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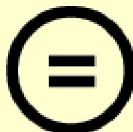
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2010년 2월

석사학위 논문

**Chiral Organotin Complexes
Stabilized by C,N-Chelating
Oxazolinyl-*o*-carboranes**

2010년 2월 25일

조선대학교 대학원

화 학 과

김 효 속

Chiral Organotin Complexes Stabilized by C,N-Chelating Oxazolinyl-*o*-carboranes

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이 논문을 이학 석사학위신청 논문으로 제출함

2009년 10월

조선대학교 대학원

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Contents

1. Abstract (영문)	1
2. Abstract (국문)	2
3. Introduction	3
4. Results and Discussion	4
4.1. Structural Study	
5. Conclusion	10
6. Experimental Section	11
6.1. General Procedures	11
6.2. Preparation of Cab^{iOxa} 1	11
6.3. Preparation of Cab^{tOxa} 2	12
6.4. General Synthesis of $(\text{Cab}^{iOxa})\text{SnMe}_2\text{Cl}$ 3	13
6.5. Synthesis of $(\text{Cab}^{iOxa})\text{SnMe}_2\text{Br}$ 4	14
6.6. Synthesis of $(\text{Cab}^{tOxa})\text{SnMe}_2\text{Cl}$ 5	14
6.7. Synthesis of $(\text{Cab}^{tOxa})\text{SnMe}_2\text{Br}$ 6	15
6.8. Preparation of Cab^{OMe} 7	16
6.9. Preparation of Cab^{OMePh} 8	16
6.10. Synthesis of the $(\text{Cab}^{C,O})\text{Me}_2\text{SnBr}$ 9	17
6.11. Synthesis of $(\text{Cab}^{C,O})\text{Me}_2\text{SnBr}$ 10	17
6.12. Crystal Structure Determination	18
7. References	20

8. Figures	24
9. X-ray Data	28
10. 감사의 글	55

1. ABSTRACT

Chiral Organotin Complexes Stabilized by *C,N*-Chelating Oxazolinyl-*o*-carboranes

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A series of chiral organotin halides containing 2-(4-*R*)-oxazolinyl-*o*-carboranes(*R* = *i*-propyl **1**, *t*-butyl **2**; Cab^{oxa}) was prepared from *o*-carborane with a chiral oxazoline auxiliary. X-ray structural analysis of the representative chiral organotin halide, [2-(4-*i*-propyl)-oxazolinyl-*o*-carboranyl]SnMe₂Br (**4**), revealed the formation of a stable penta-coordinated tin center due to a N→Sn interaction. Similar O→Sn assisted intramolecular penta-coordinated tin complexes (**9** and **10**) were prepared from methoxy-*o*-carborane ligands, MeOCH(Z)-*o*-carborane(Z = H **7**, Ph **8**; Cab^{O*Me*}), respectively, and a rigid *o*-carboranyl backbone provided the basic skeleton for the facile formation of organotin complexes.

2. 국문초록

2-(4-*R*)-oxazolinyl-*o*-carboranes (*R* = *i*-propyl **1**, *t*-butyl **2** Cab^{Oxa})를 포함하는 카이랄 유기주석 할로겐화물 시리즈는 카이랄 oxazoline에 유용한 *o*-carborane에서 얻어졌다. 카이랄 유기주석 할로겐화물을 대표하는 $[\text{2-(4-}i\text{-propyl)-oxazolinyl-}o\text{-carboranyl}] \text{SnMe}_2\text{Br}$ (**4**) X-ray 구조분석은 $\text{N} \rightarrow \text{Sn}$ 상호작용으로 인해 안정한 5-배위 주석 중심 구조를 나타낸다. 이와 유사한 분자 내 5-배위 주석화합물을 장려하는 $\text{O} \rightarrow \text{Sn}$ 은 methoxy-*o*-carborane ligands, $\text{MeOCH}(\text{Z})$ -*o*-carborane ($\text{Z} = \text{H}$ **7**, Ph **8** Cab^{OMe})로부터 얻어진다. 단단한 *o*-carboranyl backbone 은 유기주석 화합물로부터 손쉬운 구조물을 얻기 위한 기본 골격으로 공급된다.

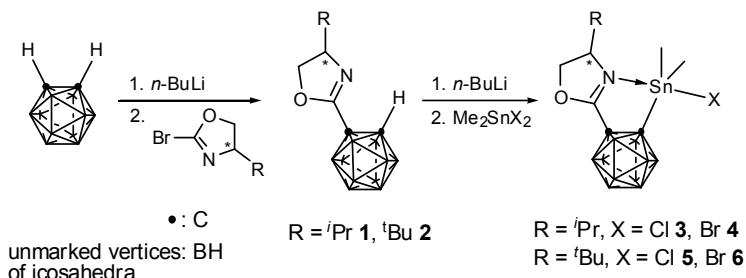
3. Introduction

Chiral organotin complexes have been developed as efficient reagents for a wide variety of organic transformations in stereospecific reactions [1-3]. The most important work involves the chiral induction of organotin complexes, one of the notable accomplishments being free-radical enantioselective reductions [4-6]. In such cases, a penta-coordinated tin center was completed with intramolecularly coordinated nitrogen atoms [7-12]. It has been reported that chiral oxazoline rings induce stereospecific reactions [13-16] due to the closer proximity of the stereogenic motif to the metal center. Such a superior chiral auxiliary can be more efficient when a suitable ligand backbone is provided. In this study, a rigid and sterically demanding *o*-carborane backbone was used to assist the proceeding stereospecific reactions [17].

Chiral oxazolinyl-*o*-carborane (Cab^{Oxa}) ligands have a nitrogen donor atom adjacent to the stereogenic carbon center at the oxazoline ring. When these ligands coordinate to the metal center, the stereogenic carbon atom will induce chiral recognition most effectively. This paper reports the synthesis and characterization of chiral organotin complexes (**3-6**) with bidentate chiral oxazoline ligands containing *o*-carborane as the rigid backbone. In addition, comparative studies using *C,O*-chelating ligands, Cab^{OMe} , have assisted in determining the relationship between the tin complexes (**9** and **10**) with respect to the structures and electronic effects of each ligand series.

4. Results and Discussion

The ligand systems, chiral [2-(4-*R*)-oxazolinyl]-*o*-carborane (*R* = *i*-propyl **1**, *t*-butyl **2**), consisted of two dissimilar coordination modes of carbon in carborane. The imine functionalities of the oxazoline unit were produced using a standard procedure [17] by reacting lithio-*o*-carborane with 2-bromo-(4-*R*)-oxazoline in a THF solution. Treatment of compounds **1** and **2** with a 1.1 equiv of *n*-BuLi and 1 equiv of Me₂SnX₂ (X = Cl, Br) in diethyl ether at -10 °C for 10 min gave the chiral oxazoline substituted *o*-carboranylorganotin halides with the general formula [2-(4-*R*)-oxazolinyl-*o*-carboranyl]SnMe₂X (*R* = *i*-propyl, X = Cl **3**, Br **4** R = *t*-butyl, X = Cl **5**, Br **6**) in good yield (**3**: 77%, **4**: 84%, **5**: 75%, **6**: 81%, Scheme 1).



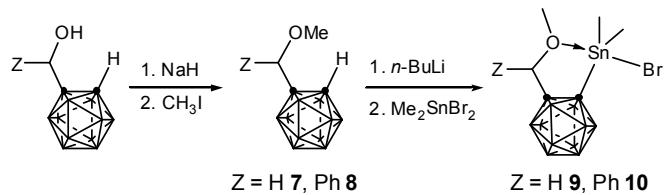
Scheme 1. Synthesis of [2-(4-*R*)-oxazolinyl-*o*-carboranyl]SnMe₂X (*R* = *i*Pr, X = Cl **3**, Br **4** *t*Bu, X = Cl **5**, Br **6**).

All new compounds were characterized by Fourier transform infrared (IR), ¹H, ¹¹B, ¹³C and ¹¹⁹Sn nuclear magnetic resonance (NMR) spectroscopy, elemental analysis, high-resolution mass spectroscopy, and single-crystal X-ray crystallography. Compounds **3-6** were moderately stable in air and decomposed only slowly when in contact with moisture. The kinetic stability of compounds

3-6 is due to the formation of a five-membered chelate ring, which protects the Sn atom from external nucleophilic attack. The ^1H NMR signals for both NCH and OCH_2 of the oxazoline ring in compounds **3-6** were observed downfield from those found in the free ligands. This can be explained by the trigonal-bipyramidal geometry with the nitrogen atom of the oxazoline unit and the halogen atom in the axial positions as well as by evidence of Sn-N coordination in solution. Information on the ligand geometry in solution at tin in compounds **3-6** was obtained from the ^{119}Sn chemical shifts and $^2J(\text{Sn}-\text{C}^1\text{H}_3)$ values. These depend on the coordination number of tin [18-20] and were compared with those of the penta-coordinated methyl-substituted organotin halides. The observed $\delta(\text{Sn})$ and $^2J(\text{Sn}-\text{C}^1\text{H}_3)$ values suggested penta-coordinate geometry at tin for compounds **3-6**. Indeed, there was close agreement of the NMR spectroscopic data between compounds **3-6** and $(\text{Ar}^{\text{Oxa}})\text{Me}_2\text{SnBr}$ [21], particularly the $^2J(\text{Sn}-\text{C}^1\text{H}_3)$ coupling constants (77.2 Hz in $(\text{Cab}^{\text{Oxa}})\text{Me}_2\text{SnBr}$ (**4**) and 75 Hz in $(\text{Ar}^{\text{Oxa}})\text{Me}_2\text{SnBr}$). The spectroscopic data suggests that complexes **3-6** have a related structure. A trigonal-bipyramidal structure for compounds **3-6** in solution was proposed based on the ^1H , ^{13}C , and ^{119}Sn NMR spectroscopy. This was expected because the tin atom in organotin halides containing a C,N -chelating ligand normally has trigonal-bipyramidal coordination geometry due to intramolecular coordination. It is believed that the *o*-carboranyl carbon atom and two alkyl ligands are at the equatorial sites, while the more electronegative nitrogen atom of oxazolinyl-*o*-carborane and halide atom reside at the axial positions.

New types of C,O -chelated organotin bromides with Sn-O intramolecular interactions were attempted as a variation of the generation of organotin compounds stabilized by *o*-carboranyl ligands. Accordingly, the synthesis and

single-crystal X-ray crystallographic studies of organotin bromides containing new types of methoxy-*o*-carborane ligands, MeOCH(Z)-*o*-carborane (Z = H **7**, Ph **8**), were carried out. *C,O*-chelating ligands, **7** and **8**, were prepared by reacting *o*-carboranyl- or *o*-carboranyl(phenyl)methanol [22] with CH₃I in the presence of 3 equiv of NaH in THF at 0 °C (Scheme 2). After ligand deprotonation of compounds **7** and **8** by *n*-BuLi at -10 °C in diethyl ether for 10 min, methathesis reactions with Me₂SnBr₂ were carried out to produce the desired intramolecularly stabilized *C,O*-chelated organotin complexes, **9** and **10**, in good yield (**9**: 84%; **10**: 83%, Scheme 2).



Scheme 2. Synthesis of [CH₃OCH(Z)-*o*-carboranyl]SnMe₂Br (Z = H **9**, Ph **10**).

The *C,O*-chelating organotin complexes were stabilized by the formation of a five-membered chelate ring. Compounds **9** and **10** were purified by low-temperature recrystallization in toluene. Satisfactory elemental analyses were obtained for compounds **9** and **10**, and the ¹H, ¹³C, and ¹¹⁹Sn NMR spectral data was consistent with the presence of methoxymethyl-*o*-carboranyl ligands. Downfield shifts of the signals for both OCH₃ and OCH₂ were observed in the ¹H NMR spectra in compounds **9** and **10**, which is in accord with the presence of Sn-O bonds. ¹H NMR suggested that compounds **9** and **10** are penta-coordinated in solution. Additional evidence for penta-coordinate tin centers in these compounds was provided by the observed absolute ¹¹⁹Sn NMR chemical

shifts values. As reported in the literature [23], $\delta^{119}\text{Sn}$) values in the range -210 to -400, -90 to -190, and 200 to -60 ppm are associated with six-, five-, and four-coordinate tin centers, respectively. Compounds **9** and **10** exhibited chemical shifts of ($\delta^{119}\text{Sn}$) -108.2 (**9**) and -110.3 (**10**) ppm) with respect to Ph₂BrSn(CH₂-16-crown-5) [24] ($\delta^{119}\text{Sn}$) -96 ppm). Overall, these results favor the existence of an intramolecular Sn-O interaction in compounds **9** and **10**, which leads to the trigonal-bipyramidal coordination of the Sn atom. The spectroscopic data indicates that complexes **9** and **10** have a related structure. It is believed that the *o*-carboranyl carbon atom and two alkyl ligands are at the equatorial sites, while the more electronegative oxygen atom of methoxymethyl-*o*-carborane and the bromide atom reside at the axial positions.

4.1. Structural Study.

The structures of compounds **4**, **7**, **8**, and **9** were determined by X-ray structural analysis. Selected interatomic distances and angles are presented in the appropriate figure caption (Figures 1–4). Detailed information on the structural determinations and structural features of all four compounds are provided in the Supporting Information. Figures 1 and 4 show the penta-coordinated organotin bromide structures tethered by chiral oxazolinyl- (**4**) and methoxymethyl- (**9**) *o*-carborane, respectively. Figures 2 and 3 show the conformations of the ligands, consisting of methoxymethyl- (**7**) and methoxy(phenyl)methyl-*o*-carborane (**8**), respectively. In compounds **4** and **9**, each central tin atom has a distorted trigonal-bipyramidal structure with the electronegative atoms (N, Br (**4**) or O, Br (**9**)) in the axial positions and all carbon atoms in equatorial positions, which is in accordance with previously published results[25]. As expected, compound **4** is

chiral, crystallizing in the orthorhombic $P2_12_12_1$ space group with the Flack parameter [26] refining to 0.00, which confirms the presence of an enantiomerically pure compound. Unfortunately, the nine non-hydrogen atoms of compound **4**, C(1), C(2), C(3), B(3), B(4), B(6), B(7), B(9), and B(10), were refined isotropically because of their non-positive temperature factors that might occur due to systematic errors in the observed amplitudes originating in possible merohedral twinning. A strong Sn-N interaction was found in compound **4** with a distance of 2.500(1) Å, which lies in the normal range of $N_{sp^2} \rightarrow \text{Sn}$ dative bonding. A shorter Sn-N distance is expected because the coordinating nitrogen atom is sp^2 -hybridized. Indeed, the Sn-N distance in compound **4** is approximately 0.15 Å shorter than the Sn- N_{sp^3} distances (2.648 (6) Å) [25]. Recently, a similar strong $N_{sp^2} \rightarrow \text{Sn}$ interaction was reported in tin complexes of 2-mercaptop-4-methylpyrimidine [27], where the Sn-N distances were varied in the range of 2.456–2.664 Å. As a consequence of the Sn-N interaction, the Sn(1)-Br(1) distance (2.614(2) Å) is longer than that observed in other hypervalent triorganotin bromides (2.599(4) Å) [28]. The structure shows that the nitrogen atom of the oxazoline ring coordinates preferentially to tin, even though Sn-O coordination would lead to a sterically less crowded molecule. Furthermore, considerable distortions from an idealized trigonal-bipyramidal are evident in the solid state due to the sp^2 C(3) and N(1) of the oxazoline ring. Therefore, the angle associated with axial ligand N(1)-Sn(1)-Br(1) deviates from linearity (169.6(3)°) due to its proximity to the sterically incumbent oxazolinyl unit.

X-ray structural determinations of compound **9** authenticated the expected trigonal-bipyramidal geometries illustrated in Figure 4. The overall geometry was similar to that observed in compound **4**. Therefore, the Sn atom has a distorted trigonal-bipyramidal geometry with the O(1) and Br(1) atoms in the axial positions and *o*-carboranyl carbon atom and two alkyl ligands in the equatorial plane. The

angular distortions of the trigonal-bipyramidal arise from the geometric constraints associated with the bite angle of the bidentate ligands [O(1)-Sn(1)-C(1)) angle of 71.4(6) $^{\circ}$] in the presence of the O(1)-Sn(1)-Br(1) bond angle (169.8(3) $^{\circ}$). Sn(1)-O(1) and Sn(1)-Br(1) bond distances of 2.579(1) and 2.537(3) Å are similar to the corresponding normal values for Sn-O (2.564(2) Å) dative and Sn-Br (2.6088(4) Å) single bonds [24].

5. Conclusion

In conclusion, chiral organotin compounds were synthesized from chiral oxazolinyl auxiliary containing *o*-carborane as a rigid backbone and their structure was determined. NMR and single-crystal X-ray crystallographic studies of compound **4** showed that the chiral oxazolinyl-*o*-carborane ligands at the tin metal center significantly affect both the stability of the starting compounds and the electronic properties of the metal center due to the strength of the Sn-N bond.

6. Experimental Section

6.1. General Procedures.

All manipulations were carried out under a dry, oxygen-free nitrogen or argon atmosphere using standard Schlenk techniques or in a Vacuum Atmosphere HE-493 drybox. Solvents were dried by standard methods and distilled prior to use. The ^1H , ^{11}B , ^{13}C and ^{119}Sn NMR spectra were recorded on a Varian Mercury 300 spectrometer operating at 300.1, 96.3, 75.4 and 111.9 MHz, respectively. The chemical shifts are reported (δ , ppm) in reference to tetramethylsilane for ^1H and ^{13}C , boron trifluoride etherate for ^{11}B , or tetramethyltin for ^{119}Sn spectroscopy. The IR spectra were recorded on a Biorad FTS-165 spectrophotometer. *o*-Carborane was purchased from KatChem, and tetrabutylammonium fluoride, paraformaldehyde, benzaldehyde, *n*-BuLi, dimethyltin dichloride and dimethyltin dibromide were purchased from Aldrich chemicals. The compounds were used without purification. 2-(4-*R*)-oxazolinyl-*o*-carboranes (*R* = *i*-propyl, *t*-butyl)⁴ and methoxymethyl- and methoxy(phenyl)methyl-*o*-carborane⁷ were prepared using literature methods. Elemental analyses were performed using a Carlo Erba Instruments CHNS-O EA1108 analyzer. The high-resolution mass spectra were measured at the Korea Basic Science Institute. All melting points were uncorrected.

6.2. Preparation of 2-(4-*i*-propyl)-oxazolinyl-*o*-carborane (**1**).

n-BuLi (2.0 mL, 5.0 mmol, 2.5 M solution in hexane) was added dropwise to a solution of *o*-carborane (0.72 g, 5.0 mmol) in 50 mL of dry THF at -78 °C with constant stirring. The mixture was allowed to stir for 30 min at -78 °C at

which time 2-bromo-4-*i*-propyl-oxazoline (1.06 g, 5.5 mmol) was added dropwise. The solution was stirred for 1 h and then warmed to ambient temperature. The reaction was quenched with water, extracted with ether, and dried over anhydrous Na₂SO₄. The solvent was evaporated and the residue was purified by silica gel column chromatography using hexane as the eluent (*R*_f 0.4) to afford compound **1** as a pale yellow oil in 74% yield (0.94 g, 3.7 mmol). Anal. Calcd for C₈H₂₁B₁₀NO: C, 37.63; H, 8.29; N, 5.48. Found: C, 37.60 H, 8.32 N, 5.44%. IR (KBr pellet, cm⁻¹) ν(C-H) 3014, 2990, 2982, ν(B-H) 2604, ν(C=N) 1700. ¹H NMR (CDCl₃) δ 0.92 (d, 3H, CH(CH₃)₂, ³J_{CH-CH₃} = 6.6 Hz), 0.99 (d, 3H, CH(CH₃)₂, ³J_{CH-CH₃} = 6.9 Hz), 1.92 (m, 1H, CH(CH₃)₂), 3.85 (brs, 1H, Cab-H), 4.16 (m, 1H, CHN), 4.19 (dd, 1H, CH₂O, ²J_{C-H} = 8.4 Hz), 4.45 (dd, 1H, CH₂O, ²J_{C-H} = 8.1 Hz). ¹³C NMR (75.4 MHz, CDCl₃) δ 14.2, 18.6 (CH(CH₃)₂); 30.5 (CH(CH₃)₂); 68.4 (Cab), 70.5, 71.2 (OCH₂CHN); 73.8 (Cab); 168.5 (C=N). ¹¹B NMR (96.3 MHz, CDCl₃) δ -14.05 (2H), -12.51 (3H), -8.93 (2H), -5.74 (3H).

6.3. Preparation of 2-(4-*t*-butyl)-oxazolinyl-*o*-carborane(**2**).

A procedure analogous to the preparation of compound **1** was used but instead starting from *o*-carborane (0.72 g, 5.0 mmol) with 2-bromo-4-*t*-butyl-oxazoline (1.33 g, 5.5 mmol). Compound **2** was obtained as a pale yellow oil by silica gel column chromatography using hexane as the eluent (*R*_f 0.36) (0.93 g, 3.5 mmol, 69%). Anal. Calcd for C₉H₂₃B₁₀NO: C, 40.13 H, 8.61 N, 5.20. Found: C, 40.10 H, 8.29 N, 5.17%. IR (KBr pellet, cm⁻¹) ν(C-H) 3007, 2989, 2984, ν(B-H) 2599, ν(C=N) 1692. ¹H NMR (CDCl₃) δ 0.96 (s, 9H, C(CH₃)₃), 3.84 (brs, 1H, Cab-H), 4.18 (t, 1H, CHN), 4.21 (dd, 1H, CH₂O, ²J_{C-H} = 8.1 Hz), 4.40 (dd, 1H, CH₂O, ²J_{C-H} = 8.2 Hz). ¹³C NMR (75.4 MHz, CDCl₃) δ 22.4 (C(CH₃)₃); 33.8

($C(CH_3)_3$); 68.1 (*Cab*), 70.9, 72.1 (OCH_2CHN); 72.6 (*Cab*); 168.7 ($C=N$). ^{11}B NMR (96.3 MHz, $CDCl_3$) δ -19.62 (4H), -16.33 (2H), -12.72 (2H), -4.68 (2H).

6.4. General Synthesis of the Chiral Organotin Halides [2-(4-*i*-propyl)-oxazolinyl-*o*-carboranyl]SnMe₂Cl (**3**).

A 2.5 M *n*-BuLi solution (1.3 mL, 3.3 mmol) was added to a stirred solution of compound **1** (0.77 g, 3.0 mmol) in diethyl ether (30 mL) at -10 °C through a syringe. The resulting solution was stirred at -10 °C for 30 min. A solution of Me₂SnCl₂ (0.66 g, 3.0 mmol) in diethyl ether (10 mL) was added slowly to the 30 mL diethyl ether solution of compound **1**·Li at -10 °C. The reaction temperature was maintained at -10 °C for 10 min. The reaction mixture was filtered and the organic solvent was evaporated. The crude product was dissolved in fresh distilled toluene. The volume of the toluene solution was reduced and the resulting concentrated solution allowed to stand at -10 °C for 2 days to allow crystallization. Compound **3** was obtained as colorless crystals in 77% yield (1.01 g, 2.3 mmol). Mp: 168-170 °C (dec). HRMS: Calcd for [$^{12}C_{10}^1H_{26}^{11}B_{10}^{35}Cl^{14}N^{16}O^{119}Sn$]⁺ 441.1655. Found: 441.1631. Anal. Calcd for C₁₀H₂₆B₁₀ClNO₁Sn: C, 27.38 H, 5.98 N, 3.19. Found: C, 27.40 H, 5.95 N, 3.21%. IR (KBr pellet, cm^{-1}) ν (C-H) 3205, 3085, 2980, ν (B-H) 2588, ν (C=N) 1690. 1H NMR ($CDCl_3$) δ 0.33 (s, 6H, Sn- CH_3 , $^2J_{119Sn-CH_3}$ = 75.3 Hz), 0.94 (d, 3H, $CH(CH_3)_2$, $^3J_{CH-CH_3}$ = 6.6 Hz), 1.11 (d, 3H, $CH(CH_3)_2$, $^3J_{CH-CH_3}$ = 6.9 Hz), 1.94 (m, 1H, $CH(CH_3)_2$), 4.23 (m, 1H, CHN), 4.22 (m, 1H, CH_2O), 4.47 (m, 1H, CH_2O). ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 4.21 (Sn- CH_3); 13.6, 16.0 ($CH(CH_3)_2$); 28.8 ($CH(CH_3)_2$); 68.6 (*Cab*); 68.9, 70.5 (OCH_2CHN); 70.3 (*Cab*); 166.3 ($C=N$). ^{11}B NMR (96.3 MHz, $CDCl_3$) δ -14.27 (2H), -11.59 (1H), -10.37 (1H), -9.16

(1H), -5.86 (3H), -3.37 (1H). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -124.4 (Sn-CH_3).

6.5. Synthesis of Organotin Halide (**4**).

A procedure analogous to the preparation of compound **3** was used but instead starting from compound **1** (0.77 g, 3.0 mmol) with Me_2SnBr_2 (0.93 g, 3.0 mmol). Compound **4** was obtained as colorless crystals (1.22 g, 2.5 mmol, 84%). Mp: 183-185 °C (dec). HRMS: Calcd for $[^{12}\text{C}_{10}\text{H}_{26}^{11}\text{B}_{10}^{80}\text{Br}^{14}\text{N}^{16}\text{O}^{119}\text{Sn}]^+$ 485.1150. Found: 485.1160. Anal. Calcd for $\text{C}_{10}\text{H}_{26}\text{B}_{10}\text{BrNO}_2\text{Sn}$: C, 24.86; H, 5.43; N, 2.90. Found: C, 24.84 H, 5.41 N, 2.93%. IR (KBr pellet, cm^{-1}) $\nu(\text{C-H})$ 3207, 3085, 2982, $\nu(\text{B-H})$ 2586, $\nu(\text{C=N})$ 1688. ^1H NMR (CDCl_3) δ 0.31 (s, 6H, Sn-CH_3 , $^2J_{119\text{Sn-CH}_3} = 77.2$ Hz), 0.94 (d, 3H, $\text{CH}(\text{CH}_3)_2$, $^3J_{\text{CH-CH}_3} = 6.6$ Hz), 1.11 (d, 3H, $\text{CH}(\text{CH}_3)_2$, $^3J_{\text{CH-CH}_3} = 6.9$ Hz), 1.94 (m, 1H, $\text{CH}(\text{CH}_3)_2$), 4.25 (m, 1H, CHN), 4.28 (m, 1H, CH_2O), 4.48 (m, 1H, CH_2O). ^{13}C NMR (75.4 MHz, CDCl_3) δ 4.18 (Sn-CH_3); 13.7, 16.4 ($\text{CH}(\text{CH}_3)_2$); 28.5 ($\text{CH}(\text{CH}_3)_2$); 68.6 (*Cab*); 68.7, 70.3 (OCH_2CHN); 70.1 (*Cab*); 166.2 (C=N). ^{11}B NMR (96.3 MHz, CDCl_3) δ -15.88 (2H), -12.39 (3H), -9.88 (2H), -6.67 (3H). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -120.1 (Sn-CH_3).

6.6. Synthesis of Organotin Halide (**5**).

A procedure analogous to the preparation of compound **3** was used but instead starting from compound **2** (0.81 g, 3.0 mmol) with Me_2SnCl_2 (0.66 g, 3.0 mmol). Compound **5** was obtained as colorless crystals (1.02 g, 2.3 mmol, 75%). Mp: 176-178 °C (dec). HRMS: Calcd for $[^{12}\text{C}_{11}\text{H}_{28}^{11}\text{B}_{10}^{35}\text{Cl}^{14}\text{N}^{16}\text{O}^{119}\text{Sn}]^+$ 455.1812.

Found: 455.1804. Anal. Calcd for $C_{11}H_{28}B_{10}ClNO_2Sn$: C, 29.19 H, 6.24 N, 3.09. Found: C, 29.22 H, 6.26 N, 3.11%. IR (KBr pellet, cm^{-1}) $\nu(\text{C-H})$ 3002, 2985, $\nu(\text{B-H})$ 2582, $\nu(\text{C=N})$ 1685. ^1H NMR (CDCl_3) δ 0.33 (s, 6H, Sn-CH_3 , $^2J_{119\text{Sn-CH}_3}$ = 75.7 Hz), 0.98 (s, 9H, $\text{C(CH}_3)_3$), 4.27 (m, 1H, CHN), 4.30 (dd, 1H, CH_2O , $^2J_{\text{C-H}} = 7.8$ Hz), 4.44 (dd, 1H, CH_2O , $^2J_{\text{C-H}} = 7.9$ Hz). ^{13}C NMR (75.4 MHz, CDCl_3) δ 4.06 (Sn-CH_3); 20.7 ($\text{C(CH}_3)_3$); 32.1 ($\text{C(CH}_3)_3$); 68.6 (*Cab*); 68.9, 71.2 (OCH_2CHN); 70.3 (*Cab*); 166.7 (C=N). ^{11}B NMR (96.3 MHz, CDCl_3) δ -17.38 (3H), -14.59 (2H), -10.76 (2H), -7.64 (1H), -6.79 (1H), -3.18 (1H). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -119.6 (Sn-CH_3).

6.7. Synthesis of Organotin Halide (**6**).

A procedure analogous to the preparation of compound **3** was used but instead starting from compound **2** (0.81 g, 3.0 mmol) with Me_2SnBr_2 (0.93 g, 3.0 mmol). Compound **6** was obtained as colorless crystals (1.21 g, 2.4 mmol, 81%). Mp: 180-182 °C (dec). HRMS: Calcd for $[^{12}\text{C}_{11}^{1}\text{H}_{28}^{11}\text{B}_{10}^{80}\text{Br}^{14}\text{N}^{16}\text{O}^{119}\text{Sn}]^+$ 499.1307. Found: 499.1300. Anal. Calcd for $\text{C}_{10}\text{H}_{26}\text{B}_{10}\text{BrNO}_2\text{Sn}$: C, 26.58 H, 5.68 N, 2.82. Found: C, 26.61 H, 5.65 N, 2.80%. IR (KBr pellet, cm^{-1}) $\nu(\text{C-H})$ 2988, 2881, $\nu(\text{B-H})$ 2586, $\nu(\text{C=N})$ 1687. ^1H NMR (CDCl_3) δ 0.31 (s, 6H, Sn-CH_3 , $^2J_{119\text{Sn-CH}_3} = 76.1$ Hz), 0.97 (s, 9H, $\text{C(CH}_3)_3$), 4.25 (m, 1H, CHN), 4.30 (dd, 1H, CH_2O , $^2J_{\text{C-H}} = 8.0$ Hz), 4.44 (dd, 1H, CH_2O , $^2J_{\text{C-H}} = 8.1$ Hz). ^{13}C NMR (75.4 MHz, CDCl_3) δ 4.01 (Sn-CH_3); 20.5 ($\text{C(CH}_3)_3$); 31.8 ($\text{C(CH}_3)_3$); 68.6 (*Cab*); 68.6, 71.0 (OCH_2CHN); 70.3 (*Cab*); 166.4 (C=N). ^{11}B NMR (96.3 MHz, CDCl_3) δ -18.44 (3H), -10.24 (3H), -8.52 (2H), -6.44 (1H), -4.21 (1H). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -117.8 (Sn-CH_3).

6.8. Preparation of Methoxymethyl-*o*-carborane (**7**).

NaH (0.36 g, 15.0 mmol) was added dropwise to a solution of *o*-carboranylmethanol (0.87 g, 5.0 mmol) in 50 mL of dry THF at 0 °C with stirring. The mixture was allowed to stir for 30 min at 0 °C at which time iodomethane (0.78 g, 5.5 mmol) was added dropwise. The solution was stirred for 1 h and then warmed to ambient temperature. The reaction was quenched with water, extracted with ether, and dried over anhydrous MgSO₄. The solvent was evaporated and the residue was purified by recrystallization in hexane to afford compound **7** as colorless crystals in 92% yield (0.87 g, 4.6 mmol). Mp: 68-70 °C. Anal. Calcd for C₄H₁₆B₁₀O: C, 25.52; H, 8.57. Found: C, 25.57 H, 8.62%. IR (KBr pellet, cm⁻¹) v(C-H) 3066, 2785, v(B-H) 2581. ¹H NMR (CDCl₃) δ 3.41 (s, 3H, OCH₃), 3.94 (brs, 1H, Cab-H), 4.14 (s, 2H, CH₂). ¹³C NMR (CDCl₃) δ 54.2 (OCH₃), 68.7 (Cab), 76.1 (Cab), 82.5 (CH₂). ¹¹B NMR (CDCl₃) δ -19.54 (4B), -16.82 (2B), -12.76 (2B), -8.33 (2B).

6.9. Preparation of Methoxy(phenyl)methyl-*o*-carborane (**8**).

A procedure analogous to the preparation of compound **7** was used but instead starting from *o*-carboranyl(phenyl)methanol (1.25 g, 5.0 mmol). Compound **8** was obtained as colorless crystals (1.19g, 4.5 mmol, 90%). Mp: 74-75 °C. Anal. Calcd for C₁₀H₂₀B₁₀O: C, 45.43; H, 7.63. Found: C, 45.33 H, 7.67%. IR (KBr pellet, cm⁻¹) v(C-H) 3070, 2781, v(B-H) 2593. ¹H NMR (CDCl₃) δ 3.44 (s, 3H, OCH₃), 3.93 (brs, 1H, Cab-H), 4.11 (s, 1H, PhCH), 7.14-7.30 (m, 5H, Ph). ¹³C NMR (CDCl₃) δ 55.8 (OCH₃), 67.1 (Cab), 71.5 (Cab), 83.4 (PhCH), 125.4,

129.2, 129.8, 134.6 (*Ph*). ^{11}B NMR (CDCl_3) δ -19.85 (4B), -17.32(2B), -11.76 (2B), -7.45 (2B).

6.10. General Synthesis of the Organotin Halides $(\text{Cab}^{C,O})\text{Me}_2\text{SnBr}$ (**9**).

A 2.5 M *n*-BuLi solution (1.3 mL, 3.3 mmol) was added to a stirred solution of compound **7** (0.56 g, 3.0 mmol) in diethyl ether (30 mL) at -10 °C through a syringe. The resulting solution was stirred at -10 °C for 30 min. A solution of Me_2SnBr_2 (0.93 g, 3.0 mmol) in diethyl ether (10 mL) was then added slowly to the 30 mL diethyl ether solution of compound **7**·Li at -10 °C. The reaction temperature was maintained at -10 °C for 10 min. The reaction mixture was then filtered and the organic solvent was evaporated. The crude product was dissolved in fresh distilled toluene. The volume of the toluene solution was reduced, and the resulting concentrated solution was allowed to stand at -10 °C for 2 days to allow crystallization. Compound **9** was obtained as colorless crystals in 84% yield (1.05 g, 2.5 mmol). Mp: 134-137 °C. HRMS: Calcd for $[\text{C}_6\text{H}_{21}\text{B}_{10}^{80}\text{Br}^{16}\text{O}^{119}\text{Sn}]^+$ 418.0728. Found: 418.0706. Anal. Calcd for $\text{C}_6\text{H}_{21}\text{B}_{10}\text{BrOSn}$: C, 17.33; H, 5.09. Found: C, 17.29 H, 5.11%. IR (KBr pellet, cm^{-1}) $\nu(\text{C-H})$ 3178, 2888, $\nu(\text{B-H})$ 2581. ^1H NMR (CDCl_3) δ 1.11 (s, 6H, Sn-CH_3 , $^2J_{119\text{Sn-CH}_3} = 69.8$ Hz), 3.50 (s, 3H, OCH_3), 4.19(d, 1H, CH_2 , $^2J_{\text{C-H}} = 6.4$ Hz), 4.25 (d, 1H, CH_2 , $^2J_{\text{C-H}} = 6.5$ Hz). ^{13}C NMR (CDCl_3) δ 4.97 (Sn-CH_3); 50.2 (OCH_3); 67.8, 76.0 (*Cab*); 79.6 (CH_2). ^{11}B NMR (CDCl_3) δ -18.47 (4B), -14.85 (1B), -10.57 (4B), -6.48 (1B). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -108.2 (Sn-CH_3).

6.11. Synthesis of Organotin Halide (**10**).

A procedure analogous to the preparation of **9** was used but instead starting from compound **8** (0.79 g, 3.0 mmol). Compound **10** was obtained as colorless crystals (1.23 g, 2.5 mmol, 83%). Mp: 140-141 °C. HRMS: Calcd for [$^{12}\text{C}_{12}\text{H}_{25}\text{B}_{10}^{80}\text{Br}^{16}\text{O}^{119}\text{Sn}]^+$ 494.1041. Found: 494.1078. Anal. Calcd for $\text{C}_{12}\text{H}_{25}\text{B}_{10}\text{BrOSn}$: C, 29.29; H, 5.12. Found: C, 29.41 H, 5.16%. IR (KBr pellet, cm^{-1}) $\nu(\text{C-H})$ 3046, 2872, $\nu(\text{B-H})$ 2580. ^1H NMR (CDCl_3) δ 1.00 (s, 6H, Sn-CH_3 , $^2J_{119\text{Sn-CH}_3} = 68.3$ Hz), 3.50 (s, 3H, OCH_3), 4.27 (s, 1H, PhCH), 7.11-7.30 (m, 5H, *Ph*). ^{13}C NMR (CDCl_3) δ 3.26 (Sn-CH_3); 54.2 (OCH_3) 66.8, 70.4 (*Cab*) 81.2 (PhCH) 124.5, 127.1, 127.8, 130.4 (*Ph*). ^{11}B NMR (CDCl_3) δ -19.51 (3B), -16.48 (1B), -14.47 (4B), -6.81 (2B). ^{119}Sn NMR (149.2 MHz, CDCl_3) δ -110.3 (Sn-CH_3).

6.12. Crystal Structure Determination.

Crystals of compounds **4**, **7**, **8**, and **9** were obtained from toluene at -10 °C, sealed in glass capillaries under argon, and mounted on the diffractometer. The preliminary examination and data collection were performed using a Bruker SMART CCD detector system in a single-crystal X-ray diffractometer equipped with a sealed-tube X-ray source (40 kV × 50 mA) using graphite-monochromated Mo K α radiation ($\lambda = 0.71073$ Å). The preliminary unit cell constants were determined using a set of 45 narrow-frame scans (0.3°in ω). The double-pass method of scanning was employed to exclude noise. The collected frames were integrated using an orientation matrix determined from the narrow-frame scans.

The SMART software package was used for data collection, and SAINT was employed for frame integration [29]. The final cell constants were determined using a global refinement of the xyz centroids of the reflections harvested from the entire data set. The structure solution and refinement were carried out using the SHELXTL-PLUS software package [30].

7. References

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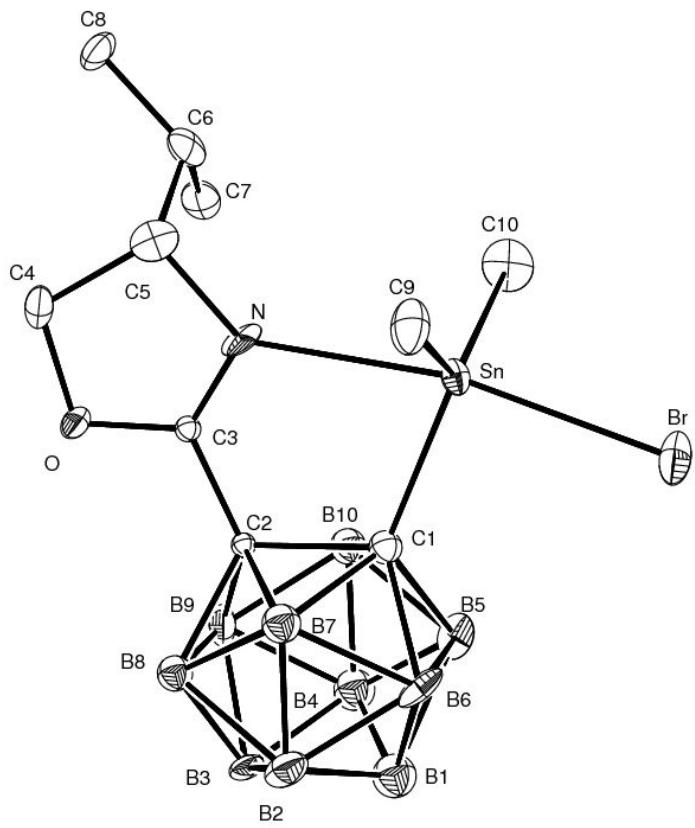


Figure 1. ORTEP presentation at the 30% probability level of the molecular structure of compound **4**. The hydrogen atoms are omitted for clarity. Selected interaction distances (\AA) and angles (deg): $\text{Sn}(1)\text{-N}(1) = 2.500(1)$, $\text{Sn}(1)\text{-Br}(1) = 2.614(2)$, $\text{Sn}(1)\text{-C}(1) = 2.197(2)$, $\text{C}(2)\text{-C}(3) = 1.492(2)$, $\text{C}(3)\text{-N}(1) = 1.241(2)$; $\text{Br}(1)\text{-Sn}(1)\text{-N}(1) = 169.6(3)$, $\text{Br}(1)\text{-Sn}(1)\text{-C}(1) = 95.3(4)$, $\text{C}(1)\text{-Sn}(1)\text{-N}(1) = 74.7(5)$, $\text{Sn}(1)\text{-N}(1)\text{-C}(3) = 114.5(1)$.

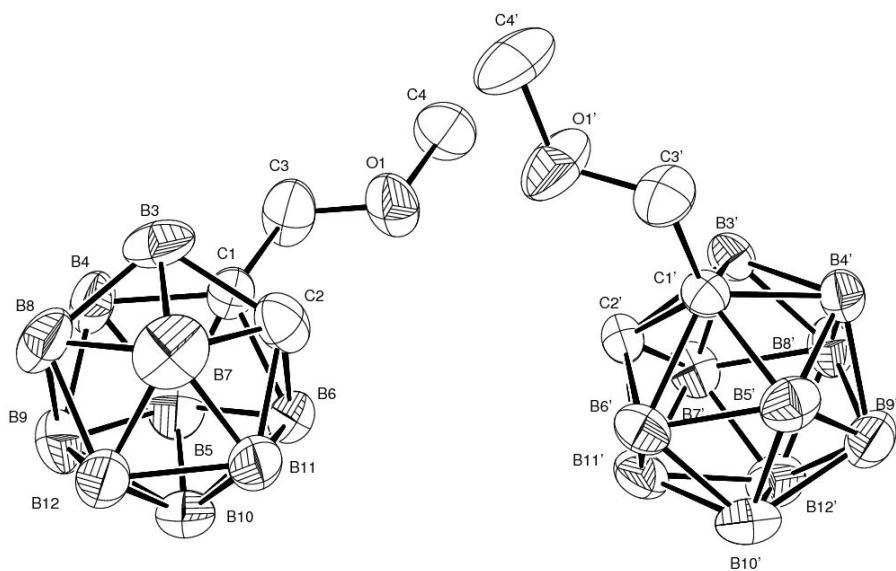


Figure 2. ORTEP presentation at the 30% probability level of the molecular structure of compound 7. The hydrogen atoms are omitted for clarity. Selected interaction distances (\AA) and angles (deg): $\text{O(1)}-\text{C(3)} = 1.327(4)$, $\text{O(1)}-\text{C(4)} = 1.425(4)$, $\text{O(1')}-\text{C(3')} = 1.336(4)$, $\text{O(1')}-\text{C(4')} = 1.420(3)$; $\text{C(3)}-\text{O(1)}-\text{C(4)} = 113.7(3)$, $\text{O(1)}-\text{C(3)}-\text{C(1)} = 111.6(3)$, $\text{C(3')}-\text{O(1')}-\text{C(4')} = 112.2(3)$, $\text{O(1')}-\text{C(3')}-\text{C(1')} = 110.9(3)$.

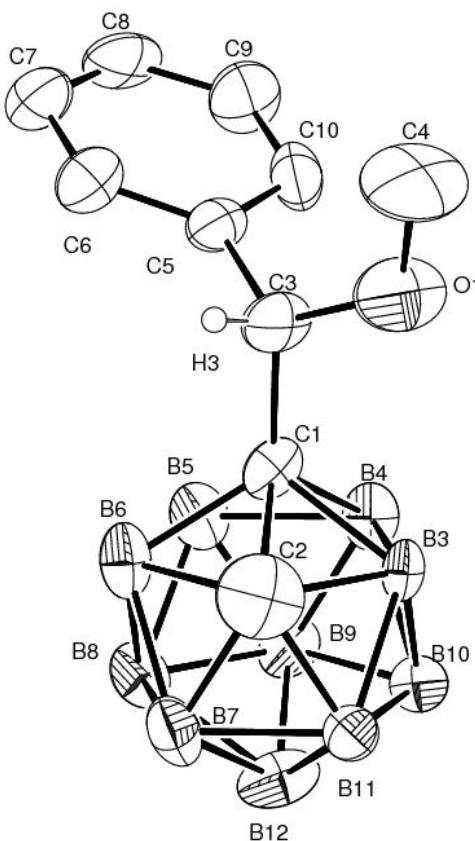


Figure 3. ORTEP presentation at the 30% probability level of the molecular structure of compound **8**. The hydrogen atoms are omitted for clarity. Selected interaction distances (\AA) and angles (deg): O(1)–C(3) = 1.297(1), O(1)–C(4) = 1.413(1); C(3)–O(1)–C(4) = 116.8(9), O(1)–C(3)–C(1) = 109.4(7), C(1)–C(3)–C(5) = 112.4(7), O(1)–C(3)–C(5) = 117.3(9).

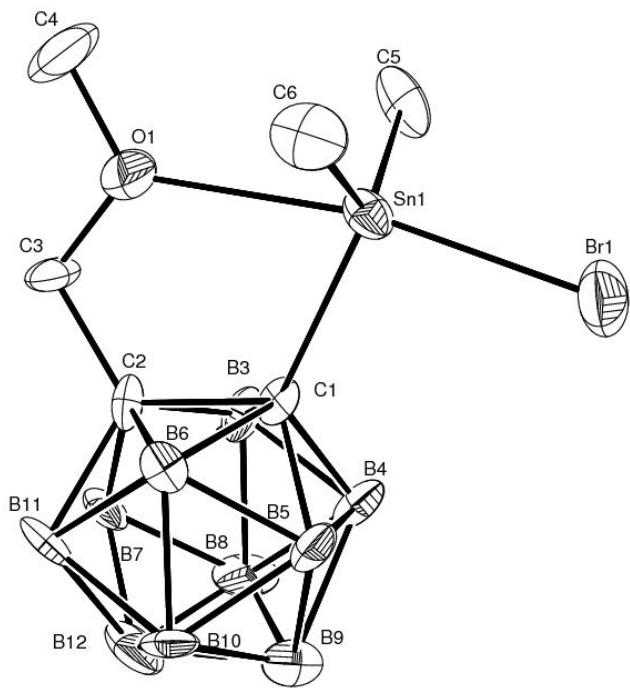


Figure 4. ORTEP presentation at the 30% probability level of the molecular structure of compound **9**. The hydrogen atoms are omitted for clarity. Selected interaction distances (\AA) and angles (deg): $\text{Sn(1)}-\text{O(1)} = 2.579(4)$, $\text{Sn(1)}-\text{Br(1)} = 2.537(3)$, $\text{Sn(1)}-\text{C(1)} = 2.193(2)$; $\text{Br(1)}-\text{Sn(1)}-\text{O(1)} = 169.8(3)$, $\text{Br(1)}-\text{Sn(1)}-\text{C(1)} = 98.4(5)$, $\text{C(1)}-\text{Sn(1)}-\text{O(1)} = 71.4(6)$, $\text{Sn(1)}-\text{O(1)}-\text{C(3)} = 121.1(1)$.

Table S1. Crystal data and structure refinement for Organotin Halide.

Identification code	F019m
Empirical formula	C ₁₀ H ₂₆ B ₁₀ BrNOSn
Formula weight	483.02
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	$a = 10.7475(7)$ Å $b = 13.3867(9)$ Å $c = 14.4795(9)$ Å 2083.2(2) Å ³
Volume	4, 1.540 g/m ³
Z, D _{calc}	3.141 mm ⁻¹
<i>m</i>	944
<i>F</i> (000)	0.80 × 0.60 × 0.40 mm
Crystal size	2.07 to 28.02 °
q range for data collection	-14 ≤ <i>h</i> ≤ 14, -17 ≤ <i>k</i> ≤ 17, -19 ≤ <i>l</i> ≤ 19
Limiting indices	
Reflections collected / unique	18270 / 4999 [R(int) = 0.0943]
Completeness to q = 25.96	99.6 %
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	4999 / 0 / 217
Goodness-of-fit on <i>F</i> ²	1.410
Final R indices [<i>I</i> >2s (<i>I</i>)]	^a R ₁ = 0.1488, ^b wR ₂ = 0.2175
R indices (all data)	^a R ₁ = 0.1615, ^b wR ₂ = 0.2214
Absolute structure parameter	0.00
Largest diff. peak and hole	2.545 and -3.281 e.Å ⁻³

Table S2. Bond lengths [Å] for Organotin Halide

Sn(1)-C(10)	2.088(2) C(6)-C(7)	1.52(3)
Sn(1)-C(9)	2.092(2) B(3)-B(4)	1.73(4)
Sn(1)-C(1)	2.171(2) B(3)-B(8)	1.78(3)
Sn(1)-N(1)	2.500(1) B(3)-B(9)	1.79(3)
Sn(1)-Br(1)	2.614(2) B(4)-B(5)	1.70(2)
O(1)-C(3)	1.307(2) B(4)-B(9)	1.73(3)
O(1)-C(4)	1.42(2) B(4)-B(10)	1.78(3)
N(1)-C(3)	1.248(2) B(5)-B(10)	1.73(3)
N(1)-C(5)	1.50(2) B(5)-B(11)	1.79(4)
C(1)-B(4)	1.69(2) B(5)-B(6)	1.80(3)
C(1)-C(2)	1.70(2) B(6)-B(11)	1.73(3)
C(1)-B(5)	1.71(2) B(6)-B(7)	1.78(3)
C(1)-B(6)	1.73(2) B(7)-B(8)	1.74(3)
C(1)-B(3)	1.73(3) B(7)-B(12)	1.77(3)
C(2)-C(3)	1.50(2) B(7)-B(11)	1.79(3)
C(2)-B(7)	1.67(2) B(8)-B(12)	1.78(3)
C(2)-B(8)	1.68(3) B(8)-B(9)	1.79(3)
C(2)-B(3)	1.69(2) B(9)-B(10)	1.72(4)
C(2)-B(6)	1.699(2) B(9)-B(12)	1.77(3)
C(4)-C(5)	1.54(3) B(10)-B(12)	1.75(3)
C(5)-C(6)	1.54(3) B(10)-B(11)	1.78(4)
C(6)-C(8)	1.51(3) B(11)-B(12)	1.84(3)

Table S3. Angles [deg] for Organotin Halide

C(10)-Sn(1)-C(9)	126.8(8) B(4)-B(5)-B(11)	110.8(2)
C(10)-Sn(1)-C(1)	115.3(7) C(1)-B(5)-B(11)	106.7(2)
C(9)-Sn(1)-C(1)	115.1(7) B(10)-B(5)-B(11)	60.9(1)
C(10)-Sn(1)-N(1)	92.1(7) B(4)-B(5)-B(6)	107.2(1)
C(9)-Sn(1)-N(1)	85.5(6) C(1)-B(5)-B(6)	59.1(1)
C(1)-Sn(1)-N(1)	74.9(5) B(10)-B(5)-B(6)	106.3(2)
C(10)-Sn(1)-Br(1)	94.6(6) B(11)-B(5)-B(6)	57.8(1)
C(9)-Sn(1)-Br(1)	96.7(5) C(2)-B(6)-C(1)	59.5(8)
C(1)-Sn(1)-Br(1)	95.2(4) C(2)-B(6)-B(11)	106.1(1)
N(1)-Sn(1)-Br(1)	169.7(3) C(1)-B(6)-B(11)	108.3(1)
C(3)-O(1)-C(4)	105.5(1) C(2)-B(6)-B(7)	57.4(9)
C(3)-N(1)-C(5)	105.1(2) C(1)-B(6)-B(7)	106.9(1)
C(3)-N(1)-Sn(1)	115.2(1) B(11)-B(6)-B(7)	61.4(1)
C(5)-N(1)-Sn(1)	139.6(1) C(2)-B(6)-B(5)	103.8(1)
B(4)-C(1)-C(2)	105.7(1) C(1)-B(6)-B(5)	58.0(9)
B(4)-C(1)-B(5)	59.9(1) B(11)-B(6)-B(5)	60.9(1)
C(2)-C(1)-B(5)	107.5(1) B(7)-B(6)-B(5)	107.5(2)
B(4)-C(1)-B(6)	110.6(1) C(2)-B(7)-B(8)	58.8(1)
C(2)-C(1)-B(6)	59.4(9) C(2)-B(7)-B(12)	106.1(1)
B(5)-C(1)-B(6)	63.0(1) B(8)-B(7)-B(12)	61.1(1)
B(4)-C(1)-B(3)	60.5(1) C(2)-B(7)-B(6)	58.9(9)
C(2)-C(1)-B(3)	59.2(1) B(8)-B(7)-B(6)	108.1(1)
B(5)-C(1)-B(3)	109.8(1) B(12)-B(7)-B(6)	108.2(2)
B(6)-C(1)-B(3)	110.2(1) C(2)-B(7)-B(11)	104.6(2)
B(4)-C(1)-Sn(1)	127.5(1) B(8)-B(7)-B(11)	110.2(2)

C(2)-C(1)-Sn(1)	115.5(8) B(12)-B(7)-B(11)	62.2(1)
B(5)-C(1)-Sn(1)	128.3(1) B(6)-B(7)-B(11)	58.0(1)
B(6)-C(1)-Sn(1)	117.7(9) C(2)-B(8)-B(7)	58.6(1)
B(3)-C(1)-Sn(1)	116.0(1) C(2)-B(8)-B(12)	105.2(2)
C(3)-C(2)-B(7)	122.7(1) B(7)-B(8)-B(12)	60.2(1)
C(3)-C(2)-B(8)	125.1(1) C(2)-B(8)-B(3)	58.5(1)
B(7)-C(2)-B(8)	62.6(1) B(7)-B(8)-B(3)	107.8(2)
C(3)-C(2)-B(3)	116.4(1) B(12)-B(8)-B(3)	108.6(2)
B(7)-C(2)-B(3)	115.5(1) C(2)-B(8)-B(9)	103.9(2)
B(8)-C(2)-B(3)	63.9(1) B(7)-B(8)-B(9)	106.8(2)
C(3)-C(2)-B(6)	113.2(1) B(12)-B(8)-B(9)	59.5(1)
B(7)-C(2)-B(6)	63.8(1) B(3)-B(8)-B(9)	60.2(1)
B(8)-C(2)-B(6)	115.2(1) B(10)-B(9)-B(4)	62.2(1)
B(3)-C(2)-B(6)	113.5(1) B(10)-B(9)-B(12)	60.4(1)
C(3)-C(2)-C(1)	111.4(1) B(4)-B(9)-B(12)	110.3(1)
B(7)-C(2)-C(1)	113.4(1) B(10)-B(9)-B(8)	108.0(2)
B(8)-C(2)-C(1)	113.5(1) B(4)-B(9)-B(8)	107.3(2)
B(3)-C(2)-C(1)	61.3(1) B(12)-B(9)-B(8)	60.2(1)
B(6)-C(2)-C(1)	61.1(9) B(10)-B(9)-B(3)	108.8(2)
N(1)-C(3)-O(1)	121.5(2) B(4)-B(9)-B(3)	58.8(1)
N(1)-C(3)-C(2)	122.7(1) B(12)-B(9)-B(3)	108.9(2)
O(1)-C(3)-C(2)	115.8(1) B(8)-B(9)-B(3)	59.9(1)
O(1)-C(4)-C(5)	104.7(1) B(9)-B(10)-B(5)	107.6(2)
N(1)-C(5)-C(4)	102.1(2) B(9)-B(10)-B(12)	61.4(1)
N(1)-C(5)-C(6)	112.9(2) B(5)-B(10)-B(12)	111.4(2)
C(4)-C(5)-C(6)	115.7(2) B(9)-B(10)-B(4)	59.2(1)

C(8)-C(6)-C(7)	112.2(2) B(5)-B(10)-B(4)	58.0(1)
C(8)-C(6)-C(5)	110.5(2) B(12)-B(10)-B(4)	108.8(2)
C(7)-C(6)-C(5)	111.0(2) B(9)-B(10)-B(11)	111(2)
C(2)-B(3)-B(4)	104.6(1) B(5)-B(10)-B(11)	61.3(2)
C(2)-B(3)-C(1)	59.6(1) B(12)-B(10)-B(11)	62.7(2)
B(4)-B(3)-C(1)	58.7(1) B(4)-B(10)-B(11)	107.5(2)
C(2)-B(3)-B(8)	57.5(1) B(6)-B(11)-B(10)	106.8(2)
B(4)-B(3)-B(8)	107.4(1) B(6)-B(11)-B(5)	61.4(1)
C(1)-B(3)-B(8)	106.9(1) B(10)-B(11)-B(5)	57.8(1)
C(2)-B(3)-B(9)	103.0(1) B(6)-B(11)-B(7)	60.7(1)
B(4)-B(3)-B(9)	58.8(1) B(10)-B(11)-B(7)	104.2(2)
C(1)-B(3)-B(9)	105.0(2) B(5)-B(11)-B(7)	107.4(2)
B(8)-B(3)-B(9)	60.0(1) B(6)-B(11)-B(12)	107.2(1)
C(1)-B(4)-B(5)	60.5(1) B(10)-B(11)-B(12)	58.0(1)
C(1)-B(4)-B(3)	60.8(1) B(5)-B(11)-B(12)	104.9(2)
B(5)-B(4)-B(3)	110.5(2) B(7)-B(11)-B(12)	58.2(1)
C(1)-B(4)-B(9)	109.4(2) B(10)-B(12)-B(7)	106.4(2)
B(5)-B(4)-B(9)	108.2(1) B(10)-B(12)-B(9)	58.2(2)
B(3)-B(4)-B(9)	62.4(1) B(7)-B(12)-B(9)	106.3(1)
C(1)-B(4)-B(10)	106.8(1) B(10)-B(12)-B(8)	106.4(2)
B(5)-B(4)-B(10)	59.4(1) B(7)-B(12)-B(8)	58.7(1)
B(3)-B(4)-B(10)	108.8(2) B(9)-B(12)-B(8)	60.3(1)
B(9)-B(4)-B(10)	58.6(1) B(10)-B(12)-B(11)	59.4(1)
B(4)-B(5)-C(1)	59.6(1) B(7)-B(12)-B(11)	59.6(1)
B(4)-B(5)-B(10)	62.6(1) B(9)-B(12)-B(11)	105.6(2)
C(1)-B(5)-B(10)	108.6(2) B(8)-B(12)-B(11)	106.3(2)

Table S4. Crystal data and structure refinement for Methoxymethyl-*o*-carborane

Identification code	Kor053
Empirical formula	C ₄ H ₁₆ B ₁₀ O
Formula weight	188.27
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ /c
Unit cell dimensions	<i>a</i> = 14.2526(8) Å <i>b</i> = 11.3858(12) Å β = 91.760(5) ° <i>c</i> = 14.4510(10) Å
Volume	2344.0(3) Å ³
Z, D _{calc}	4, 1.067 g/m ³
<i>m</i>	0.026 mm ⁻¹
<i>F</i> (000)	392
Crystal size	0.5 × 0.5 × 0.6 mm
q range for data collection	1.43 to 26.27 °
Limiting indices	0 ≤ <i>h</i> ≤ 17, 0 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 17
Reflections collected / unique	4780 / 4594 [R(int) = 0.1024]
Completeness to <i>q</i> = 25.96	92.0%
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	4594 / 0 / 293
Goodness-of-fit on <i>F</i> ²	1.151
Final R indices [<i>I</i> >2s(<i>I</i>)]	^a <i>R</i> ₁ = 0.0820, ^b <i>wR</i> ₂ = 0.2004
R indices (all data)	^a <i>R</i> ₁ = 0.1849, ^b <i>wR</i> ₂ = 0.2373
Largest diff. peak and hole	0.371 and -0.314 e.Å ⁻³

Table S5. Bond lengths [Å] for Methoxymethyl-*o*-carborane

O(1)-C(3)	1.327(4)	O(1)-C(4)	1.425(4)
C(1)-C(3)	1.521(4)	C(1)-C(2)	1.617(4)
C(1)-B(3)	1.661(5)	C(1)-B(4)	1.680(5)
C(1)-B(5)	1.691(6)	C(1)-B(6)	1.694(5)
C(2)-B(6)	1.658(5)	C(2)-B(7)	1.685(6)
C(2)-B(11)	1.698(5)	C(2)-B(3)	1.713(5)
B(3)-B(7)	1.738(6)	B(3)-B(4)	1.741(6)
B(3)-B(8)	1.742(6)	B(4)-B(8)	1.724(6)
B(4)-B(5)	1.740(6)	B(4)-B(9)	1.750(6)
B(5)-B(6)	1.700(6)	B(5)-B(9)	1.723(6)
B(5)-B(10)	1.753(7)	B(6)-B(10)	1.731(6)
B(6)-B(11)	1.733(6)	B(7)-B(11)	1.726(6)
B(7)-B(8)	1.766(7)	B(7)-B(12)	1.776(7)
B(8)-B(12)	1.756(6)	B(8)-B(9)	1.758(7)
B(9)-B(12)	1.737(7)	B(9)-B(10)	1.747(6)
B(10)-B(11)	1.719(7)	B(10)-B(12)	1.721(7)
B(11)-B(12)	1.746(6)	O(1')-C(3')	1.336(4)
O(1')-C(4')	1.420(3)	C(1')-C(3')	1.511(4)
C(1')-C(2')	1.641(4)	C(1')-B(4')	1.678(4)
C(1')-B(3')	1.689(4)	C(1')-B(5')	1.690(4)
C(1')-B(6')	1.749(4)	C(2')-B(7')	1.669(4)
C(2')-B(11')	1.705(5)	C(2')-B(3')	1.705(4)
C(2')-B(6')	1.708(5)	B(3')-B(8')	1.739(5)
B(3')-B(4')	1.759(5)	B(3')-B(7')	1.763(4)
B(4')-B(8')	1.737(5)	B(4')-B(9')	1.759(5)

B(4')-B(5')	1.761(5) B(5')-B(9')	1.742(6)
B(5')-B(6')	1.775(5) B(5')-B(10')	1.781(6)
B(6')-B(11')	1.741(5) B(6')-B(10')	1.744(6)
B(7')-B(8')	1.770(5) B(7')-B(11')	1.773(6)
B(7')-B(12')	1.776(6) B(8')-B(9')	1.761(6)
B(8')-B(12')	1.798(6) B(9')-B(12')	1.757(6)
B(9')-B(10')	1.777(6) B(10')-B(12')	1.728(6)
B(10')-B(11')	1.753(6) B(11')-B(12')	1.749(6)

Table S6. Angles [deg] for Methoxymethyl-*o*-carborane

C(3)-O(1)-C(4)	113.7(3)	C(3)-C(1)-C(2)	118.7(3)
C(3)-C(1)-B(3)	117.5(3)	C(2)-C(1)-B(3)	63.0(2)
C(3)-C(1)-B(4)	120.5(3)	C(2)-C(1)-B(4)	112.4(3)
B(3)-C(1)-B(4)	62.8(2)	C(3)-C(1)-B(5)	121.2(3)
C(2)-C(1)-B(5)	109.2(3)	B(3)-C(1)-B(5)	113.5(3)
B(4)-C(1)-B(5)	62.2(2)	C(3)-C(1)-B(6)	118.7(3)
C(2)-C(1)-B(6)	60.0(2)	B(3)-C(1)-B(6)	113.2(3)
B(4)-C(1)-B(6)	111.9(3)	B(5)-C(1)-B(6)	60.3(2)
C(1)-C(2)-B(6)	62.3(2)	C(1)-C(2)-B(7)	109.3(3)
B(6)-C(2)-B(7)	112.1(3)	C(1)-C(2)-B(11)	111.3(3)
B(6)-C(2)-B(11)	62.2(2)	B(7)-C(2)-B(11)	61.4(3)
C(1)-C(2)-B(3)	59.7(2)	B(6)-C(2)-B(3)	112.3(3)
B(7)-C(2)-B(3)	61.5(2)	B(11)-C(2)-B(3)	112.0(3)
O(1)-C(3)-C(1)	111.6(3)	C(1)-B(3)-C(2)	57.6(9)
C(1)-B(3)-B(7)	104.8(3)	C(2)-B(3)-B(7)	58.4(2)
C(1)-B(3)-B(4)	59.1(2)	C(2)-B(3)-B(4)	104.9(3)
B(7)-B(3)-B(4)	107.9(3)	C(1)-B(3)-B(8)	105.2(3)
C(2)-B(3)-B(8)	105.5(3)	B(7)-B(3)-B(8)	61.0(3)
B(4)-B(3)-B(8)	59.3(3)	C(1)-B(4)-B(8)	105.2(3)
C(1)-B(4)-B(3)	58.0(2)	B(8)-B(4)-B(3)	60.4(3)
C(1)-B(4)-B(5)	59.2(2)	B(8)-B(4)-B(5)	107.5(3)
B(3)-B(4)-B(5)	107.2(3)	C(1)-B(4)-B(9)	105.5(3)
B(8)-B(4)-B(9)	60.8(3)	B(3)-B(4)-B(9)	108.7(3)
B(5)-B(4)-B(9)	59.2(3)	C(1)-B(5)-B(6)	60.0(2)
C(1)-B(5)-B(9)	106.3(3)	B(6)-B(5)-B(9)	108.9(3)
C(1)-B(5)-B(4)	58.6(2)	B(6)-B(5)-B(4)	108.7(3)

B(9)-B(5)-B(4)	60.7(3) C(1)-B(5)-B(10)	106.5(3)
B(6)-B(5)-B(10)	60.1(3) B(9)-B(5)-B(10)	60.3(3)
B(4)-B(5)-B(10)	108.8(3) C(2)-B(6)-C(1)	57.6(9)
C(2)-B(6)-B(5)	106.9(3) C(1)-B(6)-B(5)	59.7(2)
C(2)-B(6)-B(10)	107.1(3) C(1)-B(6)-B(10)	107.3(3)
B(5)-B(6)-B(10)	61.4(3) C(2)-B(6)-B(11)	60.1(2)
C(1)-B(6)-B(11)	106.0(3) B(5)-B(6)-B(11)	108.8(3)
B(10)-B(6)-B(11)	59.5(3) C(2)-B(7)-B(11)	59.7(2)
C(2)-B(7)-B(3)	60.1(2) B(11)-B(7)-B(3)	109.5(3)
C(2)-B(7)-B(8)	105.7(3) B(11)-B(7)-B(8)	107.7(3)
B(3)-B(7)-B(8)	59.6(3) C(2)-B(7)-B(12)	105.7(3)
B(11)-B(7)-B(12)	59.8(3) B(3)-B(7)-B(12)	107.8(3)
B(8)-B(7)-B(12)	59.4(3) B(4)-B(8)-B(3)	60.3(2)
B(4)-B(8)-B(12)	108.1(3) B(3)-B(8)-B(12)	108.5(3)
B(4)-B(8)-B(9)	60.3(3) B(3)-B(8)-B(9)	108.3(3)
B(12)-B(8)-B(9)	59.3(3) B(4)-B(8)-B(7)	107.4(3)
B(3)-B(8)-B(7)	59.4(3) B(12)-B(8)-B(7)	60.6(3)
B(9)-B(8)-B(7)	107.3(3) B(5)-B(9)-B(12)	107.6(3)
B(5)-B(9)-B(10)	60.7(3) B(12)-B(9)-B(10)	59.2(3)
B(5)-B(9)-B(4)	60.1(3) B(12)-B(9)-B(4)	107.7(3)
B(10)-B(9)-B(4)	108.7(3) B(5)-B(9)-B(8)	106.7(3)
B(12)-B(9)-B(8)	60.3(3) B(10)-B(9)-B(8)	107.4(3)
B(4)-B(9)-B(8)	58.9(2) B(11)-B(10)-B(12)	61.0(3)
B(11)-B(10)-B(6)	60.3(2) B(12)-B(10)-B(6)	108.2(3)
B(11)-B(10)-B(9)	108.6(3) B(12)-B(10)-B(9)	60.1(3)
B(6)-B(10)-B(9)	106.4(3) B(11)-B(10)-B(5)	107.0(3)

B(12)-B(10)-B(5)	106.9(3) B(6)-B(10)-B(5)	58.4(3)
B(9)-B(10)-B(5)	59.0(3) C(2)-B(11)-B(10)	105.9(3)
C(2)-B(11)-B(7)	58.9(2) B(10)-B(11)-B(7)	109.0(3)
C(2)-B(11)-B(6)	57.8(2) B(10)-B(11)-B(6)	60.2(3)
B(7)-B(11)-B(6)	106.6(3) C(2)-B(11)-B(12)	106.5(3)
B(10)-B(11)-B(12)	59.6(3) B(7)-B(11)-B(12)	61.5(3)
B(6)-B(11)-B(12)	107.0(3) B(10)-B(12)-B(9)	60.7(3)
B(10)-B(12)-B(11)	59.4(3) B(9)-B(12)-B(11)	107.8(3)
B(10)-B(12)-B(8)	108.6(3) B(9)-B(12)-B(8)	60.4(3)
B(11)-B(12)-B(8)	107.3(3) B(10)-B(12)-B(7)	106.6(3)
B(9)-B(12)-B(7)	107.8(3) B(11)-B(12)-B(7)	58.7(3)
B(8)-B(12)-B(7)	60.0(3) C(3')-O(1')-C(4')	112.2(3)
C(3')-C(1')-C(2')	119.5(2) C(3')-C(1')-B(4')	119.2(2)
C(2')-C(1')-B(4')	111.3(2) C(3')-C(1')-B(3')	115.9(2)
C(2')-C(1')-B(3')	61.5(2) B(4')-C(1')-B(3')	63.0(2)
C(3')-C(1')-B(5')	120.8(3) C(2')-C(1')-B(5')	110.2(2)
B(4')-C(1')-B(5')	63.0(2) B(3')-C(1')-B(5')	114.8(2)
C(3')-C(1')-B(6')	118.7(3) C(2')-C(1')-B(6')	60.4(2)
B(4')-C(1')-B(6')	114.2(2) B(3')-C(1')-B(6')	113.7(2)
B(5')-C(1')-B(6')	62.1(2) C(1')-C(2')-B(7')	111.0(2)
C(1')-C(2')-B(11')	111.7(2) B(7')-C(2')-B(11')	63.4(2)
C(1')-C(2')-B(3')	60.6(2) B(7')-C(2')-B(3')	63.0(2)
B(11')-C(2')-B(3')	115.6(2) C(1')-C(2')-B(6')	62.9(2)
B(7')-C(2')-B(6')	114.1(3) B(11')-C(2')-B(6')	61.3(2)
B(3')-C(2')-B(6')	115.0(2) O(1')-C(3')-C(1')	110.9(3)
C(1')-B(3')-C(2')	57.8(2) C(1')-B(3')-B(8')	104.0(2)

C(2')-B(3')-B(8')	104.2(2)	C(1')-B(3')-B(4')	58.2(2)
C(2')-B(3')-B(4')	104.6(2)	B(8')-B(3')-B(4')	59.5(2)
C(1')-B(3')-B(7')	104.3(2)	C(2')-B(3')-B(7')	57.5(2)
B(8')-B(3')-B(7')	60.7(2)	B(4')-B(3')-B(7')	108.0(2)
C(1')-B(4')-B(8')	104.6(2)	C(1')-B(4')-B(9')	104.5(3)
B(8')-B(4')-B(9')	60.5(2)	C(1')-B(4')-B(3')	58.8(2)
B(8')-B(4')-B(3')	59.6(2)	B(9')-B(4')-B(3')	108.0(3)
C(1')-B(4')-B(5')	58.8(2)	B(8')-B(4')-B(5')	107.7(3)
B(9')-B(4')-B(5')	59.3(2)	B(3')-B(4')-B(5')	108.0(2)
C(1')-B(5')-B(9')	104.7(3)	C(1')-B(5')-B(4')	58.1(2)
B(9')-B(5')-B(4')	60.3(2)	C(1')-B(5')-B(6')	60.6(2)
B(9')-B(5')-B(6')	107.6(3)	B(4')-B(5')-B(6')	108.9(3)
C(1')-B(5')-B(10')	105.5(3)	B(9')-B(5')-B(10')	60.6(2)
B(4')-B(5')-B(10')	108.9(3)	B(6')-B(5')-B(10')	58.7(2)
C(2')-B(6')-B(11')	59.2(2)	C(2')-B(6')-B(10')	105.0(3)
B(11')-B(6')-B(10')	60.4(2)	C(2')-B(6')-C(1')	56.7(2)
B(11')-B(6')-C(1')	105.0(3)	B(10')-B(6')-C(1')	104.6(3)
C(2')-B(6')-B(5')	103.4(2)	B(11')-B(6')-B(5')	108.6(3)
B(10')-B(6')-B(5')	60.8(2)	C(1')-B(6')-B(5')	57.3(2)
C(2')-B(7')-B(3')	59.5(2)	C(2')-B(7')-B(8')	104.4(2)
B(3')-B(7')-B(8')	59.0(2)	C(2')-B(7')-B(11')	59.3(2)
B(3')-B(7')-B(11')	109.3(2)	B(8')-B(7')-B(11')	108.4(3)
C(2')-B(7')-B(12')	104.1(3)	B(3')-B(7')-B(12')	108.0(3)
B(8')-B(7')-B(12')	60.9(2)	B(11')-B(7')-B(12')	59.0(2)
B(4')-B(8')-B(3')	60.8(2)	B(4')-B(8')-B(9')	60.4(2)
B(3')-B(8')-B(9')	108.9(3)	B(4')-B(8')-B(7')	108.7(3)

B(3')-B(8')-B(7')	60.3(2)	B(9')-B(8')-B(7')	107.5(3)
B(4')-B(8')-B(12')	107.7(3)	B(3')-B(8')-B(12')	108.1(3)
B(9')-B(8')-B(12')	59.1(2)	B(7')-B(8')-B(12')	59.7(2)
B(5')-B(9')-B(12')	107.4(3)	B(5')-B(9')-B(4')	60.4(2)
B(12')-B(9')-B(4')	108.6(3)	B(5')-B(9')-B(8')	107.5(3)
B(12')-B(9')-B(8')	61.5(2)	B(4')-B(9')-B(8')	59.1(2)
B(5')-B(9')-B(10')	60.8(2)	B(12')-B(9')-B(10')	58.5(2)
B(4')-B(9')-B(10')	109.1(3)	B(8')-B(9')-B(10')	108.2(3)
B(12')-B(10')-B(6')	107.8(3)	B(12')-B(10')-B(11')	60.3(2)
B(6')-B(10')-B(11')	59.7(2)	B(12')-B(10')-B(9')	60.1(2)
B(6')-B(10')-B(9')	107.5(3)	B(11')-B(10')-B(9')	108.2(3)
B(12')-B(10')-B(5')	107.0(3)	B(6')-B(10')-B(5')	60.5(2)
B(11')-B(10')-B(5')	107.8(3)	B(9')-B(10')-B(5')	58.6(2)
C(2')-B(11')-B(6')	59.4(2)	C(2')-B(11')-B(12')	103.7(3)
B(6')-B(11')-B(12')	107.0(3)	C(2')-B(11')-B(10')	104.8(3)
B(6')-B(11')-B(10')	59.9(2)	B(12')-B(11')-B(10')	59.1(2)
C(2')-B(11')-B(7')	57.3(2)	B(6')-B(11')-B(7')	107.5(3)
B(12')-B(11')-B(7')	60.5(2)	B(10')-B(11')-B(7')	107.8(3)
B(10')-B(12')-B(11')	60.6(3)	B(10')-B(12')-B(9')	61.3(2)
B(11')-B(12')-B(9')	109.3(3)	B(10')-B(12')-B(7')	108.8(3)
B(11')-B(12')-B(7')	60.4(2)	B(9')-B(12')-B(7')	107.4(3)
B(10')-B(12')-B(8')	108.7(3)	B(11')-B(12')-B(8')	108.2(3)
B(9')-B(12')-B(8')	59.4(2)	B(7')-B(12')-B(8')	59.4(2)

Table S7. Crystal data and structure refinement for
Methoxy(phenyl)methyl-*o*-carborane

Identification code	Kor056
Empirical formula	C ₁₀ H ₂₀ B ₁₀ O
Formula weight	264.35
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Orthorhombic, <i>Pna</i> 2 ₁
Unit cell dimensions	$a = 12.7870(12)$ Å $b = 15.077(3)$ Å $c = 8.1932(14)$ Å
Volume	1579.6(4) Å ³
Z, D _{calc}	4, 1.107 g/m ³
<i>m</i>	0.057 mm ⁻¹
F(000)	548
Crystal size	0.4 × 0.4 × 0.5 mm
q range for data collection	2.09 to 25.98 °
Limiting indices	0 ≤ h ≤ 15, 0 ≤ k ≤ 18, 0 ≤ l ≤ 10
Reflections collected / unique	1813 / 1665 [R(int) = 0.0000]
Completeness to q = 28.29	99.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1665 / 1 / 237
Goodness-of-fit on F^2	1.062
Final R indices [I>2s(I)]	^a R ₁ = 0.0812, ^b wR ₂ = 0.2199
R indices (all data)	^a R ₁ = 0.1056, ^b wR ₂ = 0.2542
Absolute structure parameter	3(5)
Largest diff. peak and hole	0.552 and -0.279 e.Å ⁻³

Table S8. Bond lengths [Å] for Methoxy(phenyl)methyl-*o*-carborane

O(1)-C(3)	1.357(8) O(1)-C(4)	1.406(9)
C(1)-C(3)	1.553(8) C(1)-B(3)	1.648(7)
C(1)-B(5)	1.698(8) C(1)-B(6)	1.701(7)
C(1)-B(4)	1.704(8) C(1)-C(2)	1.732(8)
C(2)-B(3)	1.698(8) C(2)-B(7)	1.747(1)
C(2)-B(11)	1.771(1) C(2)-B(6)	1.790(9)
C(3)-C(5)	1.522(8) C(5)-C(6)	1.369(9)
C(5)-C(10)	1.396(9) C(6)-C(7)	1.370(1)
C(7)-C(8)	1.360(1) C(8)-C(9)	1.349(1)
C(9)-C(10)	1.366(1) B(3)-B(4)	1.684(9)
B(3)-B(8)	1.692(9) B(3)-B(7)	1.693(8)
B(4)-B(9)	1.718(1) B(4)-B(8)	1.726(1)
B(4)-B(5)	1.768(8) B(5)-B(10)	1.750(1)
B(5)-B(6)	1.758(9) B(5)-B(9)	1.761(1)
B(6)-B(10)	1.776(9) B(6)-B(11)	1.784(9)
B(7)-B(12)	1.758(1) B(7)-B(11)	1.779(9)
B(7)-B(8)	1.780(1) B(8)-B(9)	1.747(1)
B(8)-B(12)	1.748(9) B(9)-B(12)	1.791(1)
B(9)-B(10)	1.804(9) B(10)-B(11)	1.766(1)
B(10)-B(12)	1.802(1) B(11)-B(12)	1.778(1)

Table S9. Angles [deg] for Methoxy(phenyl)methyl-*o*-carborane

C(3)-O(1)-C(4)	112.9(6) C(3)-C(1)-B(3)	116.7(4)
C(3)-C(1)-B(5)	120.9(5) B(3)-C(1)-B(5)	110.2(4)
C(3)-C(1)-B(6)	124.4(4) B(3)-C(1)-B(6)	110.7(4)
B(5)-C(1)-B(6)	62.3(4) C(3)-C(1)-B(4)	114.0(4)
B(3)-C(1)-B(4)	60.3(3) B(5)-C(1)-B(4)	62.6(4)
B(6)-C(1)-B(4)	113.7(4) C(3)-C(1)-C(2)	120.1(5)
B(3)-C(1)-C(2)	60.3(3) B(5)-C(1)-C(2)	113.3(4)
B(6)-C(1)-C(2)	62.9(3) B(4)-C(1)-C(2)	111.9(4)
B(3)-C(2)-C(1)	57.4(3) B(3)-C(2)-B(7)	58.8(4)
C(1)-C(2)-B(7)	105.3(5) B(3)-C(2)-B(11)	104.9(5)
C(1)-C(2)-B(11)	104.2(5) B(7)-C(2)-B(11)	60.7(4)
B(3)-C(2)-B(6)	104.3(5) C(1)-C(2)-B(6)	57.7(3)
B(7)-C(2)-B(6)	108.8(5) B(11)-C(2)-B(6)	60.1(4)
O(1)-C(3)-C(5)	115.7(6) O(1)-C(3)-C(1)	107.9(5)
C(5)-C(3)-C(1)	113.0(4) C(6)-C(5)-C(10)	119.1(6)
C(6)-C(5)-C(3)	120.5(6) C(10)-C(5)-C(3)	120.4(6)
C(5)-C(6)-C(7)	119.5(7) C(8)-C(7)-C(6)	120.8(7)
C(9)-C(8)-C(7)	120.3(7) C(8)-C(9)-C(10)	120.3(8)
C(9)-C(10)-C(5)	119.8(7) C(1)-B(3)-B(4)	61.5(3)
C(1)-B(3)-B(8)	111.2(4) B(4)-B(3)-B(8)	61.5(4)
C(1)-B(3)-B(7)	111.8(4) B(4)-B(3)-B(7)	114.1(5)
B(8)-B(3)-B(7)	63.4(4) C(1)-B(3)-C(2)	62.3(3)
B(4)-B(3)-C(2)	114.7(4) B(8)-B(3)-C(2)	114.7(5)
B(7)-B(3)-C(2)	62.0(4) B(3)-B(4)-C(1)	58.2(3)
B(3)-B(4)-B(9)	106.7(5) C(1)-B(4)-B(9)	106.7(4)

B(3)-B(4)-B(8)	59.5(4) C(1)-B(4)-B(8)	106.9(4)
B(9)-B(4)-B(8)	61.0(4) B(3)-B(4)-B(5)	105.3(4)
C(1)-B(4)-B(5)	58.5(3) B(9)-B(4)-B(5)	60.7(4)
B(8)-B(4)-B(5)	109.1(5) C(1)-B(5)-B(10)	106.0(5)
C(1)-B(5)-B(6)	58.9(3) B(10)-B(5)-B(6)	60.8(4)
C(1)-B(5)-B(9)	105.0(4) B(10)-B(5)-B(9)	61.8(4)
B(6)-B(5)-B(9)	110.0(5) C(1)-B(5)-B(4)	58.8(3)
B(10)-B(5)-B(4)	107.8(5) B(6)-B(5)-B(4)	107.9(4)
B(9)-B(5)-B(4)	58.3(4) C(1)-B(6)-B(5)	58.8(3)
C(1)-B(6)-B(10)	104.7(4) B(5)-B(6)-B(10)	59.4(4)
C(1)-B(6)-B(11)	105.0(4) B(5)-B(6)-B(11)	106.9(5)
B(10)-B(6)-B(11)	59.5(4) C(1)-B(6)-C(2)	59.4(3)
B(5)-B(6)-C(2)	107.7(4) B(10)-B(6)-C(2)	107.1(4)
B(11)-B(6)-C(2)	59.4(4) B(3)-B(7)-C(2)	59.1(4)
B(3)-B(7)-B(12)	104.2(5) C(2)-B(7)-B(12)	108.7(5)
B(3)-B(7)-B(11)	104.8(4) C(2)-B(7)-B(11)	60.3(4)
B(12)-B(7)-B(11)	60.4(4) B(3)-B(7)-B(8)	58.2(4)
C(2)-B(7)-B(8)	108.0(5) B(12)-B(7)-B(8)	59.2(4)
B(11)-B(7)-B(8)	107.4(5) B(3)-B(8)-B(4)	59.0(4)
B(3)-B(8)-B(9)	105.1(5) B(4)-B(8)-B(9)	59.3(4)
B(3)-B(8)-B(12)	104.7(4) B(4)-B(8)-B(12)	108.4(5)
B(9)-B(8)-B(12)	61.7(4) B(3)-B(8)-B(7)	58.3(4)
B(4)-B(8)-B(7)	107.8(4) B(9)-B(8)-B(7)	109.0(5)
B(12)-B(8)-B(7)	59.7(4) B(4)-B(9)-B(8)	59.7(4)
B(4)-B(9)-B(5)	61.1(4) B(8)-B(9)-B(5)	108.4(5)
B(4)-B(9)-B(12)	106.8(5) B(8)-B(9)-B(12)	59.2(4)

B(5)-B(9)-B(12)	107.0(5) B(4)-B(9)-B(10)	107.6(5)
B(8)-B(9)-B(10)	107.7(5) B(5)-B(9)-B(10)	58.8(4)
B(12)-B(9)-B(10)	60.2(4) B(5)-B(10)-B(11)	108.0(5)
B(5)-B(10)-B(6)	59.8(4) B(11)-B(10)-B(6)	60.5(4)
B(5)-B(10)-B(12)	107.0(5) B(11)-B(10)-B(12)	59.8(4)
B(6)-B(10)-B(12)	107.7(4) B(5)-B(10)-B(9)	59.4(4)
B(11)-B(10)-B(9)	107.6(5) B(6)-B(10)-B(9)	107.3(4)
B(12)-B(10)-B(9)	59.6(4) B(10)-B(11)-C(2)	108.4(5)
B(10)-B(11)-B(12)	61.1(4) C(2)-B(11)-B(12)	106.8(4)
B(10)-B(11)-B(7)	108.4(5) C(2)-B(11)-B(7)	59.0(4)
B(12)-B(11)-B(7)	59.2(4) B(10)-B(11)-B(6)	60.0(4)
C(2)-B(11)-B(6)	60.5(4) B(12)-B(11)-B(6)	108.4(5)
B(7)-B(11)-B(6)	107.7(4) B(8)-B(12)-B(7)	61.0(4)
B(8)-B(12)-B(11)	108.8(5) B(7)-B(12)-B(11)	60.4(4)
B(8)-B(12)-B(9)	59.1(4) B(7)-B(12)-B(9)	108.0(5)
B(11)-B(12)-B(9)	107.6(5) B(8)-B(12)-B(10)	107.7(5)
B(7)-B(12)-B(10)	107.7(5) B(11)-B(12)-B(10)	59.1(4)
B(9)-B(12)-B(10)	60.3(4)	

Table S10. Crystal data and structure refinement for Organotin Halides
 $(\text{C}_6\text{H}_{21}\text{B}_{10}\text{BrO})\text{Me}_2\text{SnBr}$

Identification code	kor080
Empirical formula	$\text{C}_6\text{H}_{21}\text{B}_{10}\text{BrO}\text{Sn}$
Formula weight	415.93
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Orthorhombic, $Pna2_1$
Unit cell dimensions	$a = 17.9292(15)$ Å $b = 7.2066(4)$ Å $c = 13.0582(10)$ Å
Volume	1687.2(2) Å ³
Z, D _{calc}	4, 1.637 g/m ³
m	3.862 mm ⁻¹
F(000)	800
Crystal size	0.55 × 0.42 × 0.31 mm
q range for data collection	2.27 to 25.96 °
Limiting indices	0 ≤ h ≤ 22, 0 ≤ k ≤ 8, 0 ≤ l ≤ 16
Reflections collected / unique	1724 / 1724 [R(int) = 0.0000]
Completeness to q = 28.32	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1724 / 1 / 185
Goodness-of-fit on F^2	0.985
Final R indices [I>2s(I)]	^a R ₁ = 0.0572, ^b wR ₂ = 0.0987
R indices (all data)	^a R ₁ = 0.1984, ^b wR ₂ = 0.1322
Absolute structure parameter	-0.01(5)
Largest diff. peak and hole	0.852 and -0.800 e.Å ⁻³

Table S11. Bond lengths [Å] for Organotin Halides ($\text{Ca}^{C,O}\text{B}_2\text{SnBr}$)

Sn(1)-C(5)	2.109(2) B(3)-B(7)	1.81(3)
Sn(1)-C(6)	2.13(2) B(4)-B(5)	1.75(3)
Sn(1)-C(1)	2.193(2) B(4)-B(8)	1.82(3)
Sn(1)-Br(1)	2.537(3) B(4)-B(9)	1.84(3)
Sn(1)-O(1)	2.579(1) B(5)-B(6)	1.73(3)
O(1)-C(3)	1.37(2) B(5)-B(10)	1.74(3)
O(1)-C(4)	1.43(3) B(5)-B(9)	1.76(4)
C(1)-C(2)	1.63(2) B(6)-B(10)	1.81(3)
C(1)-B(4)	1.65(3) B(6)-B(11)	1.84(3)
C(1)-B(6)	1.68(3) B(7)-B(12)	1.65(5)
C(1)-B(5)	1.68(3) B(7)-B(8)	1.70(4)
C(1)-B(3)	1.72(3) B(7)-B(11)	1.80(3)
C(2)-C(3)	1.55(3) B(8)-B(12)	1.68(5)
C(2)-B(6)	1.66(3) B(8)-B(9)	1.79(3)
C(2)-B(11)	1.70(3) B(9)-B(10)	1.77(4)
C(2)-B(3)	1.72(3) B(9)-B(12)	1.77(4)
C(2)-B(7)	1.78(3) B(10)-B(11)	1.82(3)
B(3)-B(4)	1.74(3) B(10)-B(12)	1.84(5)
B(3)-B(8)	1.79(3) B(11)-B(12)	1.76(4)

Table S12. Angles [deg] for Organotin Halides ($\text{Ca}^{C,O}_b$) Me_2SnBr

C(5)-Sn(1)-C(6)	125.5(9) C(2)-B(6)-B(5)	104.6(2)
C(5)-Sn(1)-C(1)	112.4(8) C(1)-B(6)-B(5)	59.2(1)
C(6)-Sn(1)-C(1)	113.5(8) C(2)-B(6)-B(10)	104.3(2)
C(5)-Sn(1)-Br(1)	101.3(5) C(1)-B(6)-B(10)	105.7(2)
C(6)-Sn(1)-Br(1)	99.5(7) B(5)-B(6)-B(10)	59.0(1)
C(1)-Sn(1)-Br(1)	98.4(5) C(2)-B(6)-B(11)	57.9(1)
C(5)-Sn(1)-O(1)	83.6(6) C(1)-B(6)-B(11)	105.9(2)
C(6)-Sn(1)-O(1)	84.5(8) B(5)-B(6)-B(11)	106.6(2)
C(1)-Sn(1)-O(1)	71.4(6) B(10)-B(6)-B(11)	59.9(1)
Br(1)-Sn(1)-O(1)	169.8(3) C(2)-B(6)-Sn(1)	75.9(9)
C(3)-O(1)-C(4)	111.4(2) C(1)-B(6)-Sn(1)	36.6(8)
C(3)-O(1)-Sn(1)	121.1(1) B(5)-B(6)-Sn(1)	78.7(1)
C(4)-O(1)-Sn(1)	127.4(1) B(10)-B(6)-Sn(1)	136.7(1)
C(2)-C(1)-B(4)	110.1(2) B(11)-B(6)-Sn(1)	133.5(1)
C(2)-C(1)-B(6)	60.2(1) B(12)-B(7)-B(8)	60.0(2)
B(4)-C(1)-B(6)	115.3(2) B(12)-B(7)-C(2)	103(2)
C(2)-C(1)-B(5)	108.0(2) B(8)-B(7)-C(2)	103.5(1)
B(4)-C(1)-B(5)	63.2(1) B(12)-B(7)-B(11)	61.3(2)
B(6)-C(1)-B(5)	62.0(1) B(8)-B(7)-B(11)	109.1(2)
C(2)-C(1)-B(3)	61.6(1) C(2)-B(7)-B(11)	56.7(1)
B(4)-C(1)-B(3)	61.9(1) B(12)-B(7)-B(3)	108.1(2)
B(6)-C(1)-B(3)	114.3(2) B(8)-B(7)-B(3)	61.1(1)
B(5)-C(1)-B(3)	113.1(2) C(2)-B(7)-B(3)	57.3(1)
C(2)-C(1)-Sn(1)	119.1(1) B(11)-B(7)-B(3)	106.6(2)
B(4)-C(1)-Sn(1)	121.0(1) B(12)-B(8)-B(7)	58.4(2)

B(6)-C(1)-Sn(1)	116.3(1) B(12)-B(8)-B(3)	108(2)
B(5)-C(1)-Sn(1)	122.8(1) B(7)-B(8)-B(3)	62.4(1)
B(3)-C(1)-Sn(1)	116.7(1) B(12)-B(8)-B(9)	61(2)
C(3)-C(2)-C(1)	118.7(1) B(7)-B(8)-B(9)	109(2)
C(3)-C(2)-B(6)	118.5(2) B(3)-B(8)-B(9)	108.2(2)
C(1)-C(2)-B(6)	61.2(1) B(12)-B(8)-B(4)	109(2)
C(3)-C(2)-B(11)	119.1(1) B(7)-B(8)-B(4)	108.3(2)
C(1)-C(2)-B(11)	114.6(2) B(3)-B(8)-B(4)	57.6(1)
B(6)-C(2)-B(11)	66.3(1) B(9)-B(8)-B(4)	61.3(1)
C(3)-C(2)-B(3)	113.8(2) B(5)-B(9)-B(10)	59.2(1)
C(1)-C(2)-B(3)	61.8(1) B(5)-B(9)-B(12)	106(2)
B(6)-C(2)-B(3)	115.3(2) B(10)-B(9)-B(12)	62.7(2)
B(11)-C(2)-B(3)	115.8(2) B(5)-B(9)-B(8)	106.0(2)
C(3)-C(2)-B(7)	117.9(2) B(10)-B(9)-B(8)	107.9(2)
C(1)-C(2)-B(7)	111.5(1) B(12)-B(9)-B(8)	56.0(2)
B(6)-C(2)-B(7)	116.4(2) B(5)-B(9)-B(4)	57.9(1)
B(11)-C(2)-B(7)	62.4(1) B(10)-B(9)-B(4)	106.0(2)
B(3)-C(2)-B(7)	62.4(1) B(12)-B(9)-B(4)	103(2)
O(1)-C(3)-C(2)	109.5(1) B(8)-B(9)-B(4)	60.0(1)
C(2)-B(3)-C(1)	56.6(1) B(5)-B(10)-B(9)	60.3(1)
C(2)-B(3)-B(4)	102.3(2) B(5)-B(10)-B(6)	58.3(1)
C(1)-B(3)-B(4)	57.1(1) B(9)-B(10)-B(6)	107.3(2)
C(2)-B(3)-B(8)	102.3(2) B(5)-B(10)-B(11)	106.8(2)
C(1)-B(3)-B(8)	104.6(2) B(9)-B(10)-B(11)	107.2(2)
B(4)-B(3)-B(8)	62.0(2) B(6)-B(10)-B(11)	60.8(1)
C(2)-B(3)-B(7)	60.4(1) B(5)-B(10)-B(12)	104(2)

C(1)-B(3)-B(7)	105.9(2) B(9)-B(10)-B(12)	58.8(2)
B(4)-B(3)-B(7)	107.1(2) B(6)-B(10)-B(12)	104.3(2)
B(8)-B(3)-B(7)	56.5(1) B(11)-B(10)-B(12)	57.6(2)
C(1)-B(4)-B(3)	61.0(1) C(2)-B(11)-B(12)	101.3(2)
C(1)-B(4)-B(5)	59.2(1) C(2)-B(11)-B(7)	61.0(1)
B(3)-B(4)-B(5)	109.3(2) B(12)-B(11)-B(7)	55.1(2)
C(1)-B(4)-B(8)	106.4(2) C(2)-B(11)-B(10)	102.2(1)
B(3)-B(4)-B(8)	60.4(1) B(12)-B(11)-B(10)	61.8(2)
B(5)-B(4)-B(8)	105.8(2) B(7)-B(11)-B(10)	106.5(2)
C(1)-B(4)-B(9)	105.7(2) C(2)-B(11)-B(6)	55.8(1)
B(3)-B(4)-B(9)	108.4(2) B(12)-B(11)-B(6)	106.3(2)
B(5)-B(4)-B(9)	58.8(1) B(7)-B(11)-B(6)	106.9(1)
B(8)-B(4)-B(9)	58.7(1) B(10)-B(11)-B(6)	59.2(1)
C(1)-B(5)-B(6)	58.8(1) B(7)-B(12)-B(8)	62(2)
C(1)-B(5)-B(10)	108.4(2) B(7)-B(12)-B(11)	64(2)
B(6)-B(5)-B(10)	62.7(1) B(8)-B(12)-B(11)	112(3)
C(1)-B(5)-B(4)	57.6(1) B(7)-B(12)-B(9)	113(2)
B(6)-B(5)-B(4)	107.9(2) B(8)-B(12)-B(9)	62.6(2)
B(10)-B(5)-B(4)	111.4(2) B(11)-B(12)-B(9)	109(2)
C(1)-B(5)-B(9)	107.9(2) B(7)-B(12)-B(10)	112(2)
B(6)-B(5)-B(9)	110.8(2) B(8)-B(12)-B(10)	110(2)
B(10)-B(5)-B(9)	60.5(1) B(11)-B(12)-B(10)	60.6(2)
B(4)-B(5)-B(9)	63.3(2) B(9)-B(12)-B(10)	58.5(2)
C(2)-B(6)-C(1)	58.6(1)	

감사의 글

먼저, 부족한 게 많은 저에게 첫 제자라는 이유로 무한한 관심과 애정을 갖고 지도해주신 이 종대 교수님께 깊은 감사의 말씀을 전하고 싶습니다. 화학에 대한 재미를 알게 해 주시고 연구하는 학문적인 가르침뿐만 아니라 정신적, 생활적인 면에서도 잘못된 부분을 바로 잡아 주시어 제가 한 단계 더 성장해 갈 수 있도록 이끌어주셔서 정말 감사합니다.

여학생들의 좋은 본보기가 되어 달라며 격려와 응원을 아끼지 않으셨던 송기동 교수님, 조성동 교수님, 이범규 교수님, 고문주 교수님, 손홍래 교수님, 류설 교수님께도 감사의 말씀을 올립니다. 지난 1년 동안 의과대학 연구조교 생활을 할 때 많은 도움을 주셨던 문영래 교수님, 최철희 교수님, 박건 교수님께도 감사의 말씀을 올립니다. 학생을 대하실 때 늘 자상하신 조대원 교수님, 그리고 좋은 조건에서 실험을 배울 수 있도록 배려해주신 고려대학교 강상우 교수님께도 감사의 말씀을 올립니다.

학부 시절부터 항상 챙겨주고 힘이 되어주었던 화학과 많은 선배들과 후배들, 승현오빠, 영대오빠, 지훈오빠, 이성기오빠, 경선오빠, 진석오빠, 태은오빠, 보민오빠, 성용오빠, 성훈오빠, 정민언니, 보연언니, 내동기현, 김성기오빠, 용희오빠, 날응원해준 서린언니, 보배언니, 규용오빠, 현정이, 일반화학연습조교를 하면서 친해지고 잘 따라주었던 1학년 후배들과 동아리 후배인 학회원들에게 감사의 말을 전합니다.

의대 약리학 식구들과 병원에서 알게 된 진단검사학과 PCR 식구들, 고등학교 친구이자 의대에서든 병원에서든 내가 힘들어 할 때 힘이 되어준 미선에게도 감사합니다. 그리고 석사과정 동안 함께 고생하고 의지해온 하나뿐인 동기 하연에게도 고맙다는 말을 전합니다. 또한 고려대학교 유기금속화학 연구실 대학원생들에게도 감사하다는 말을 전합니다.

겨울이 막 시작되는 코끝이 매섭도록 찬바람이 불던 이 시기쯤 대학원에 진학하겠다고 면접을 보았던 것 같은데, 벌써 졸업을 앞두고 감사의 글을 써내려가고 있는 2년이라는 시간이 지난 지금, 가슴이 뭉클해지고 그 동안의 기억들이 펄름처럼 머릿속을 스쳐 지나갑니다. 돌이켜보면 즐거웠던 기억보

다 힘들었던 기억이 더 많습니다. 주변으로부터 ‘처음시작이라 어려울 것이다’라는 말을 많이 들었지만 아직까지 노력이 많이 부족했던 모양입니다. 그럴 때마다 주변사람들의 응원과 격려가 저를 일으켜주었고, 저 또한 주저앉지 않으려 했습니다. 또, 지금의 고생과 노력이 훗날 저의 밝은 미래에 밑거름이 될 거라 생각하고 기꺼이 이 어려운 상황을 받아들이고 잘 견뎌 내리라 다짐했습니다. 그렇게 지나온 시간이 분명 저에게 약이 되는 시간이 될 것이고 제가 한 단계 더 성장할 수 있도록 만들어 줄 거라 믿었기 때문입니다. 교수님께서는 ‘사람은 꿈과 목표가 있어야 한다. 분명한 목표의식과 하고자 하는 의지만 있다면 반드시 그 꿈은 이뤄진다’고 말씀하셨습니다. 이 말을 항상 되새기면서 늘 발전하는 사람이 되도록 노력할 것입니다. 다시 한 번 제게 도움을 주신 모든 분들께 감사의 말씀을 전합니다.

마지막으로 늘 저를 믿어주시고 지원해주시는 사랑하는 부모님과 효미, 효주, 재명이, 그리고 나의 친구들, 진심으로 고맙고 사랑합니다.

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논문제목	한글 : C,N-Chelating oxazolinyl-o-carborane에 의해 안정화된 카이랄 유기주석 화합물 영문 : Chiral Organotin Complexes Stabilized by C,N-Chelating Oxazolinyl-o-carboranes				

본인이 저작한 위의 저작물에 대하여 다음과 같은 조건아래 조선대학교가 저작물을 이용할 수 있도록 허락하고 동의합니다.

- 다 음 -

- 저작물의 DB구축 및 인터넷을 포함한 정보통신망에의 공개를 위한 저작물의 복제, 기억장치에의 저장, 전송 등을 허락함.
- 위의 목적을 위하여 필요한 범위 내에서의 편집·형식상의 변경을 허락함. 다만, 저작물의 내용변경은 금지함.
- 배포·전송된 저작물의 영리적 목적을 위한 복제, 저장, 전송 등은 금지함.
- 저작물에 대한 이용기간은 5년으로 하고, 기간종료 3개월 이내에 별도의 의사표시가 없을 경우에는 저작물의 이용기간을 계속 연장함.
- 해당 저작물의 저작권을 타인에게 양도하거나 또는 출판을 허락을 하였을 경우에는 1개월 이내에 대학에 이를 통보함.
- 조선대학교는 저작물의 이용허락 이후 해당 저작물로 인하여 발생하는 타인에 의한 권리 침해에 대하여 일체의 법적 책임을 지지 않음
- 소속대학의 협정기관에 저작물의 제공 및 인터넷 등 정보통신망을 이용한 저작물의 전송·출력을 허락함.

2009년 12월 8일

저작자: 김효숙 (서명 또는 인)

조선대학교 총장 귀하