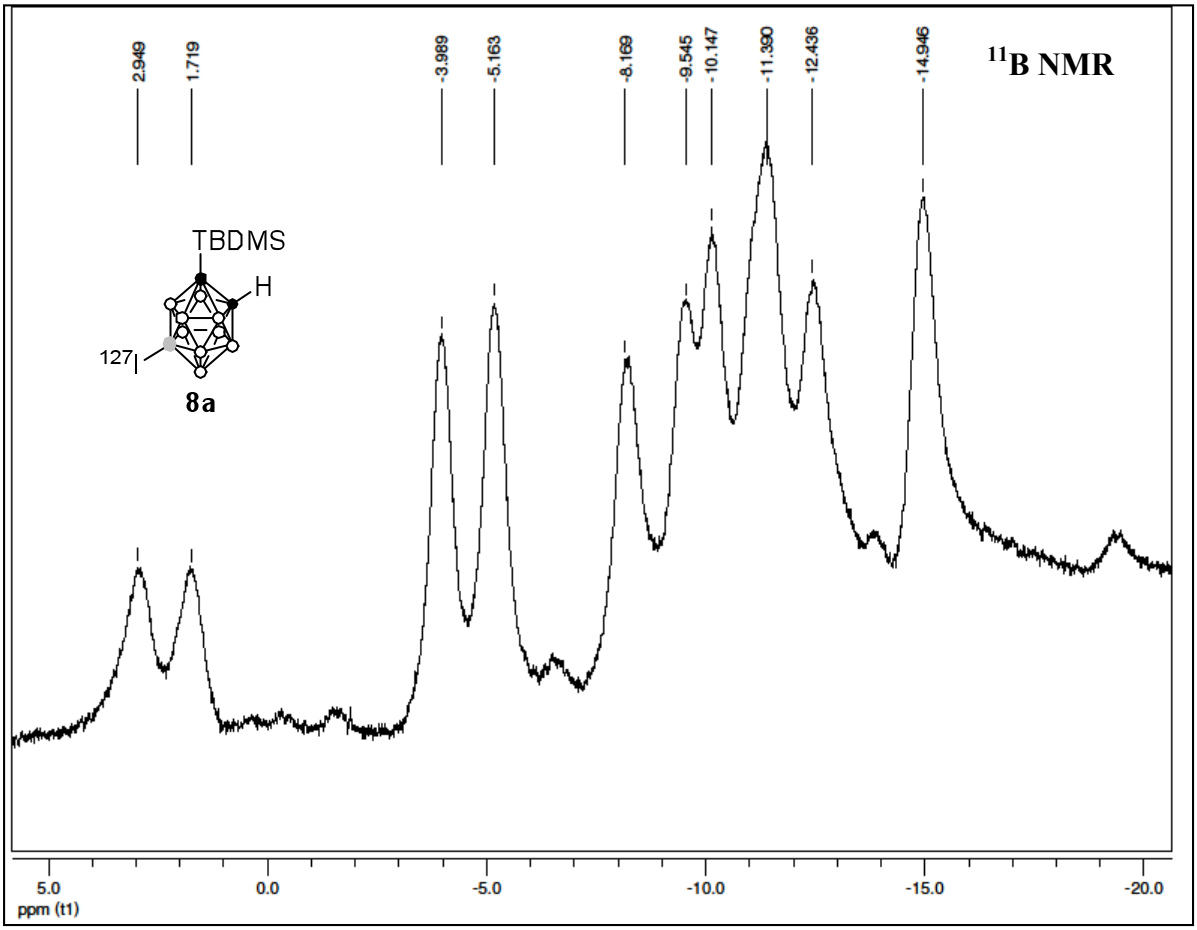


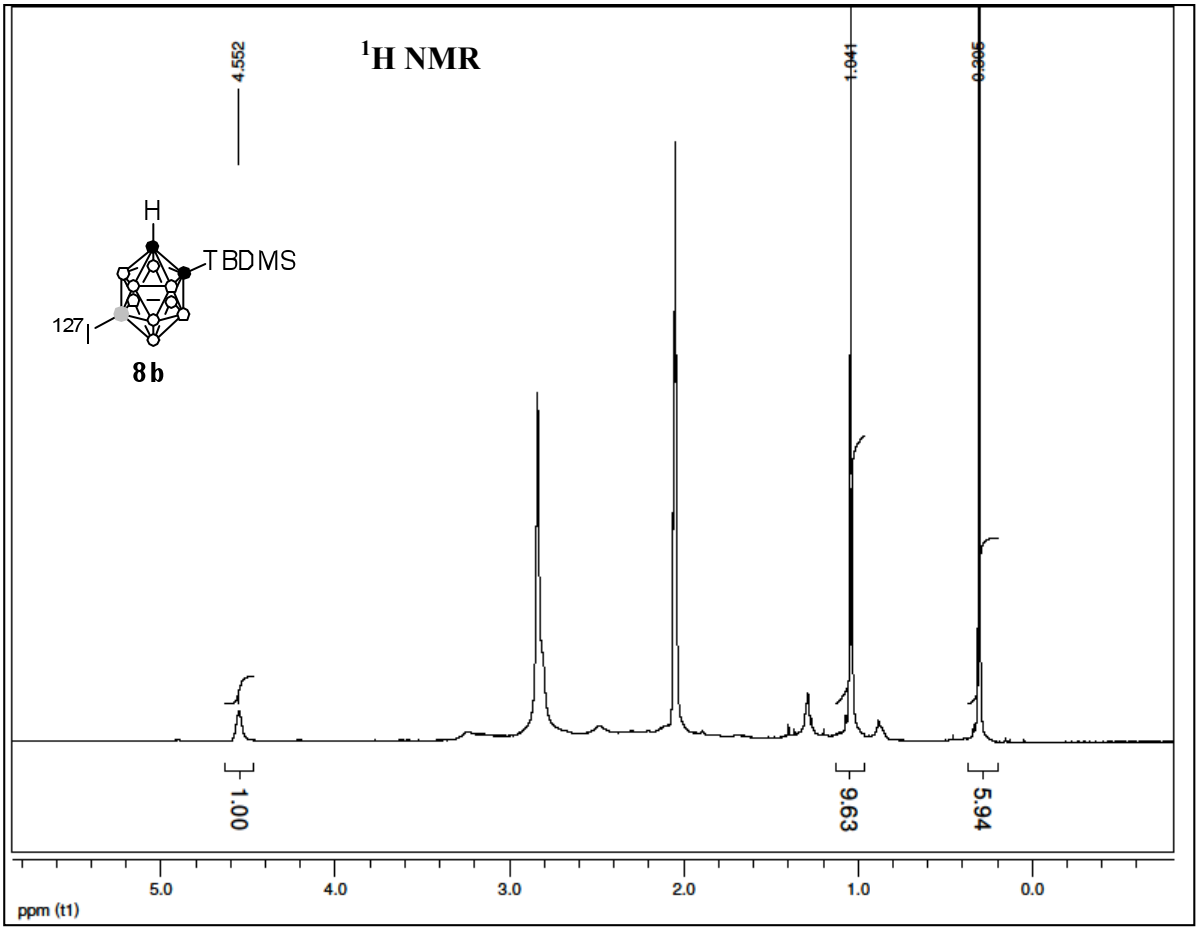



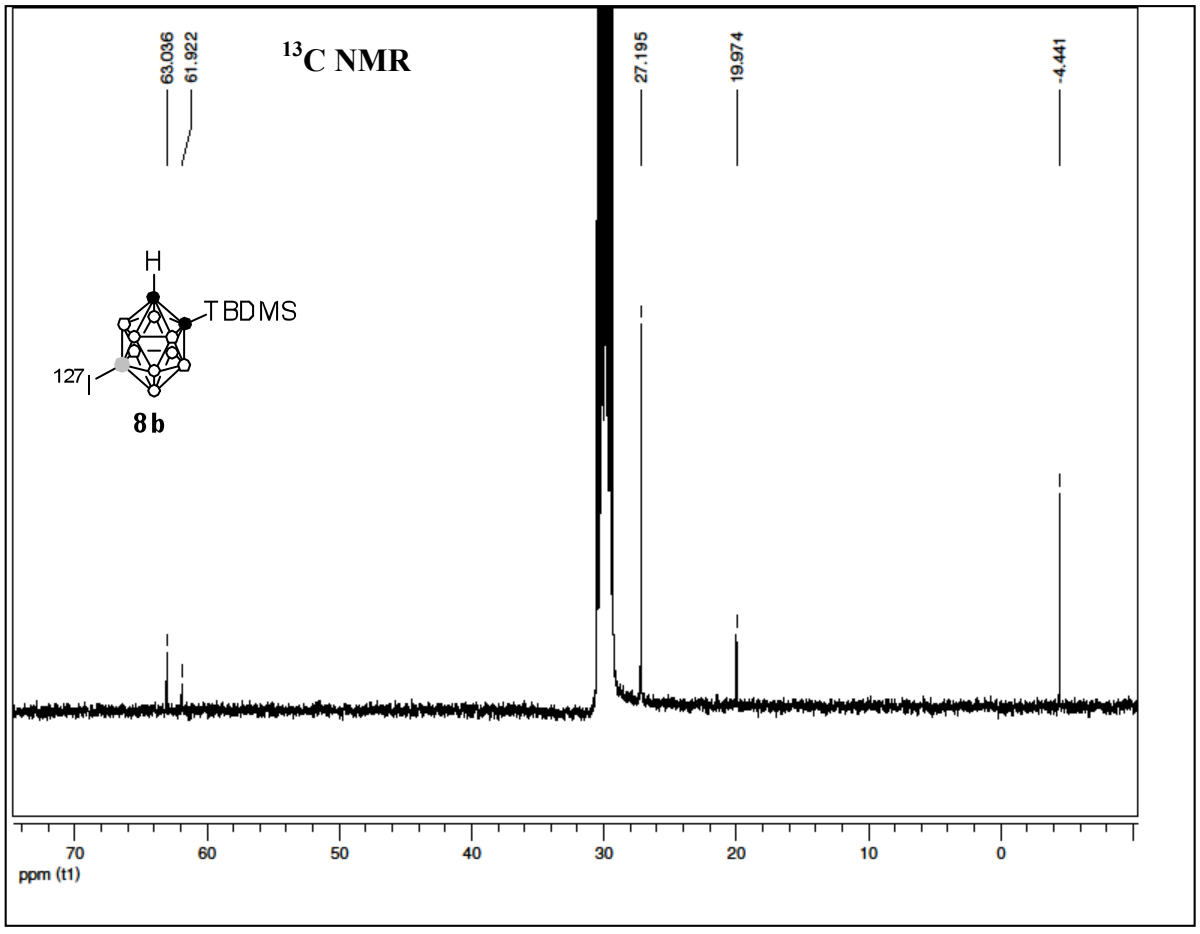

$^{1}$H NMR
4.769
1.691
0.897
TBDMS
H
127
8a
1.00
10.62
7.13
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

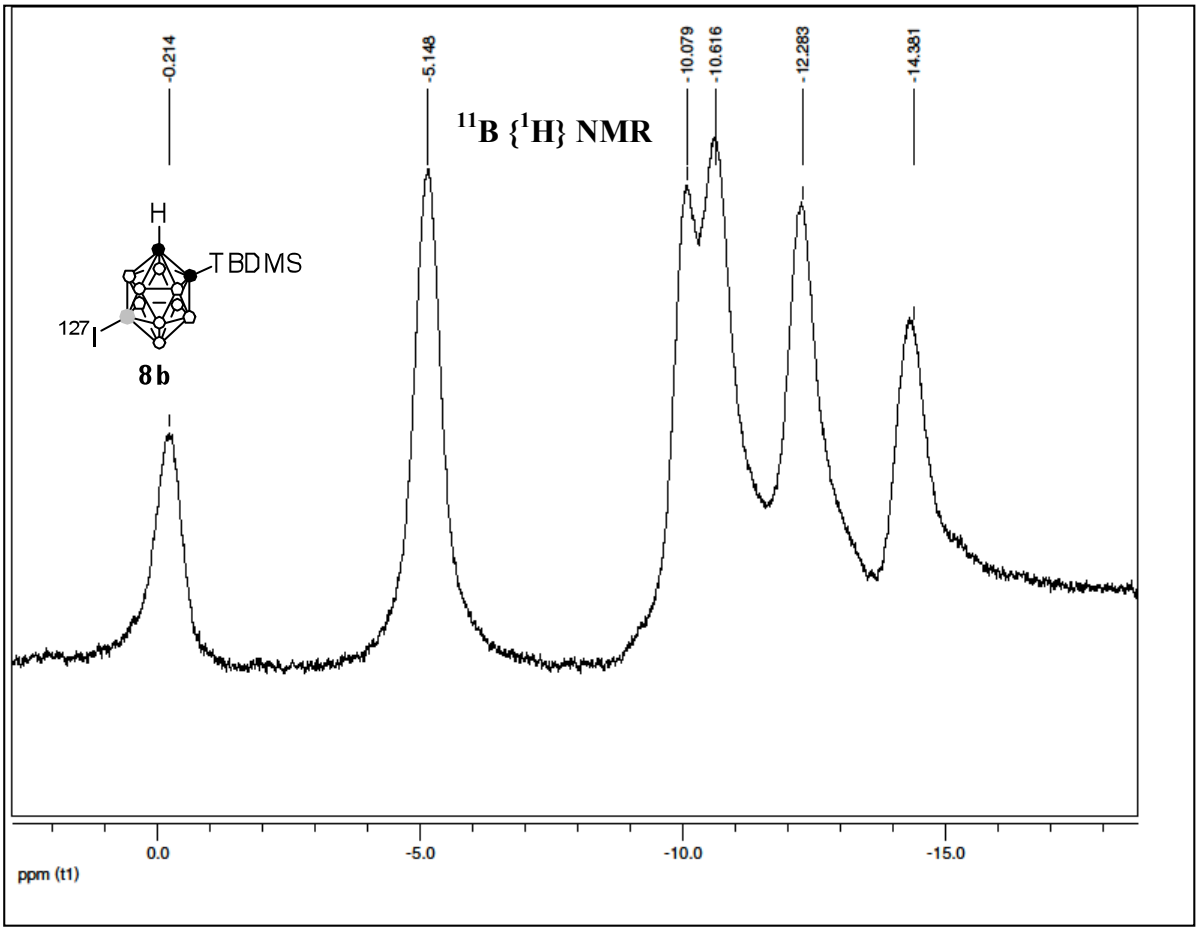

$^{13}$C NMR
58.689
27.225
20.062
-4.440
TBDMS
H
127
8a
70
60
50
40
30
20
10
0
-10
ppm (t1)

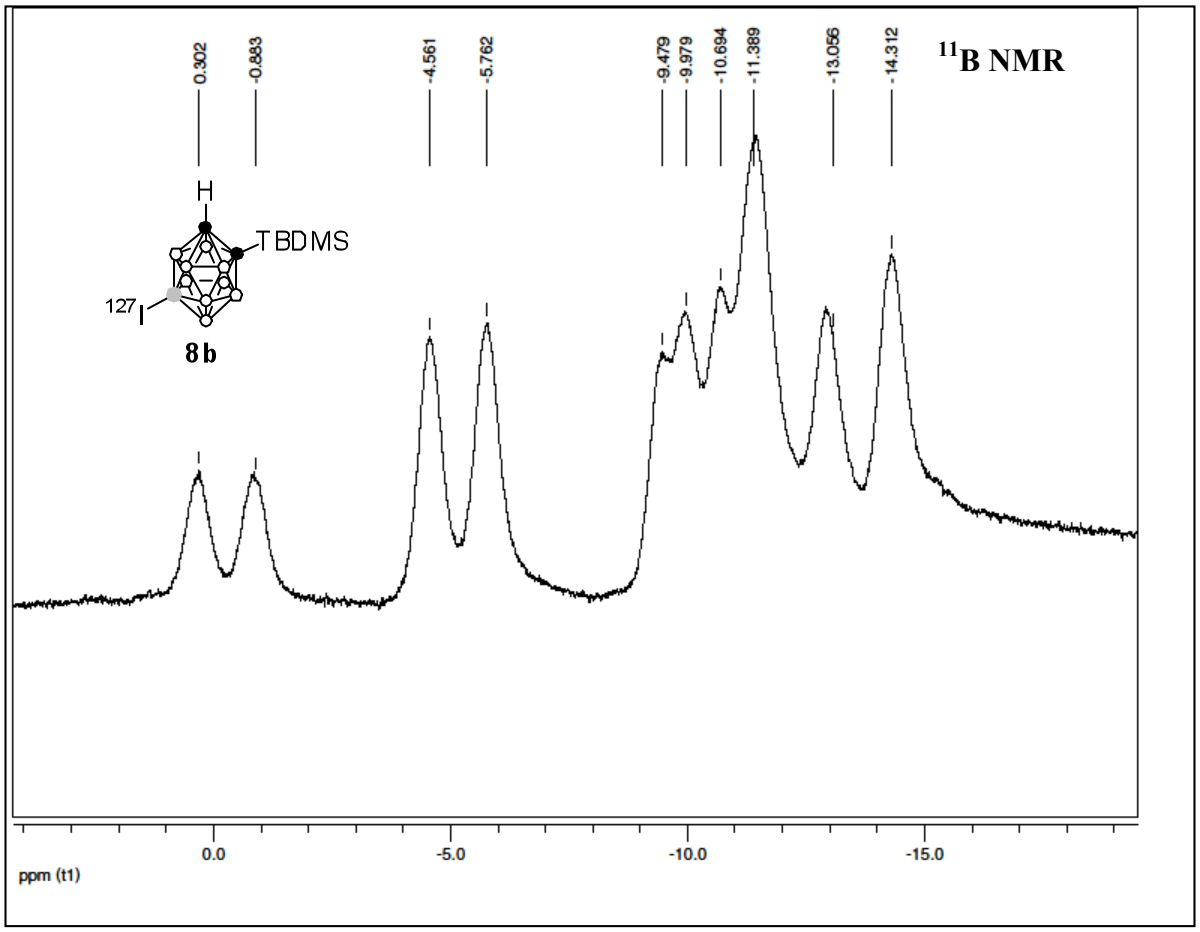

$^{11}$B {$^{1}$H} NMR
2.324
-4.578
-8.880
-10.877
-11.815
-14.985
TBDMS
H
127I
8a
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

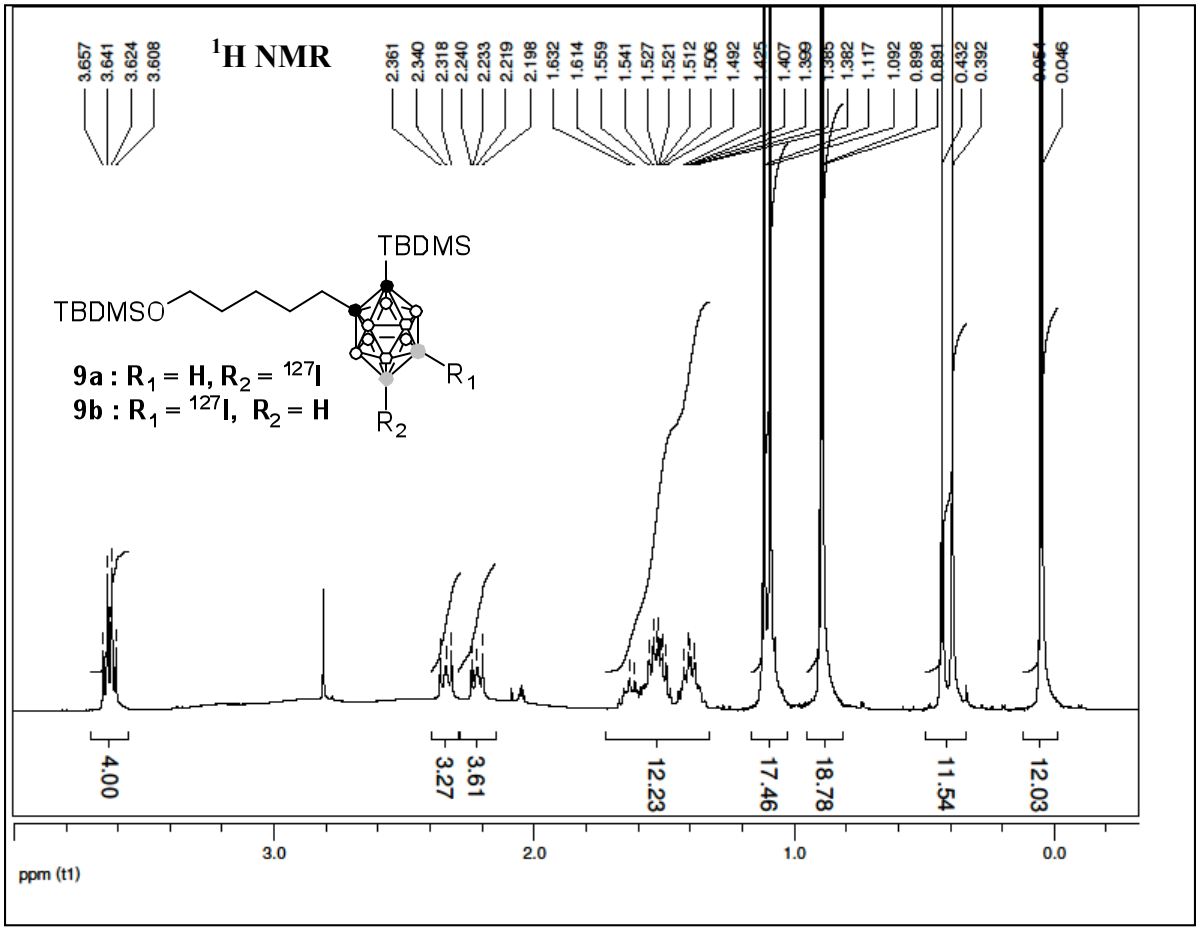

$^{11}$B NMR
2.949
1.719
-3.989
-5.163
-8.169
-9.545
-10.147
-11.390
-12.436
-14.946
TBDMS
H
127I
8a
5.0
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

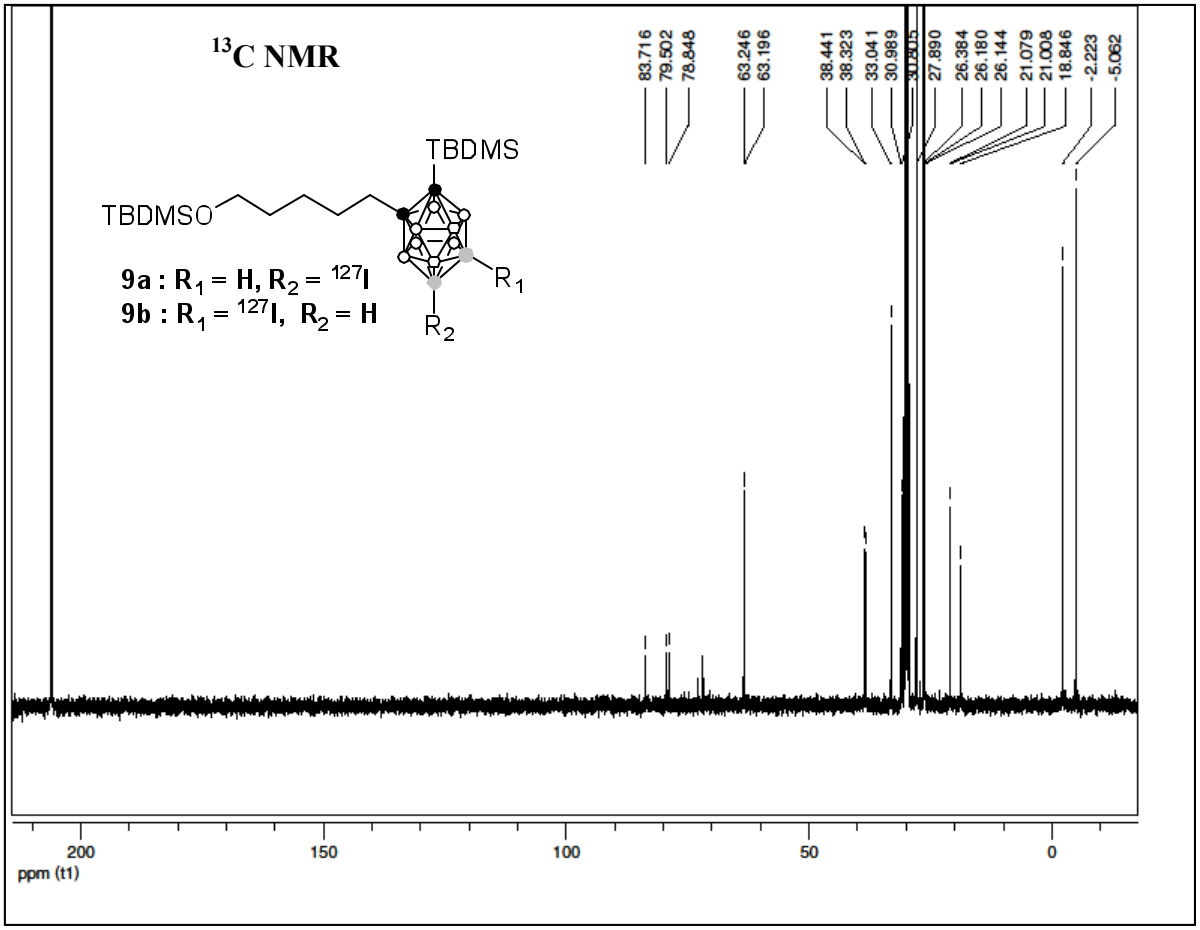

$^{1}$H NMR
4.552
1.041
0.905
H
TBDMS
127
I
8b
1.00
9.63
5.94
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

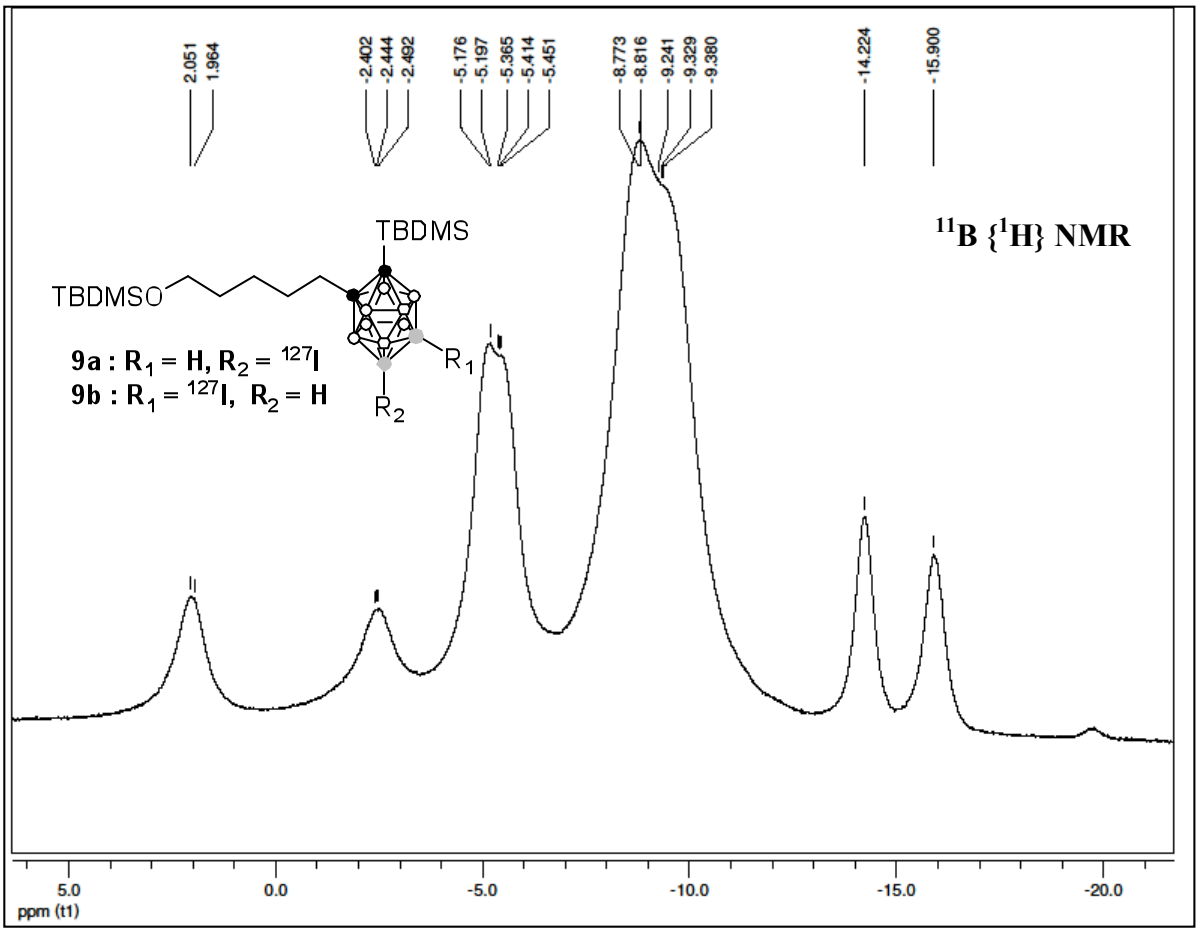

$^{13}$C NMR
63.036
61.922
27.195
19.974
-4.441
H
TBDMS
127
I
8b
70
60
50
40
30
20
10
0
ppm (t1)

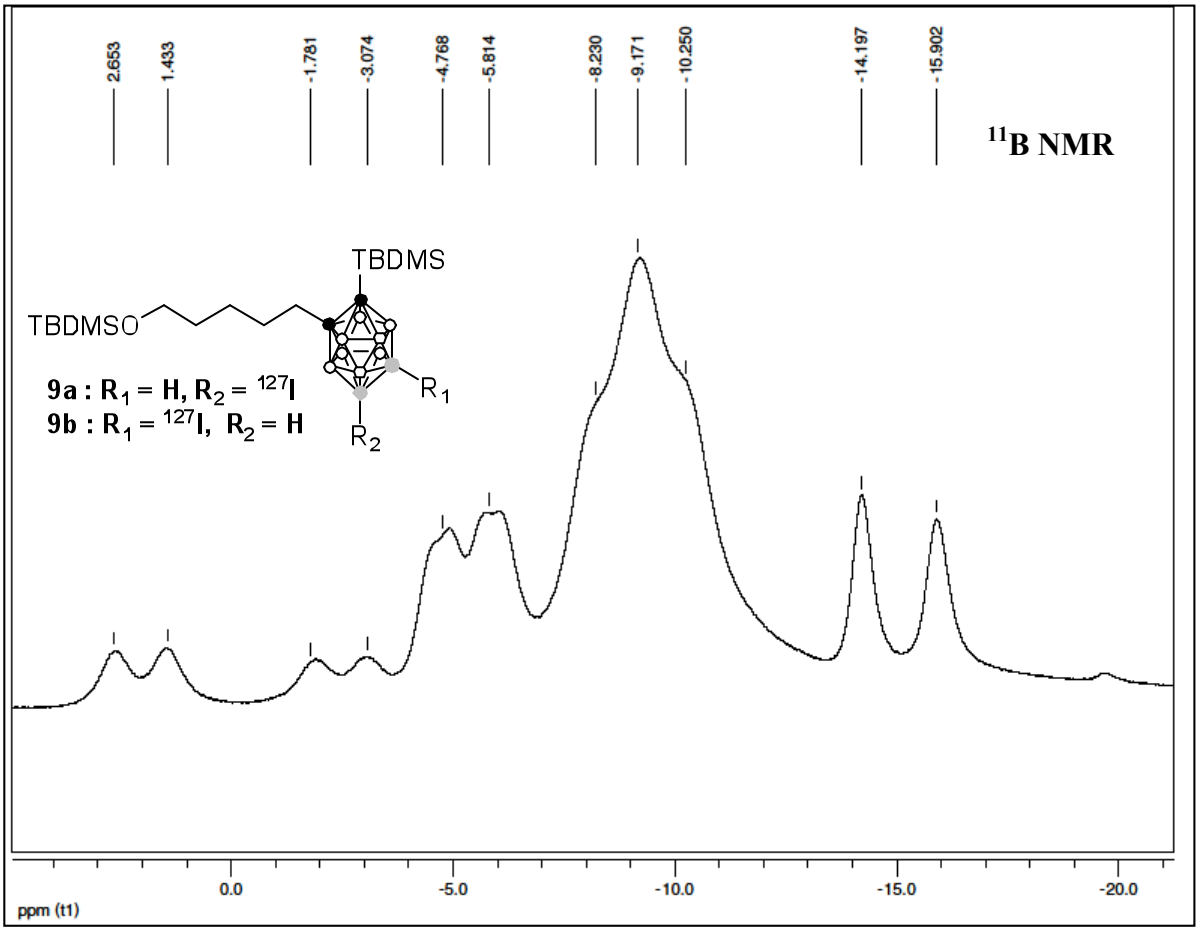

$^{11}$B {$^{1}$H} NMR
-0.214
-5.148
-10.079
-10.616
-12.283
-14.381
H
TBDMS
127
I
8b
0.0
-5.0
-10.0
-15.0
ppm (t1)

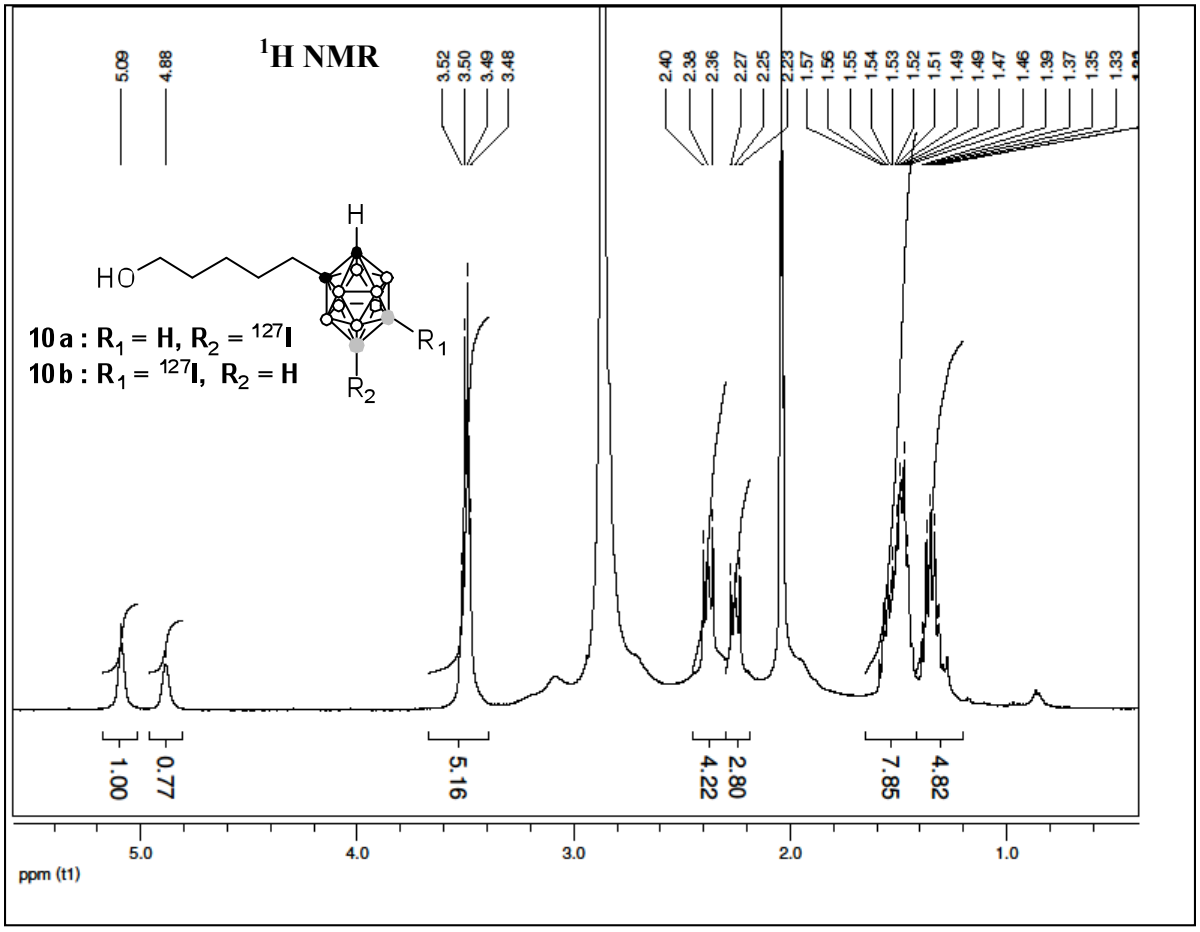

$^{11}$B NMR
0.302
-0.883
-4.561
-5.762
-9.479
-9.979
-10.694
-11.389
-13.056
-14.312
H
TBDMS
127
I
8b
0.0
-5.0
-10.0
-15.0
ppm (t1)

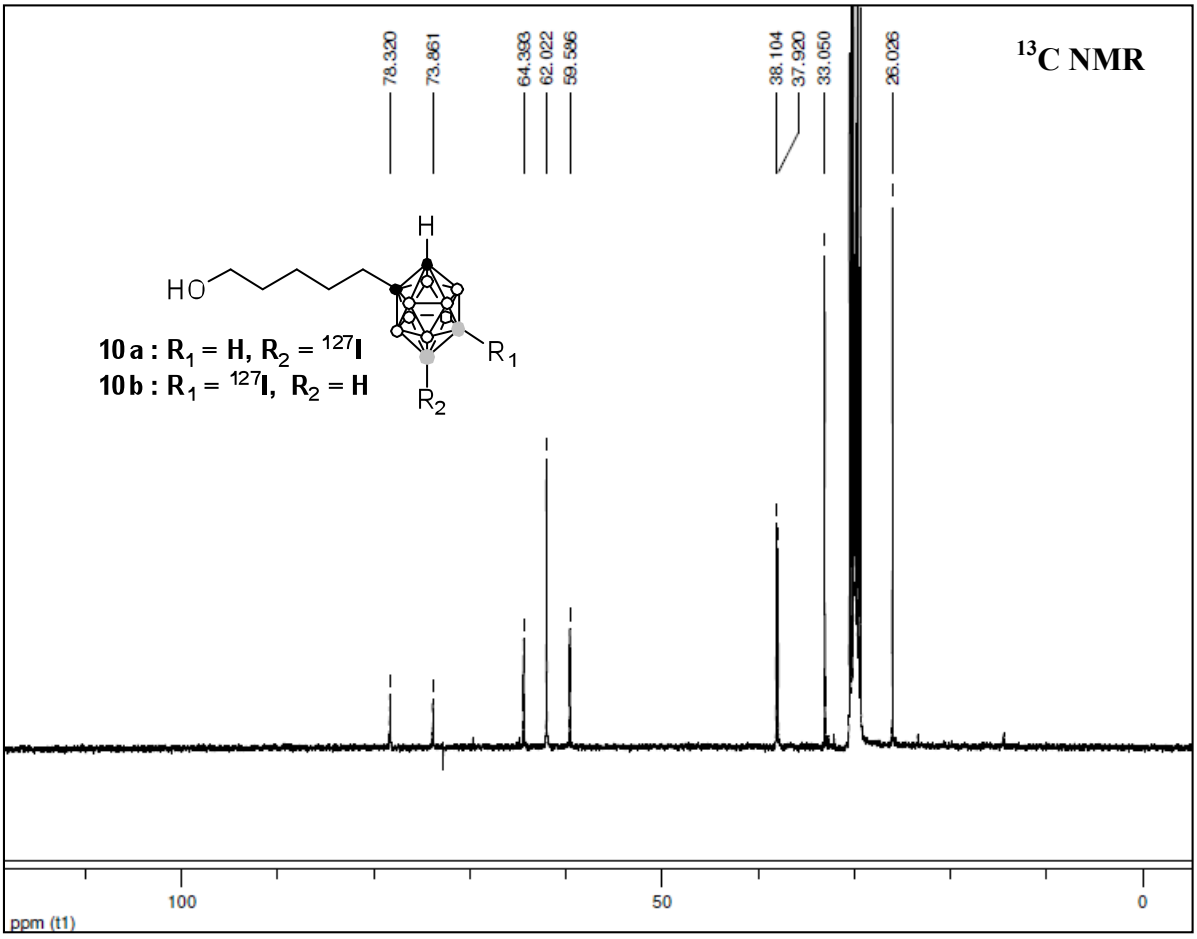

$^{1}$H NMR
3.657
3.641
3.624
3.608
2.361
2.340
2.318
2.240
2.233
2.219
2.198
1.632
1.614
1.559
1.541
1.527
1.521
1.512
1.506
1.492
1.425
1.407
1.399
1.385
1.382
1.117
1.092
0.898
0.891
0.432
0.392
0.051
0.046
TBDMS
TBDMSO
R1
R2
9a : R1 = H, R2 = 127I
9b : R1 = 127I, R2 = H
4.00
3.27
3.61
12.23
17.46
18.78
11.54
12.03
3.0
2.0
1.0
0.0
ppm (t1)

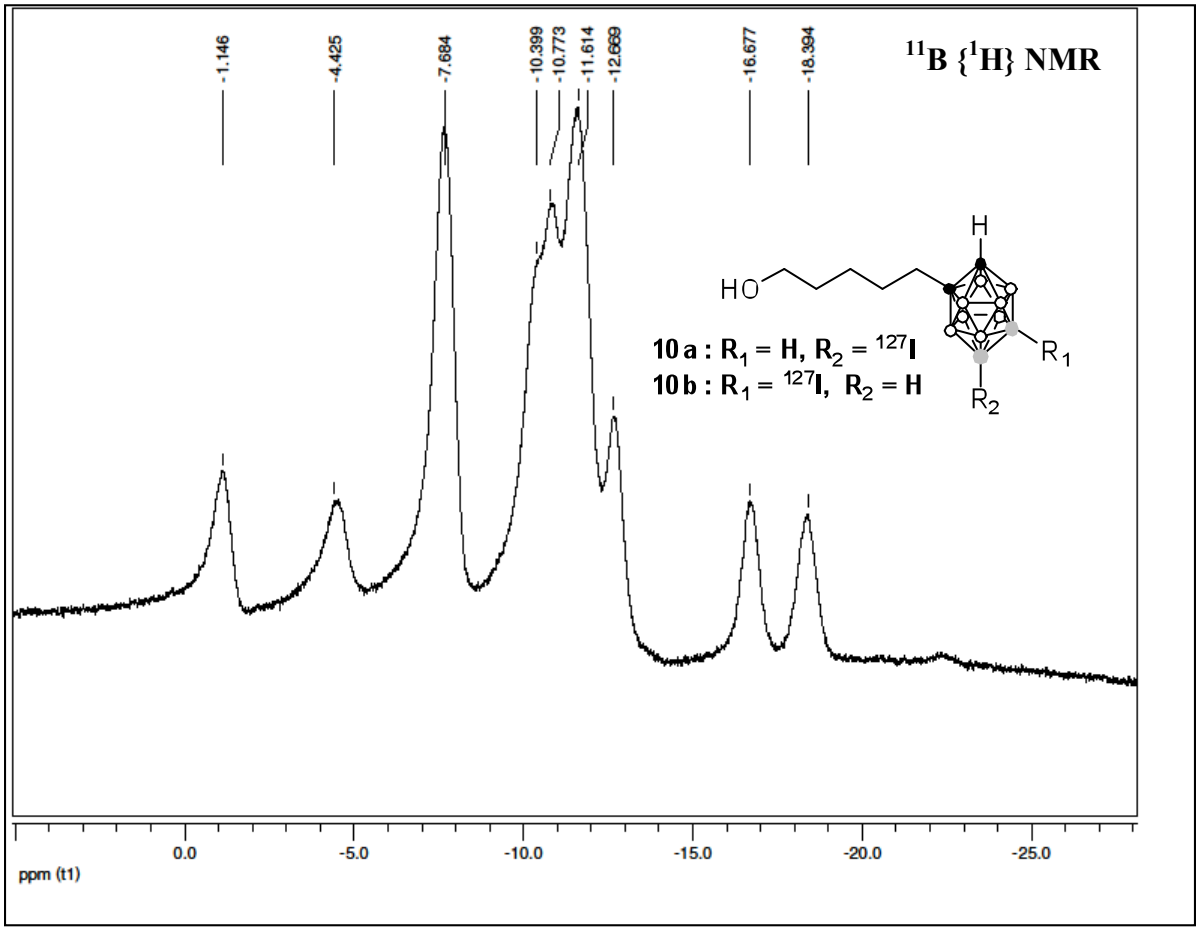

$^{13}$C NMR
83.716
79.502
78.848
63.246
63.196
38.441
38.323
33.041
30.989
27.890
26.384
26.180
26.144
21.079
21.008
18.846
-2.223
-5.062
TBDMS
TBDMSO
R1
R2
9a : R1 = H, R2 = 127I
9b : R1 = 127I, R2 = H
200
150
100
50
0
ppm (t1)

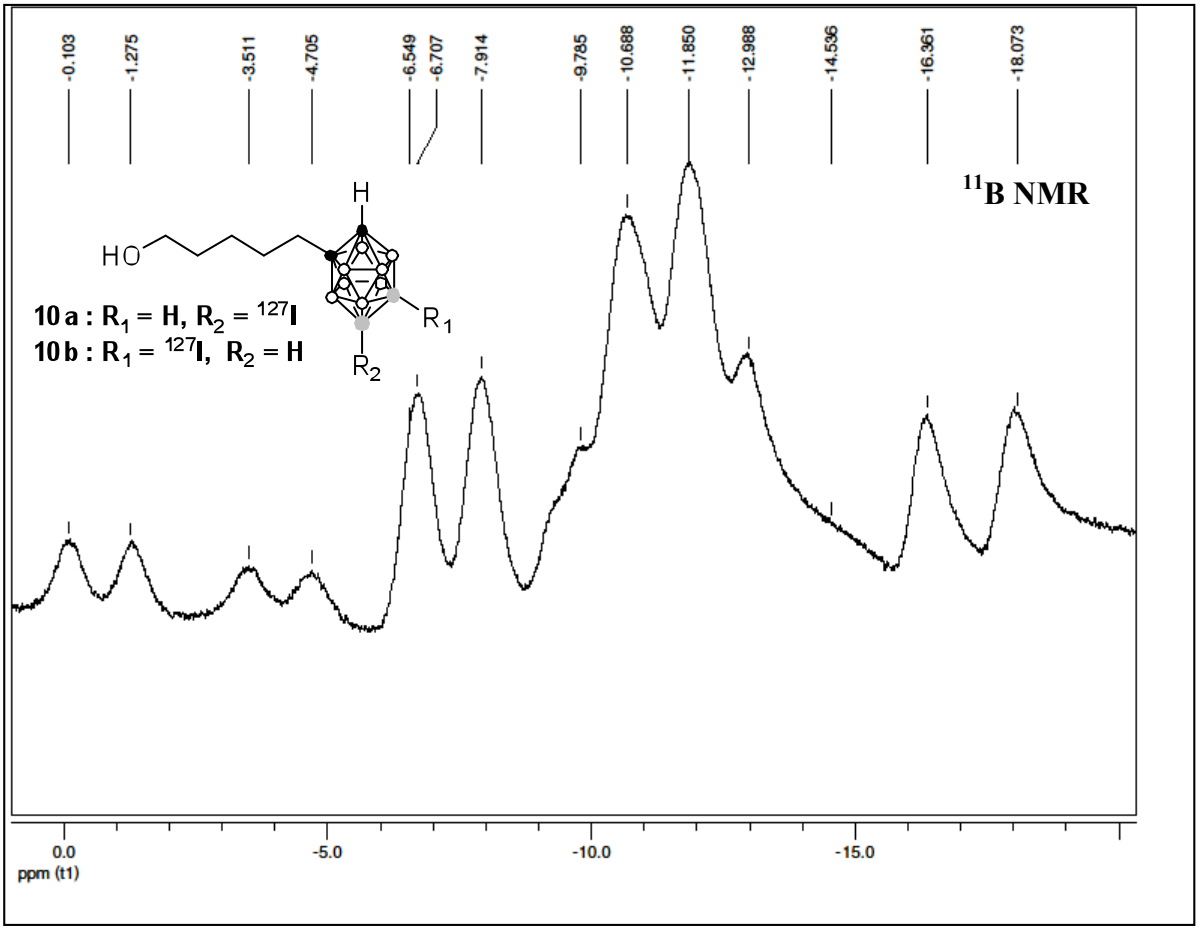

2.051
1.964
-2.402
-2.444
-2.492
-5.176
-5.197
-5.365
-5.414
-5.451
-8.773
-8.816
-9.241
-9.329
-9.380
-14.224
-15.900
TBDMS
TBDMSO
R1
R2
9a : R1 = H, R2 = 127I
9b : R1 = 127I, R2 = H
11B {1H} NMR
5.0
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

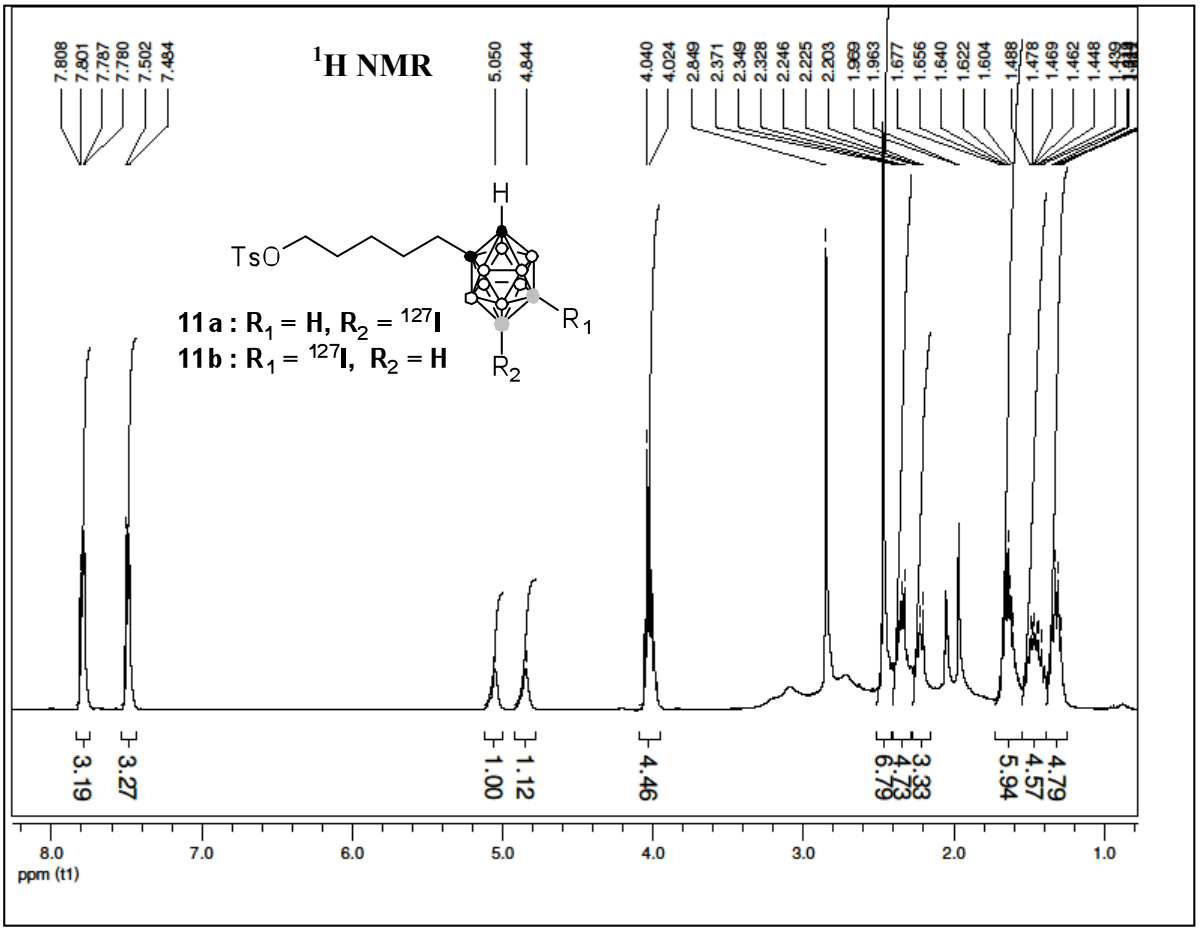

2.653
1.433
-1.781
-3.074
-4.768
-5.814
-8.230
-9.171
-10.250
-14.197
-15.902
TBDMS
TBDMSO
R1
R2
9a : R1 = H, R2 = 127I
9b : R1 = 127I, R2 = H
11B NMR
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

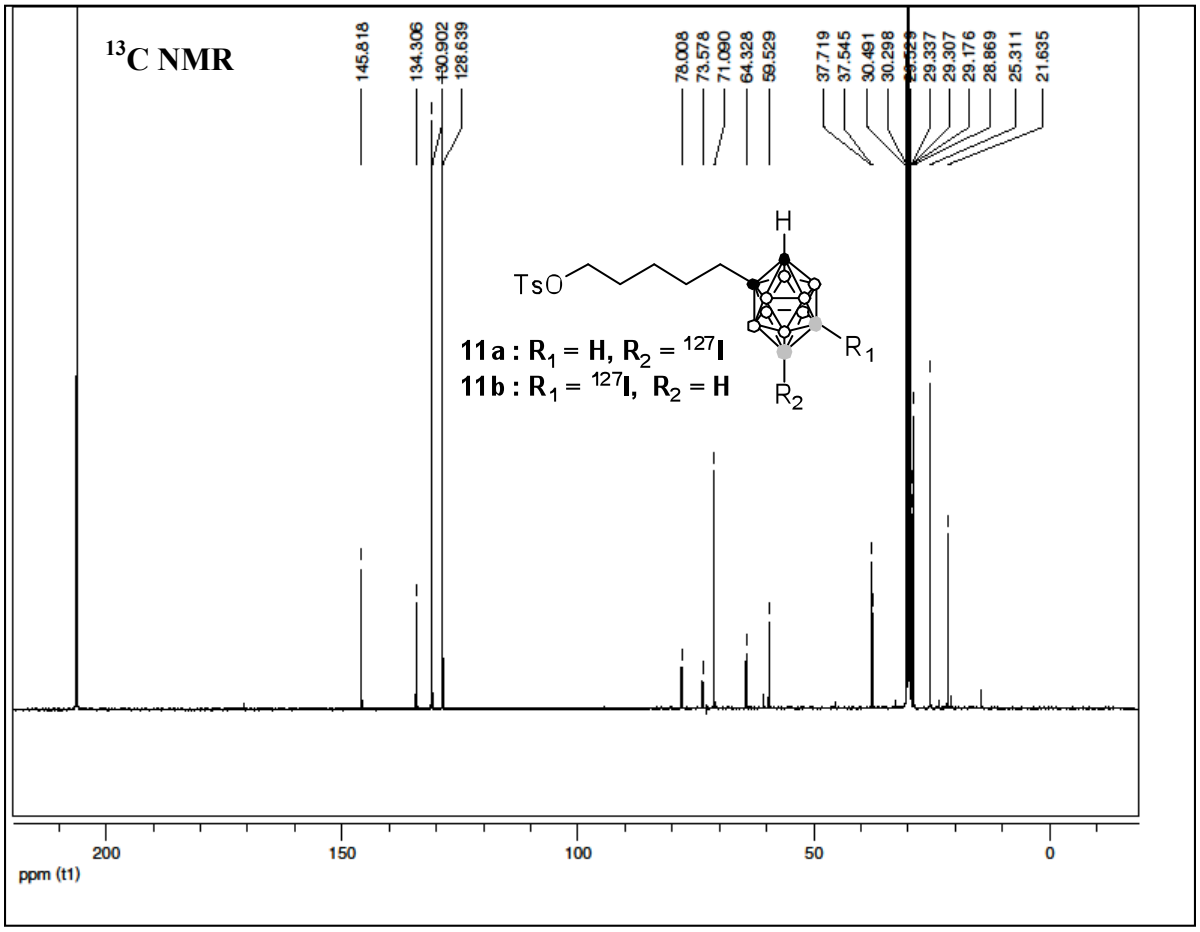

$^{1}$H NMR
5.09
4.88
3.52
3.50
3.49
3.48
2.40
2.38
2.36
2.27
2.25
2.23
1.57
1.56
1.55
1.54
1.53
1.52
1.51
1.49
1.49
1.47
1.46
1.39
1.37
1.35
1.33
HO
H
R1
R2
10 a : R1 = H, R2 = 127I
10 b : R1 = 127I, R2 = H
1.00
0.77
5.16
4.22
2.80
7.85
4.82
5.0
4.0
3.0
2.0
1.0
ppm (t1)

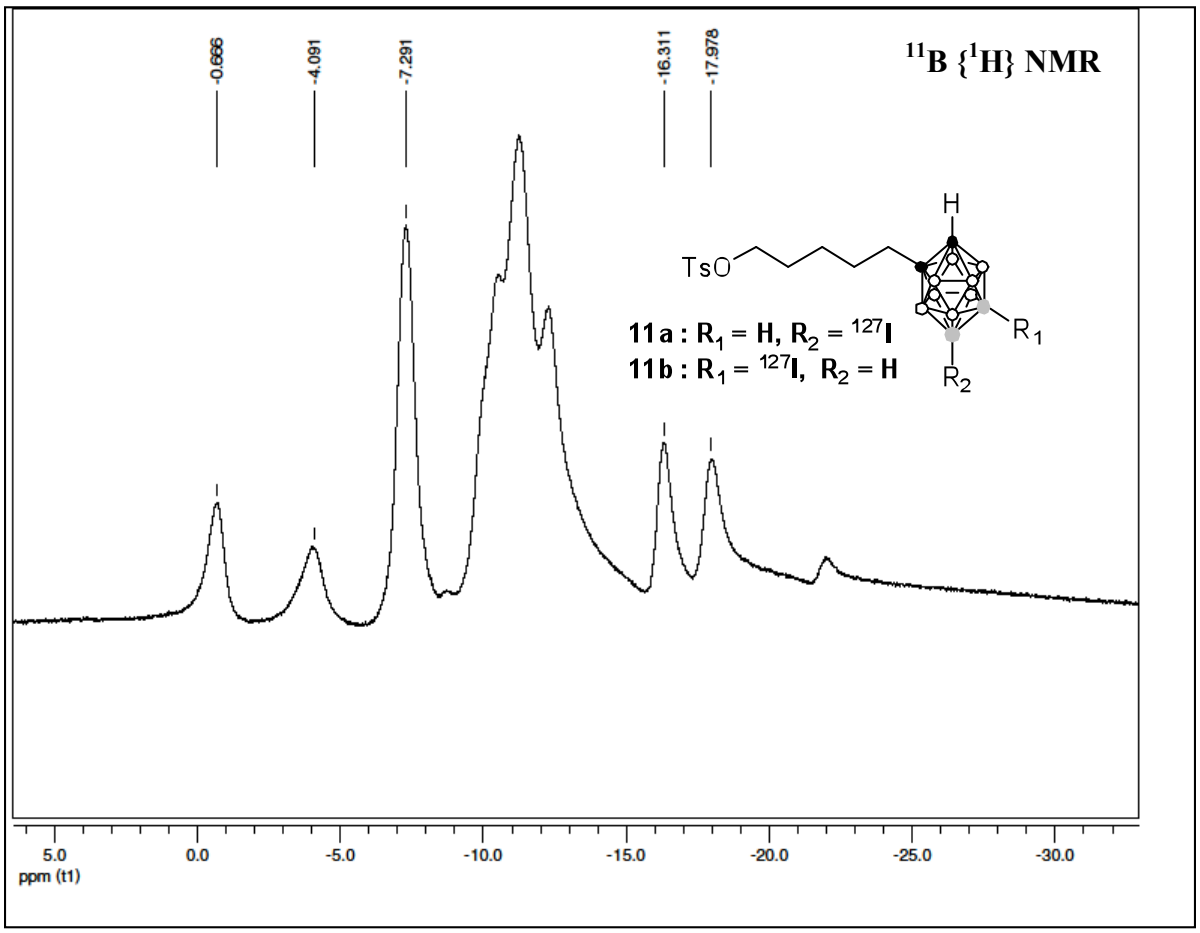

$^{13}$C NMR
78.320
73.861
64.393
62.022
59.596
38.104
37.920
33.050
26.026
HO
H
R1
R2
10 a : R1 = H, R2 = 127I
10 b : R1 = 127I, R2 = H
100
50
0
ppm (t1)

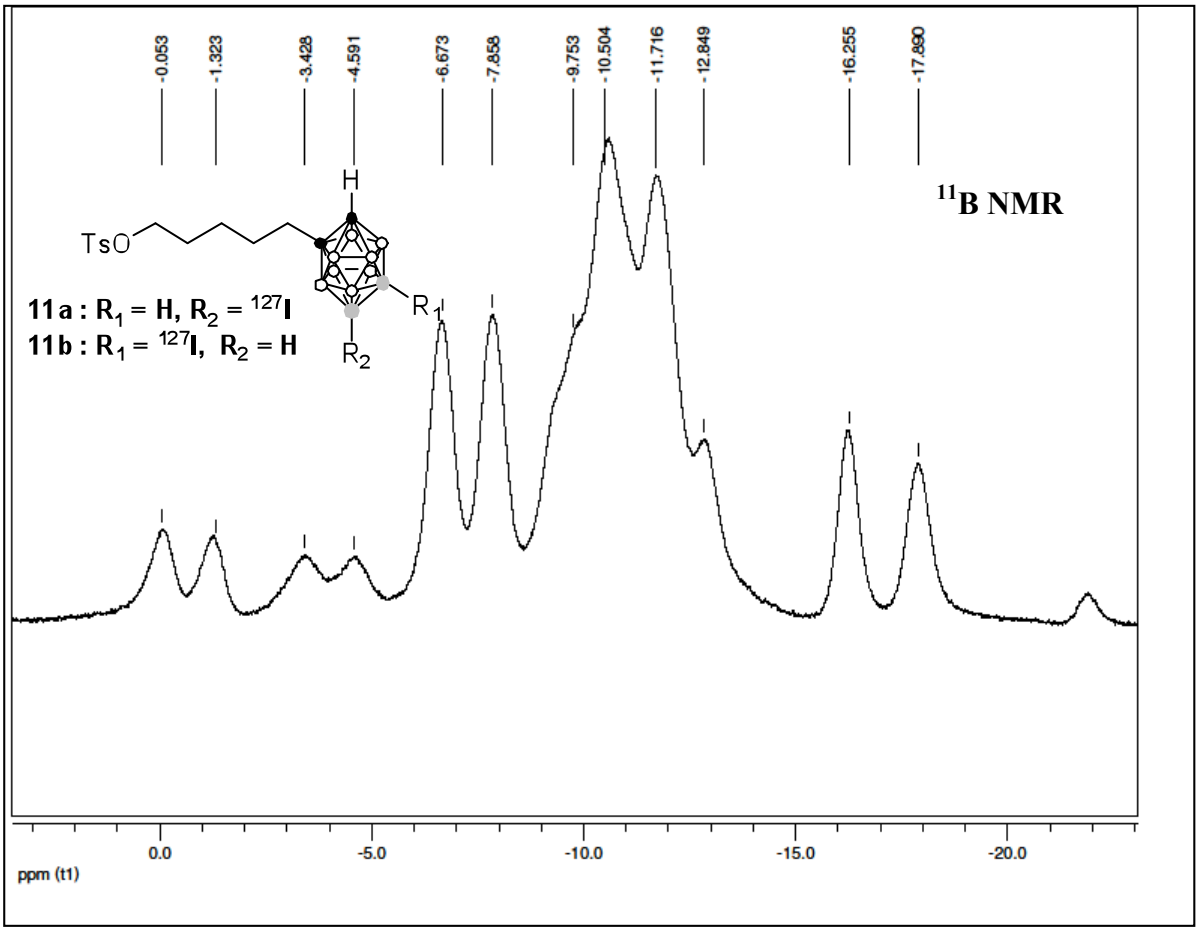

$^{11}$B {$^{1}$H} NMR
-1.146
-4.425
-7.684
-10.399
-10.773
-11.614
-12.669
-16.677
-18.394
HO
H
R1
R2
10 a : R1 = H, R2 = 127I
10 b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
-20.0
-25.0
ppm (t1)

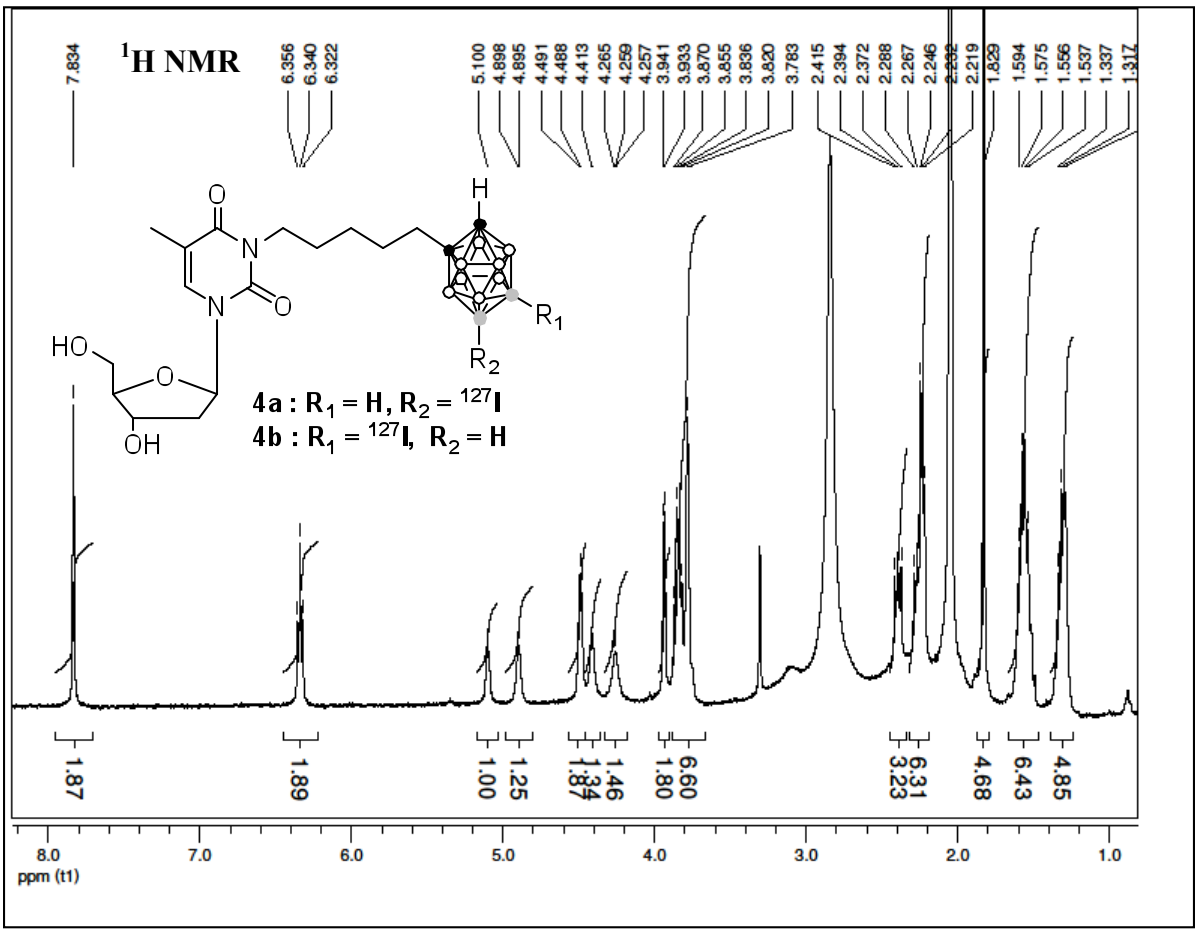

$^{11}$B NMR
-0.103
-1.275
-3.511
-4.705
-6.549
-6.707
-7.914
-9.785
-10.688
-11.850
-12.988
-14.536
-16.361
-18.073
HO
H
R1
R2
10 a : R1 = H, R2 = 127I
10 b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
ppm (t1)

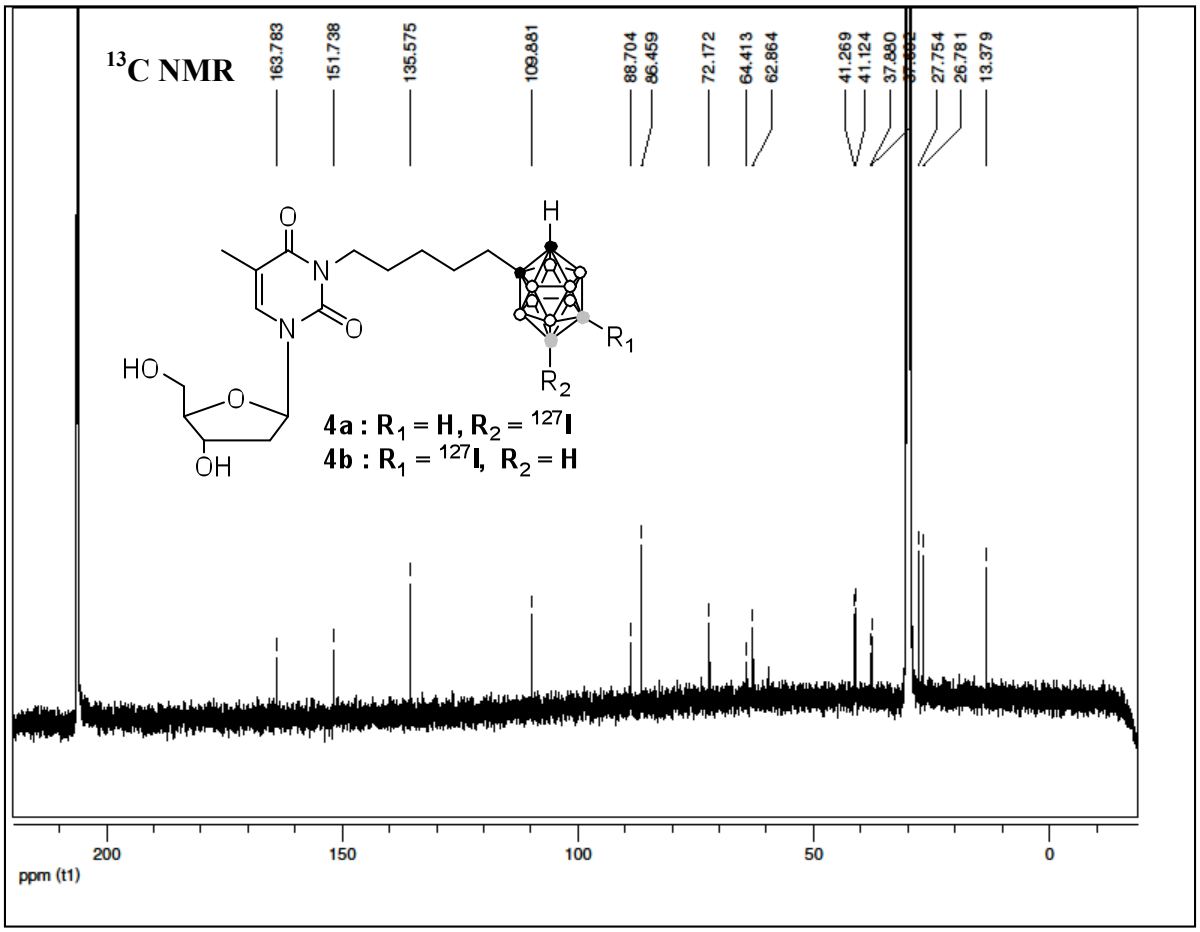

$^{1}$H NMR
7.808
7.801
7.787
7.780
7.502
7.484
5.050
4.844
4.040
4.024
2.849
2.371
2.349
2.328
2.246
2.225
2.203
1.969
1.963
1.677
1.656
1.640
1.622
1.604
1.488
1.478
1.469
1.462
1.448
TsO
H
R1
R2
11a : R1 = H, R2 = 127I
11b : R1 = 127I, R2 = H
3.19
3.27
1.00
1.12
4.46
6.79
3.33
5.94
4.79
4.57
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

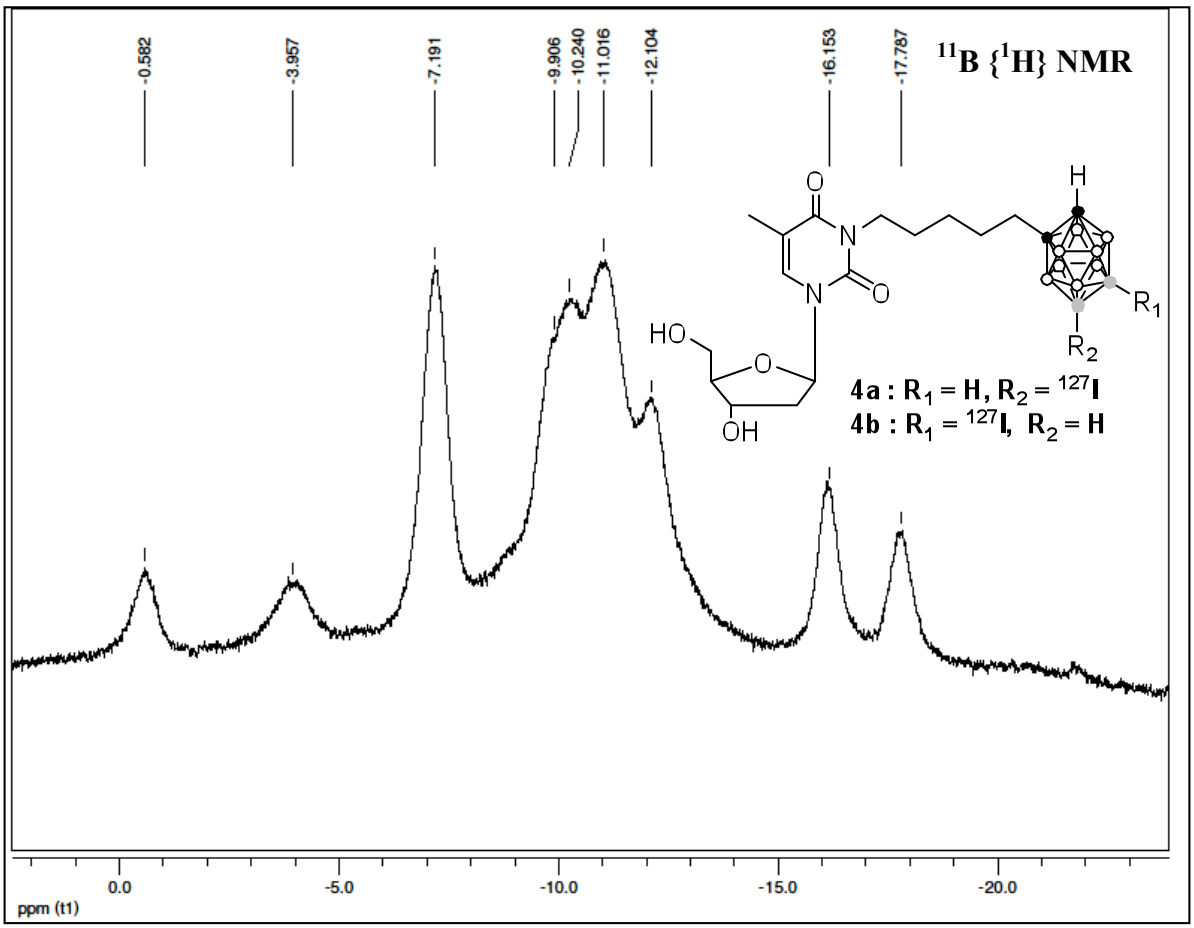

$^{13}$C NMR
145.818
134.306
130.902
128.639
78.008
73.578
71.090
64.328
59.529
37.719
37.545
30.491
30.298
29.337
29.307
29.176
28.869
25.311
21.635
TsO
H
R1
R2
11a : R1 = H, R2 = 127I
11b : R1 = 127I, R2 = H
200
150
100
50
0
ppm (t1)

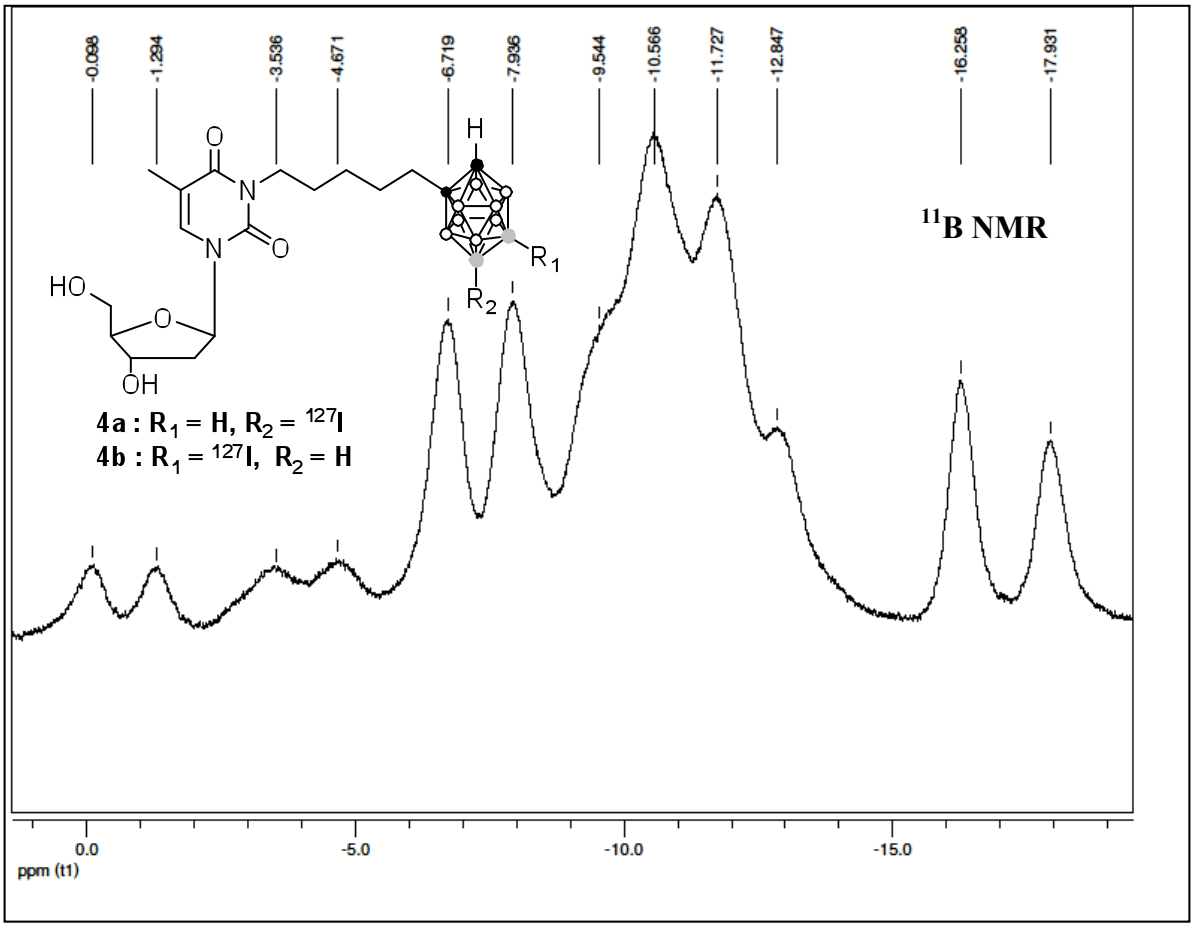

$^{11}$B {$^{1}$H} NMR
-0.666
-4.091
-7.291
-16.311
-17.978
TsO
H
R1
R2
11a : R1 = H, R2 = 127I
11b : R1 = 127I, R2 = H
5.0
0.0
-5.0
-10.0
-15.0
-20.0
-25.0
-30.0
ppm (t1)

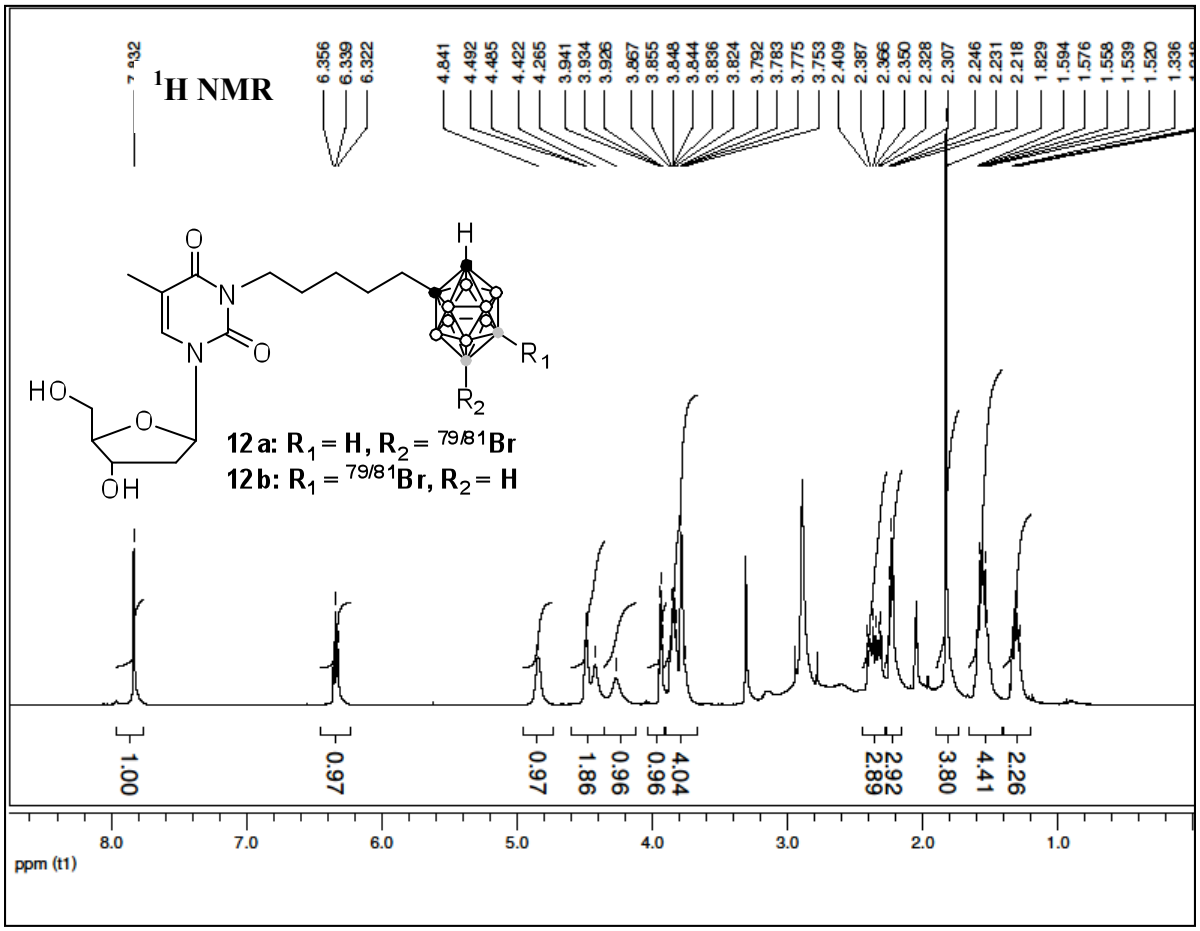

$^{11}$B NMR
-0.053
-1.323
-3.428
-4.591
-6.673
-7.858
-9.753
-10.504
-11.716
-12.849
-16.255
-17.890
TsO
H
R1
R2
11a : R1 = H, R2 = 127I
11b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

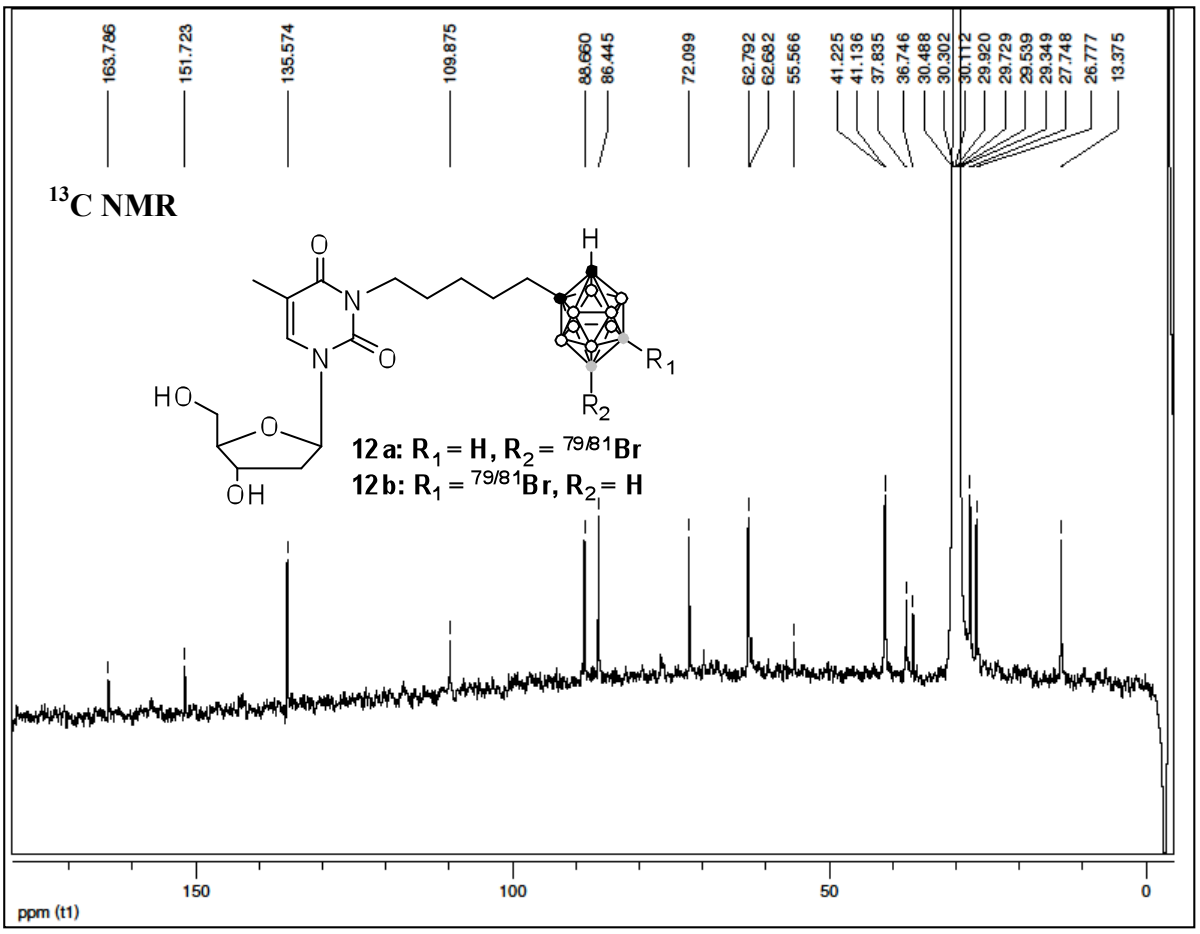

$^{1}$H NMR
4a : $R_1$ = H, $R_2$ = $^{127}$I
4b : $R_1$ = $^{127}$I, $R_2$ = H
ppm (t1)

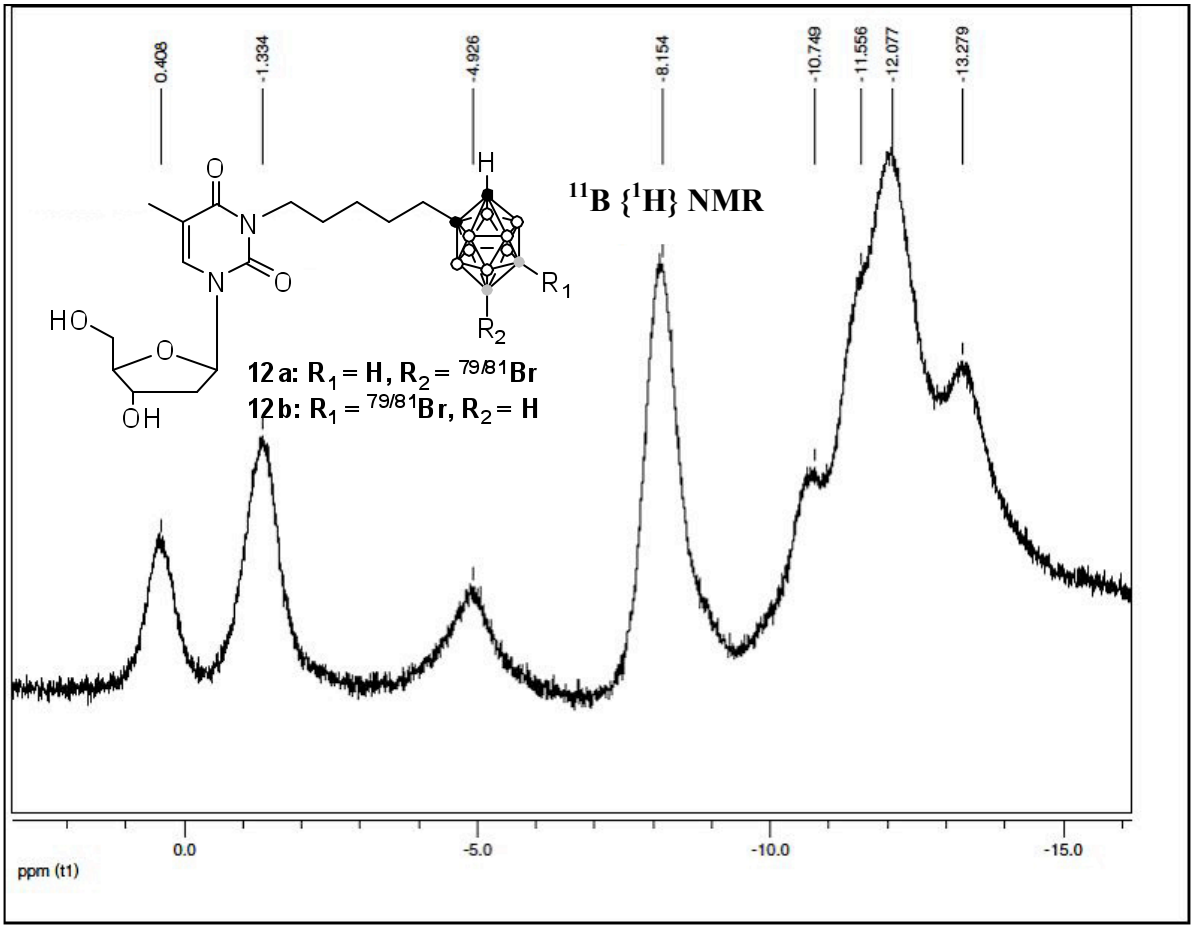

$^{13}$C NMR
4a : $R_1$ = H, $R_2$ = $^{127}$I
4b : $R_1$ = $^{127}$I, $R_2$ = H
ppm (t1)

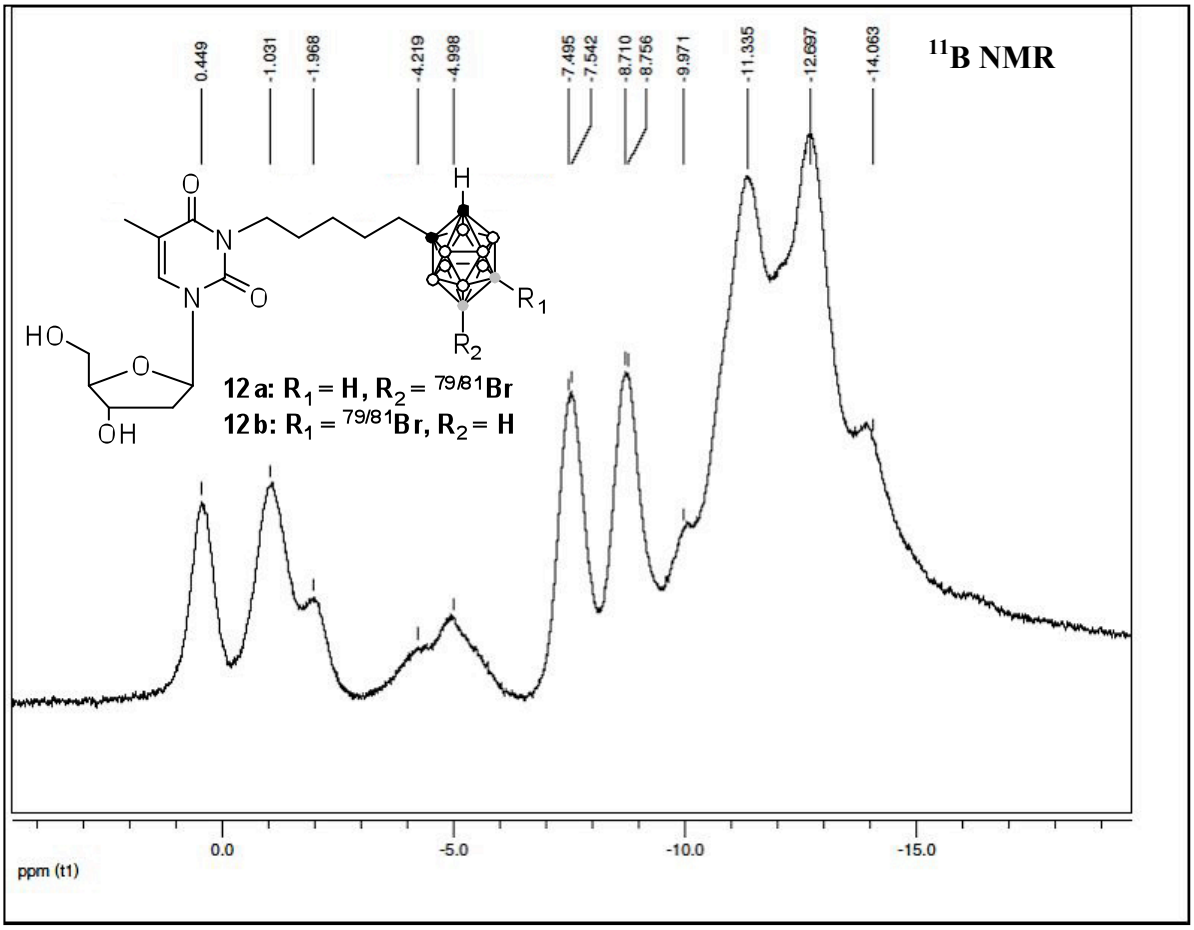

$^{11}$B {$^{1}$H} NMR
-0.582
-3.957
-7.191
-9.906
-10.240
-11.016
-12.104
-16.153
-17.787
4a : R1 = H, R2 = 127I
4b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)

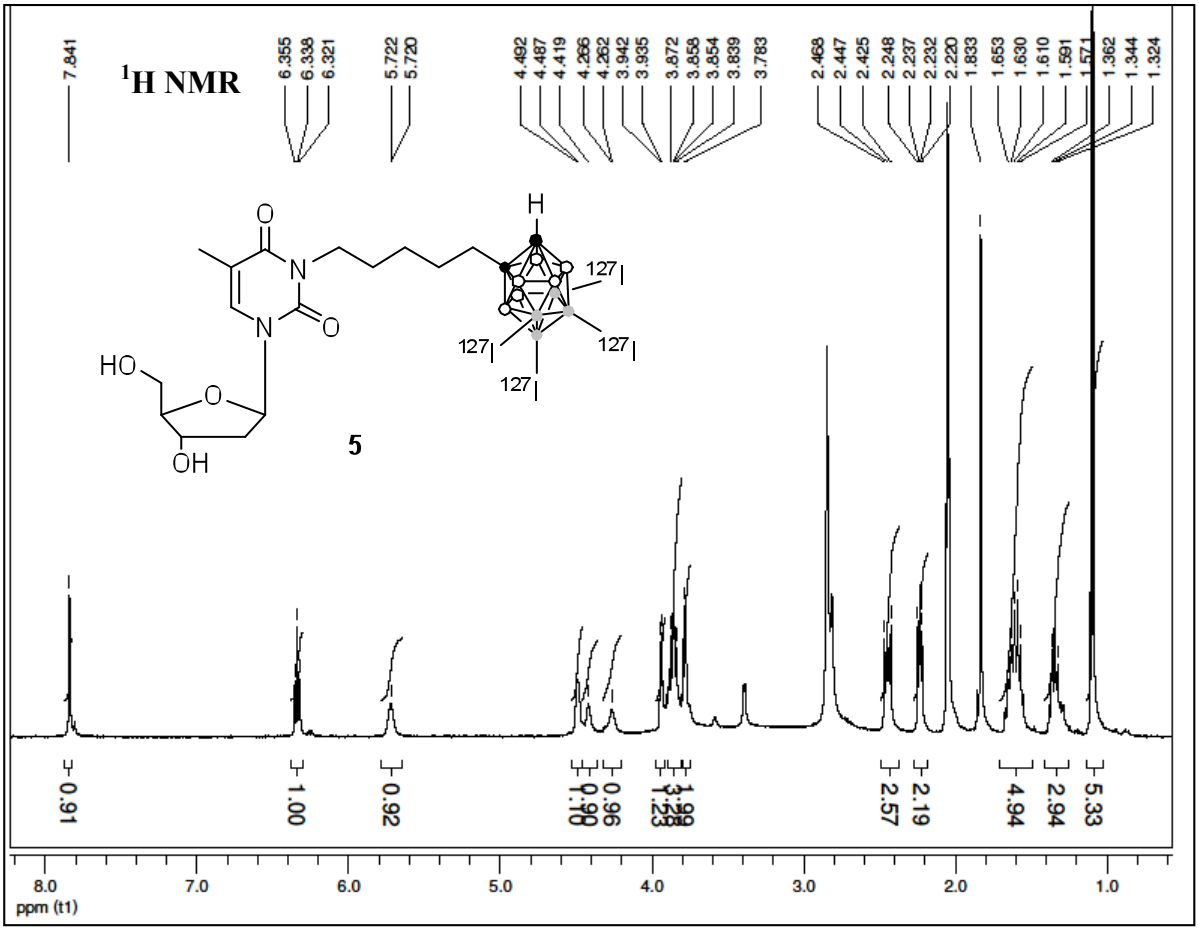

$^{11}$B NMR
-0.098
-1.294
-3.536
-4.671
-6.719
-7.936
-9.544
-10.566
-11.727
-12.847
-16.258
-17.931
4a : R1 = H, R2 = 127I
4b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
ppm (t1)

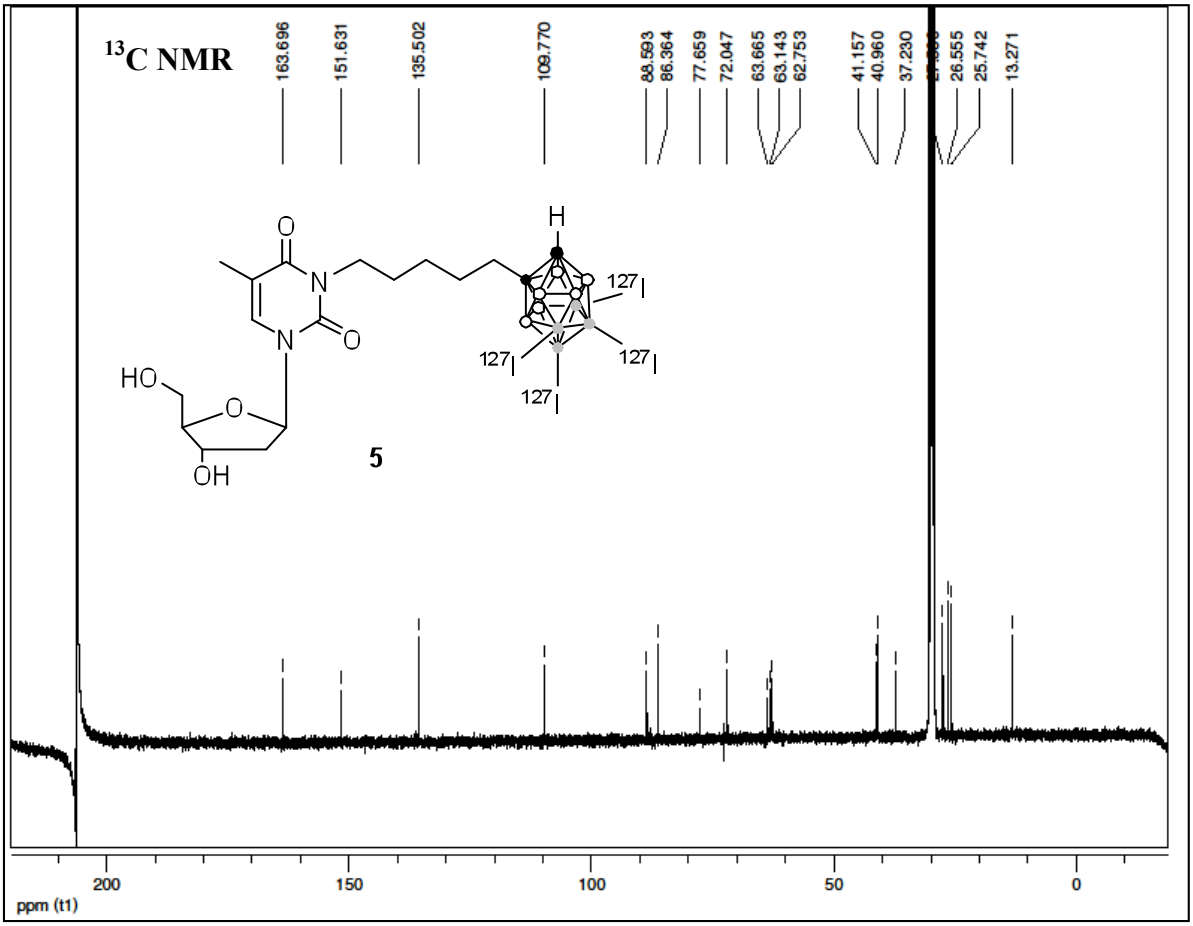

$^{1}$H NMR
12 a: $R_1$ = H, $R_2$ = $^{79/81}$Br
12 b: $R_1$ = $^{79/81}$Br, $R_2$ = H
ppm (t1)

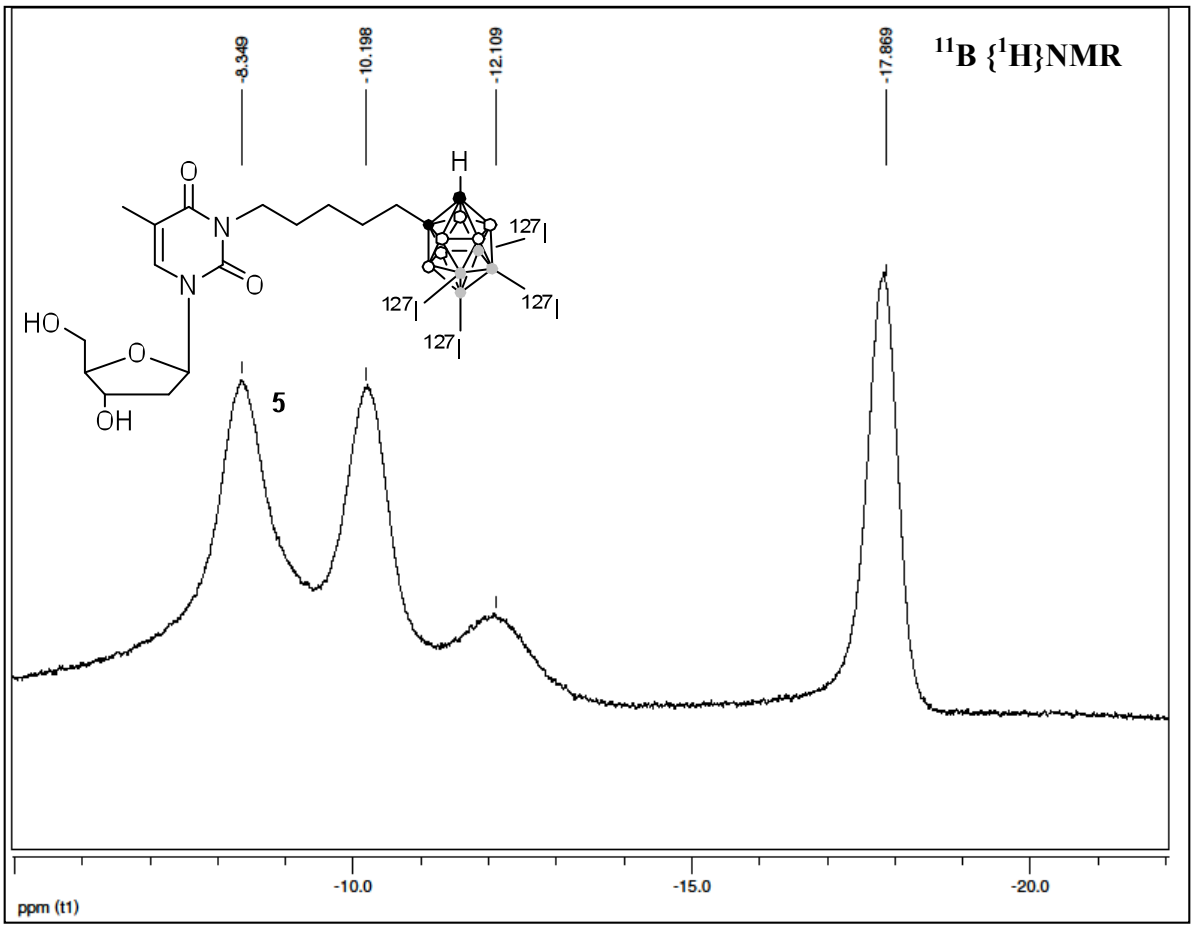

$^{13}$C NMR
12 a: $R_1$ = H, $R_2$ = $^{79/81}$Br
12 b: $R_1$ = $^{79/81}$Br, $R_2$ = H
ppm (t1)

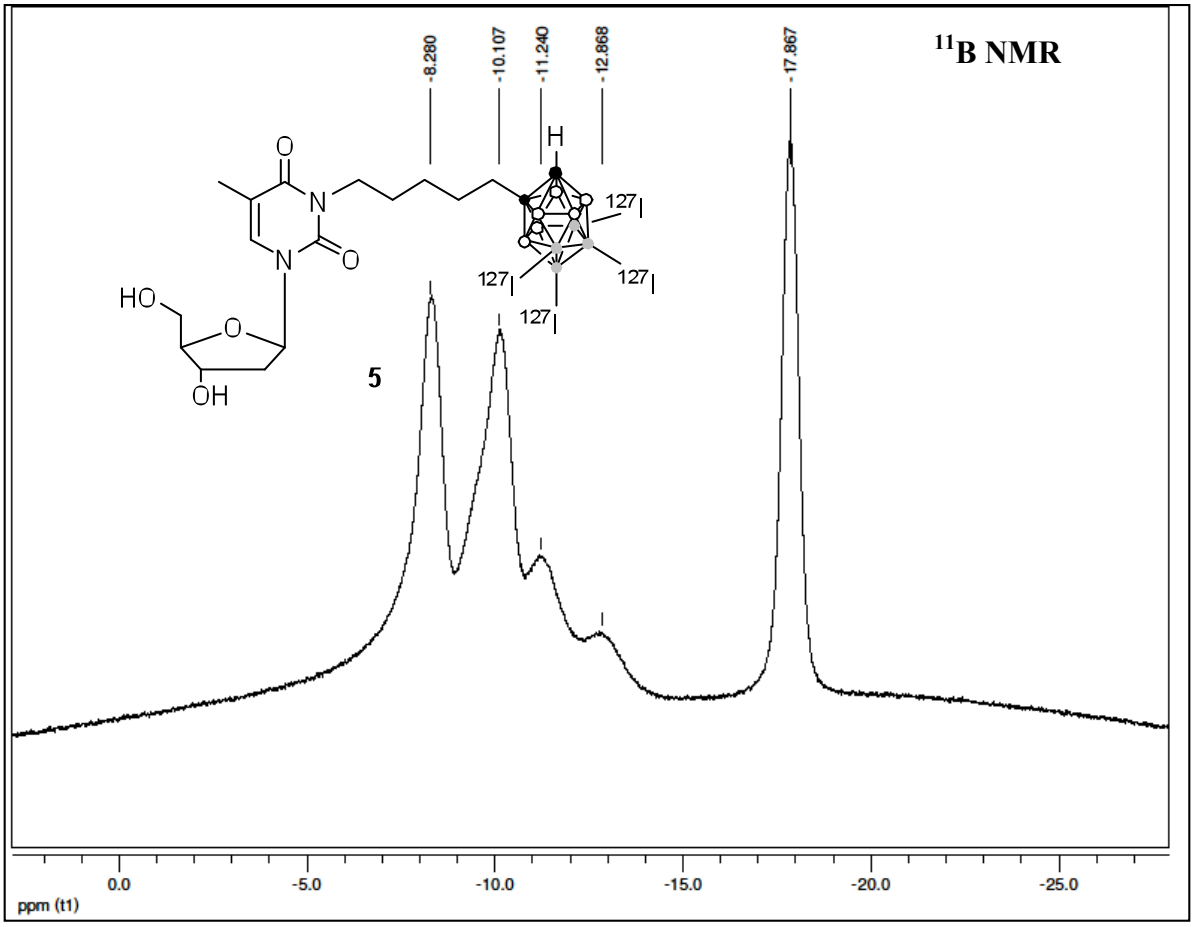

0.408
-1.334
-4.926
-8.154
-10.749
-11.556
-12.077
-13.279
$^{11}$B {$^{1}$H} NMR
12a: $R_1$ = H, $R_2$ = $^{79/81}$Br
12b: $R_1$ = $^{79/81}$Br, $R_2$ = H
0.0
-5.0
-10.0
-15.0
ppm (t1)

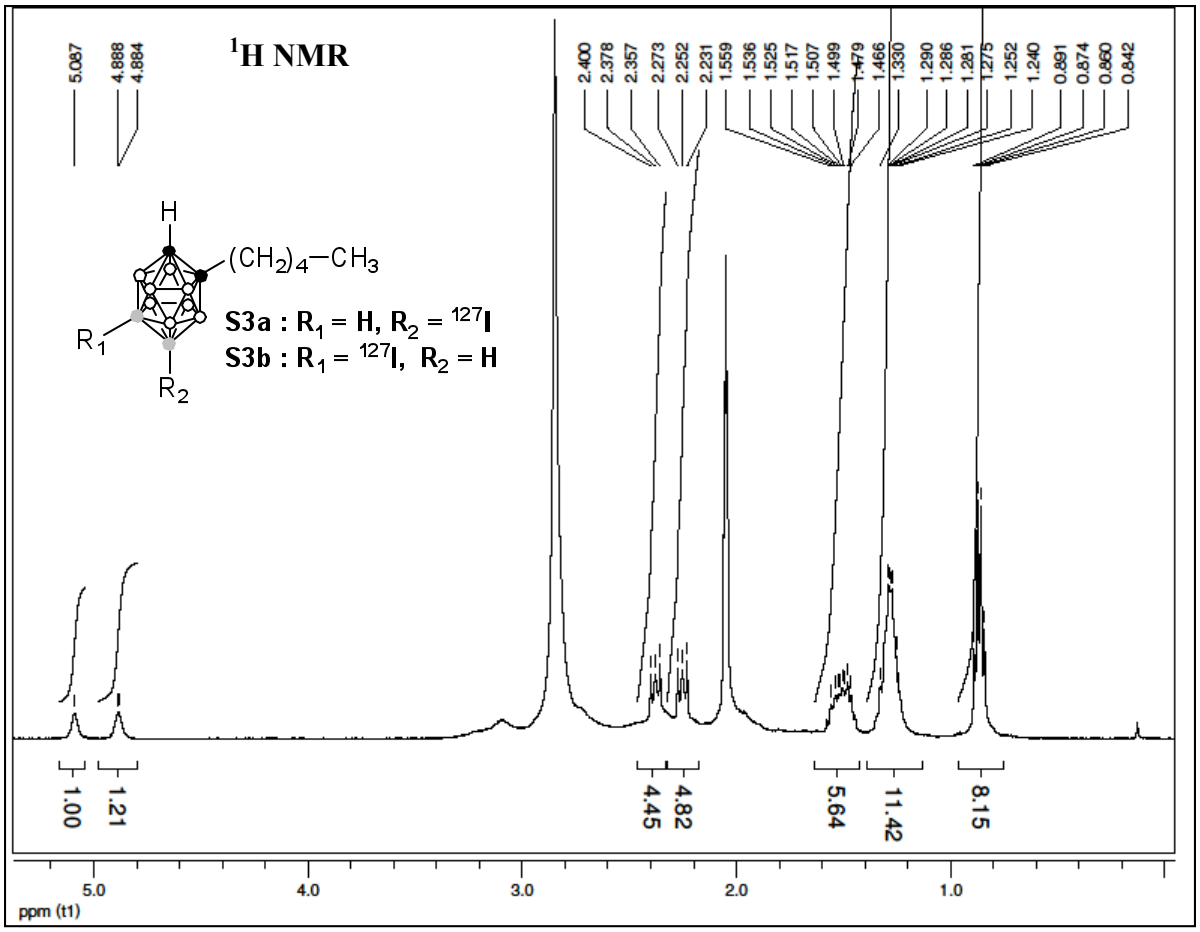

0.449
-1.031
-1.968
-4.219
-4.998
-7.495
-7.542
-8.710
-8.756
-9.971
-11.335
-12.697
-14.063
$^{11}$B NMR
12a: $R_1$ = H, $R_2$ = $^{79/81}$Br
12b: $R_1$ = $^{79/81}$Br, $R_2$ = H
0.0
-5.0
-10.0
-15.0
ppm (t1)

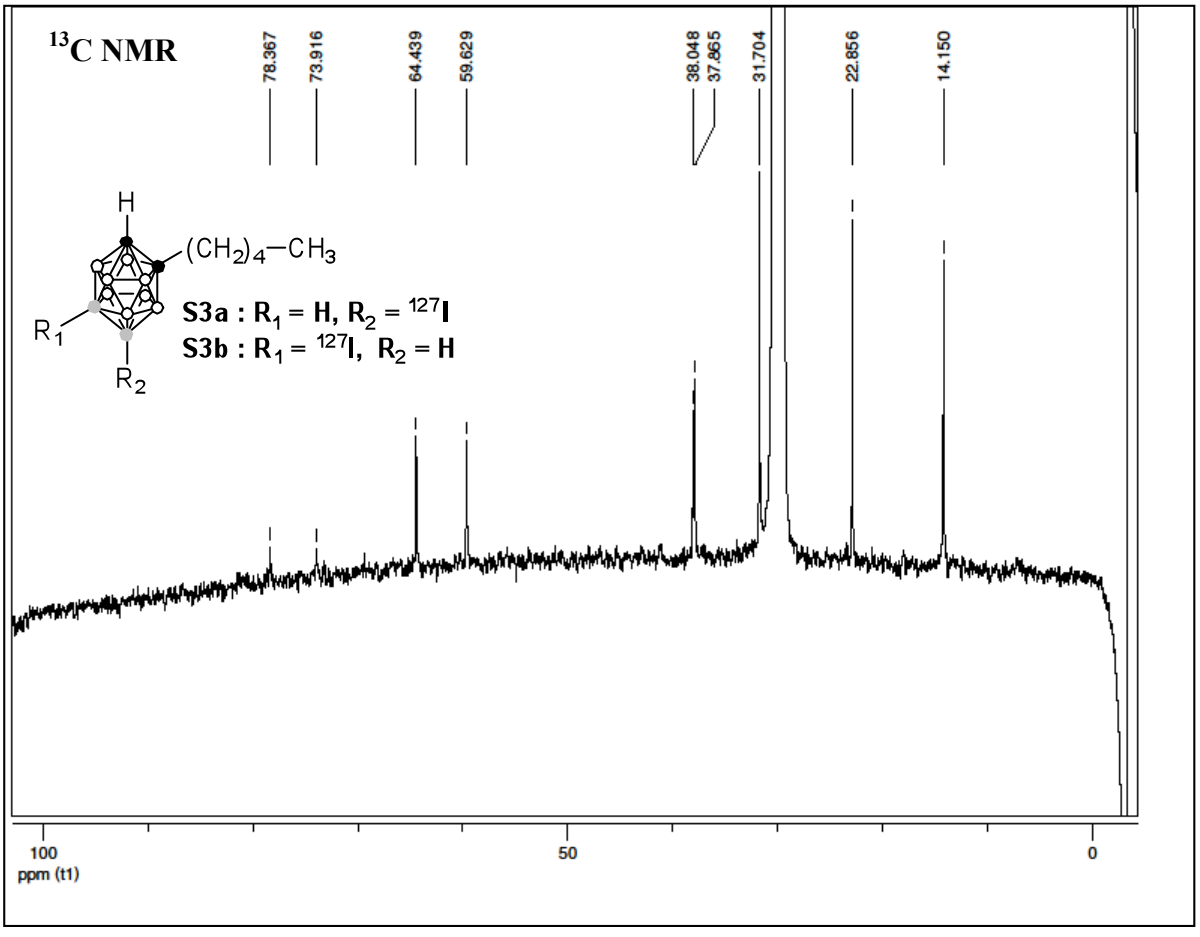

$^{1}$H NMR
7.841
6.355
6.338
6.321
5.722
5.720
4.492
4.487
4.419
4.266
4.262
3.942
3.935
3.872
3.858
3.854
3.839
3.783
2.468
2.447
2.425
2.248
2.237
2.232
2.220
1.833
1.653
1.630
1.610
1.591
1.571
1.362
1.344
1.324
O
N
N
O
HO
O
OH
H
127
127
127
127
5
0.91
1.00
0.92
1.10
0.90
0.96
1.23
2.57
2.19
4.94
2.94
5.33
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

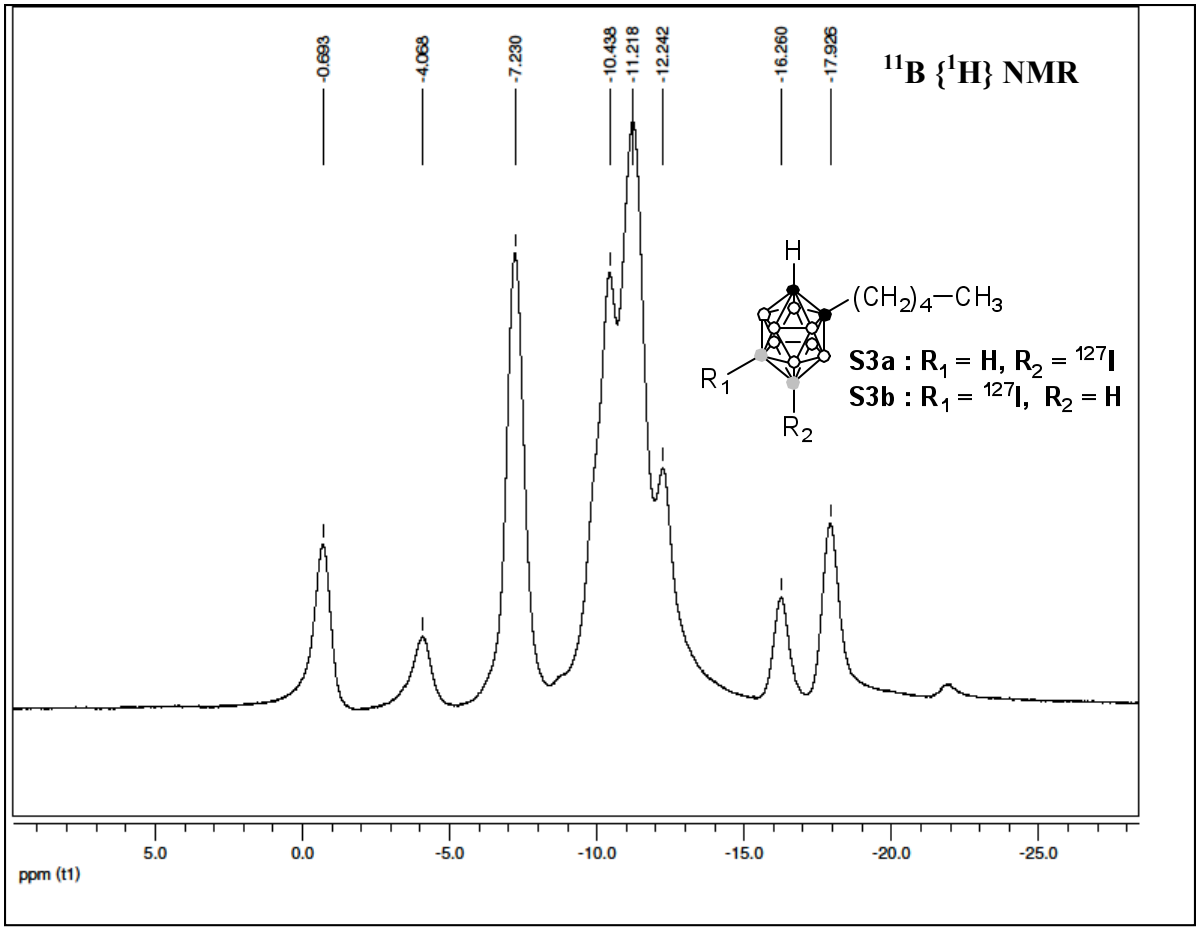

$^{13}$C NMR
163.696
151.631
135.502
109.770
88.593
86.364
77.659
72.047
63.665
63.143
62.753
41.157
40.960
37.230
26.555
25.742
13.271
O
N
N
O
HO
O
OH
H
127
127
127
127
5
200
150
100
50
0
ppm (t1)

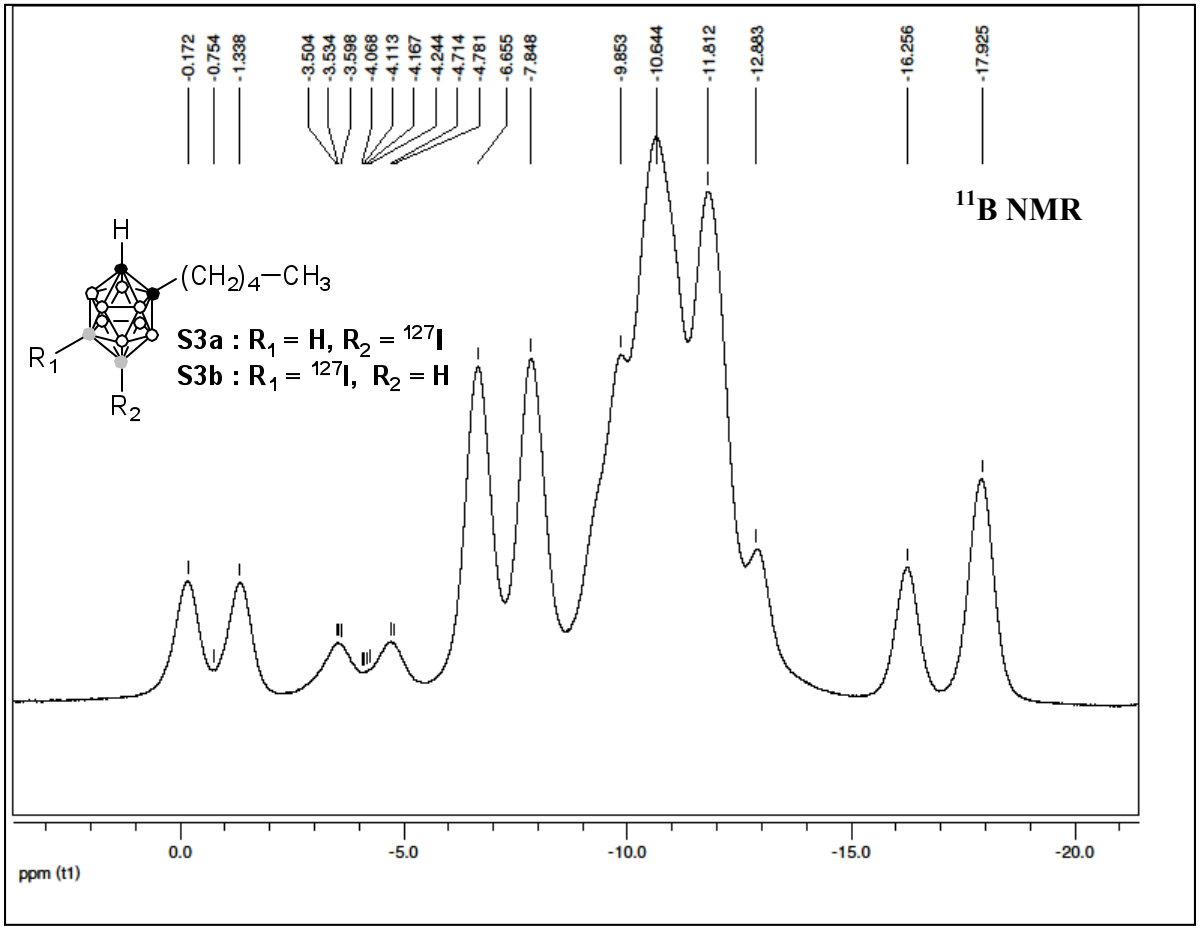

$^{11}$B {$^{1}$H}NMR
-8.349
-10.198
-12.109
-17.869
5
-10.0
-15.0
-20.0
ppm (t1)

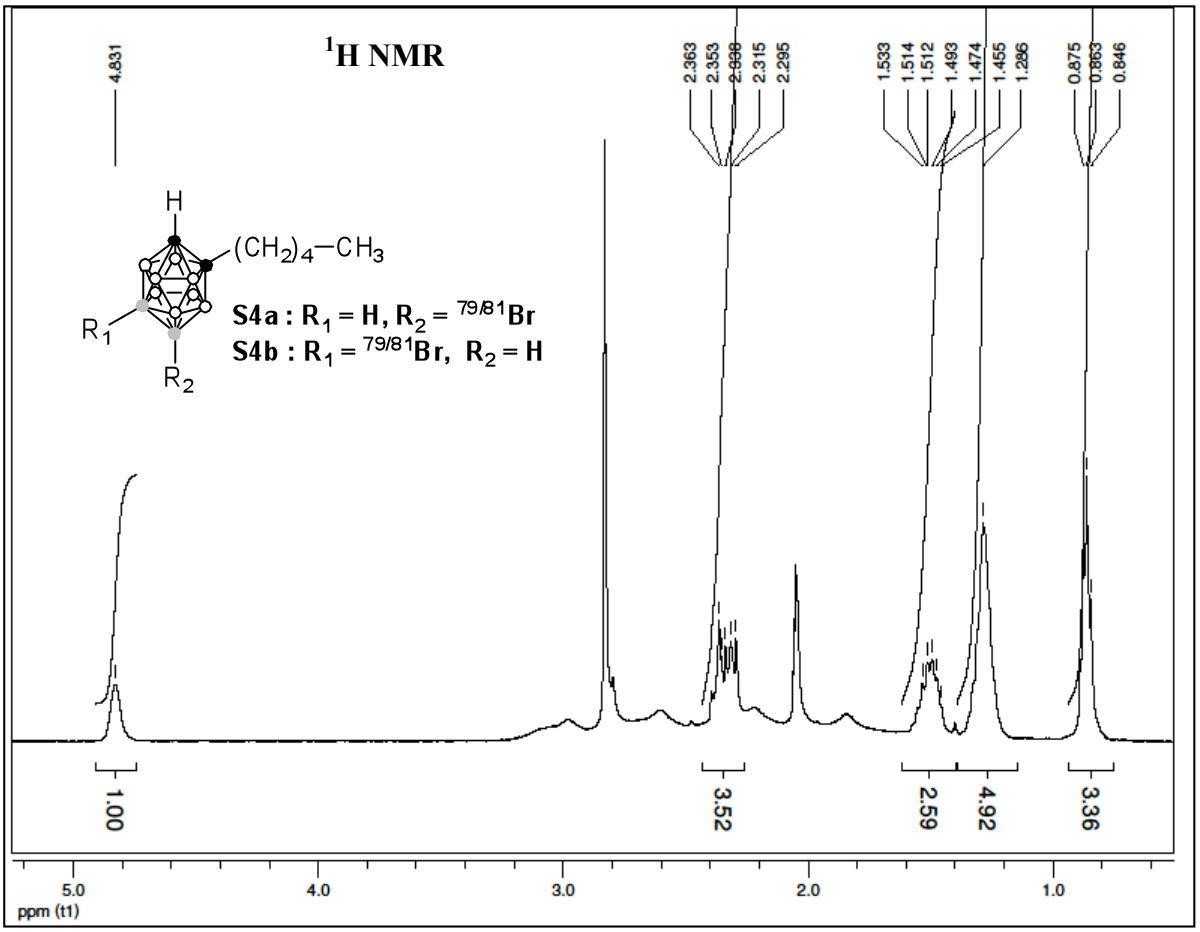

$^{11}$B NMR
-8.280
-10.107
-11.240
-12.868
-17.867
5
0.0
-5.0
-10.0
-15.0
-20.0
-25.0
ppm (t1)

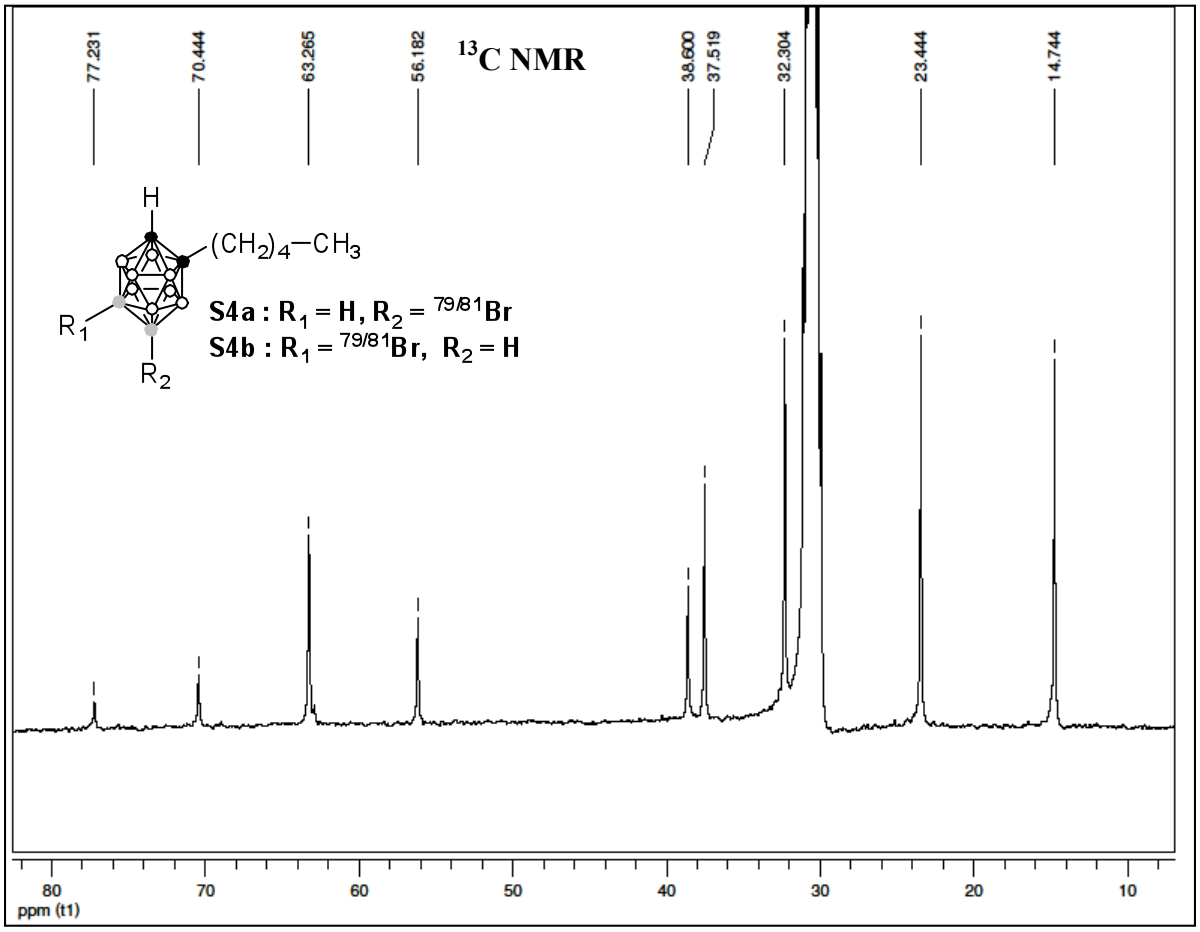

$^{1}$H NMR
5.087
4.888
4.884
2.400
2.378
2.357
2.273
2.252
2.231
1.559
1.536
1.525
1.517
1.507
1.499
1.479
1.466
1.330
1.290
1.286
1.281
1.275
1.252
1.240
0.891
0.874
0.860
0.842
H
(CH2)4—CH3
R1
R2
S3a : R1 = H, R2 = 127I
S3b : R1 = 127I, R2 = H
1.00
1.21
4.45
4.82
5.64
11.42
8.15
5.0
4.0
3.0
2.0
1.0
ppm (t1)

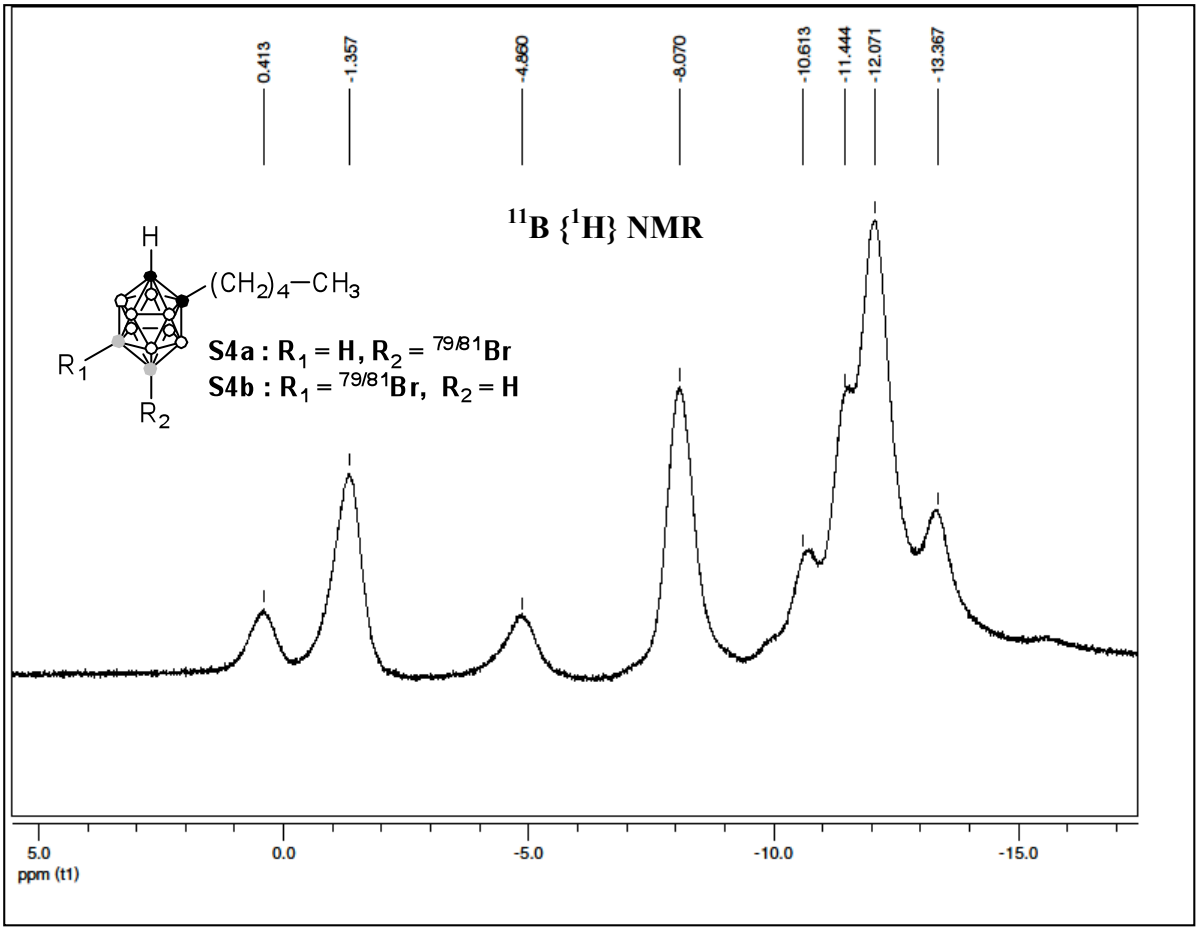

$^{13}$C NMR
78.367
73.916
64.439
59.629
38.048
37.865
31.704
22.856
14.150
H
(CH2)4—CH3
R1
R2
S3a : R1 = H, R2 = 127I
S3b : R1 = 127I, R2 = H
100
50
0
ppm (t1)

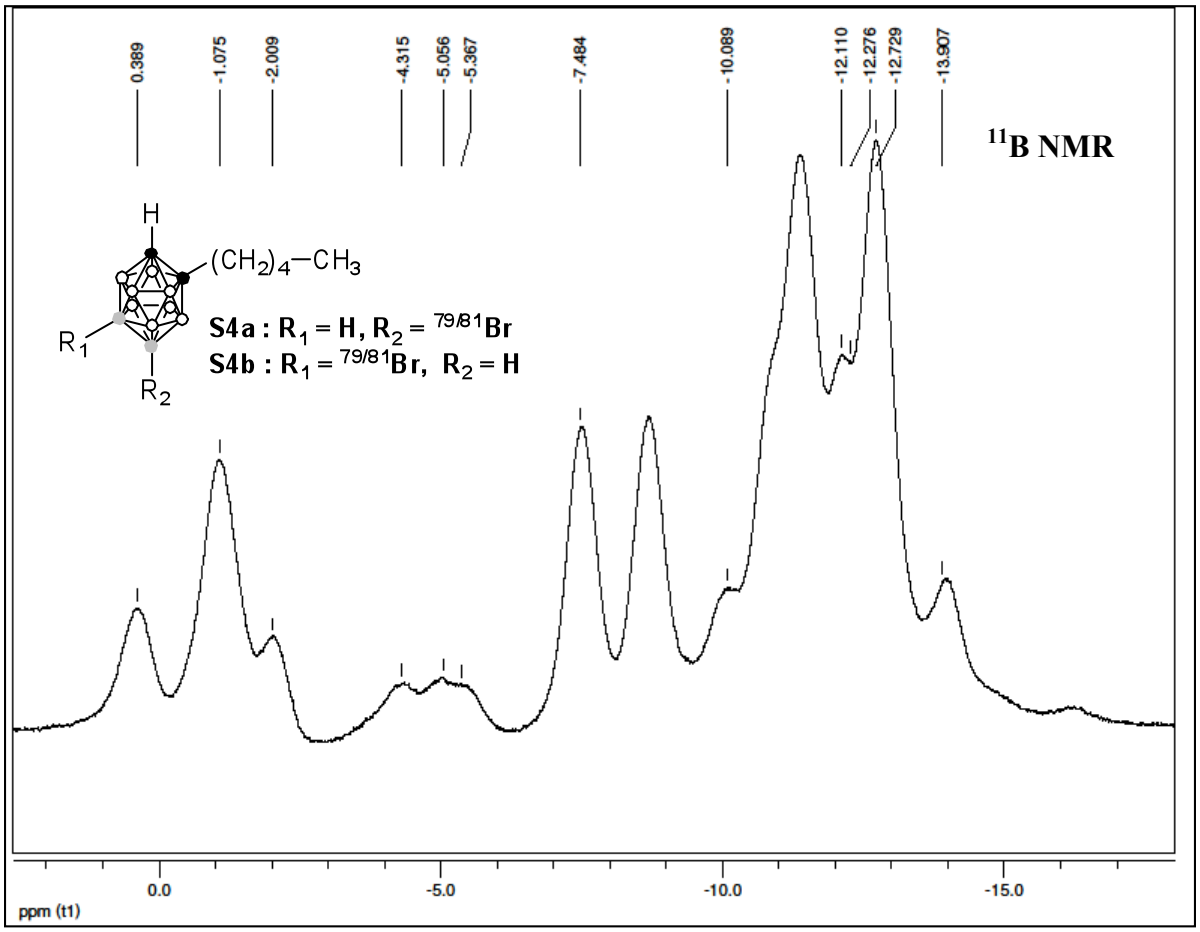

-0.693
-4.068
-7.230
-10.433
-11.218
-12.242
-16.260
-17.926
$^{11}$B {$^{1}$H} NMR
H
(CH2)4—CH3
R1
R2
S3a : R1 = H, R2 = 127I
S3b : R1 = 127I, R2 = H
5.0
0.0
-5.0
-10.0
-15.0
-20.0
-25.0
ppm (t1)


-0.172
-0.754
-1.338
-3.504
-3.534
-3.598
-4.068
-4.113
-4.167
-4.244
-4.714
-4.781
-6.655
-7.848
-9.853
-10.644
-11.812
-12.883
-16.256
-17.925
$^{11}$B NMR
H
(CH2)4—CH3
R1
R2
S3a : R1 = H, R2 = 127I
S3b : R1 = 127I, R2 = H
0.0
-5.0
-10.0
-15.0
-20.0
ppm (t1)


$^{1}$H NMR
4.831
2.363
2.353
2.338
2.315
2.295
1.533
1.514
1.512
1.493
1.474
1.455
1.286
0.875
0.863
0.846
H
(CH2)4—CH3
R1
R2
S4a : R1 = H, R2 = 79/81Br
S4b : R1 = 79/81Br, R2 = H
1.00
3.52
2.59
4.92
3.36
5.0
4.0
3.0
2.0
1.0
ppm (t1)


$^{13}$C NMR
77.231
70.444
63.265
56.182
38.600
37.519
32.304
23.444
14.744
H
(CH2)4—CH3
R1
R2
S4a : R1 = H, R2 = 79/81Br
S4b : R1 = 79/81Br, R2 = H
80
70
60
50
40
30
20
10
ppm (t1)


0.413
-1.357
-4.860
-8.070
-10.613
-11.444
-12.071
-13.367
$^{11}$B {$^{1}$H} NMR
H
(CH2)4—CH3
R1
R2
S4a : R1 = H, R2 = 79/81Br
S4b : R1 = 79/81Br, R2 = H
5.0
0.0
-5.0
-10.0
-15.0
ppm (t1)


0.389
-1.075
-2.009
-4.315
-5.056
-5.367
-7.484
-10.089
-12.110
-12.276
-12.729
-13.907
$^{11}$B NMR
H
(CH2)4—CH3
R1
R2
S4a : R1 = H, R2 = 79/81Br
S4b : R1 = 79/81Br, R2 = H
0.0
-5.0
-10.0
-15.0
ppm (t1)

## 9) References


(1) Marshall, W. J.: Young, R. J., Jr.: Grushin, V. V. *Organometallics* **2001**, *20*, 523-533.

(2) Stanko, V. I.; Iroshnikova, N. G. *Zh. Obshch. Khim.* **1970**, *40*, 311-315.

(3) Winberg, K. J.; Barbera, G.; Eriksson, L.; Teixidor, F.; Tolmachev, V.; Vinas, C.; Sjoberg, S. *J. Organomet. Chem.* **2003**, *680*, 188-192.

(4) Winberg, K. J.; Mume, E.; Tolmachev, V.; Sjoeberg, S. *J. Labelled Comp. Radiopharm.* **2005**, *48*, 195-202.

(5) Morkiw, R. T.; Canellakis, E. S. *J. Org. Chem.* **1969**, *34*, 3707-3709.

(6) Otwinowski, Z.; Minor, W. *Meth. Enzymol.* **1997**, *276*, 307-326.

(7) Blessing, R. H. *J. Appl. Cryst.* **1989**, *22*, 396-397.

(8) Blessing, R. H. *Cryst. Rev.* **1987**, *1*, 3-58.

(9) Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112-122.

(10) Farrugia, L. J. *J. Appl. Cryst.* **1999**, *32*, 837-838.

(11) International Tables for Crystallography Vol. C, Wilson, A.J.C. (Ed.) Kluwer Academic Publishers, Dordrecht, The Netherlands, 1992.