The ^{11}B chemical shift of **3** (50.8 ppm) is slightly upfield compared to that of **1** (53.6 ppm) and **11** (54.6 ppm) and is comparable to that of **10** (49.5 ppm). Although the π electrons are delocalized toward boron (**3D**), the observed ^{11}B chemical shift of **3** reveals a substantial σ polarization from boron toward the neighboring carbon atoms.[2,9]

In order to confirm the characteristic features of the electronic structure, ab initio molecular orbital calculations of **3** (R = H) were performed with the STO-3G basis set. The optimization of the planar geometry followed by the vibrational analysis indicates that the planar structure is stable since all of the calculated frequencies are positive. Charge densities and π electron densities (in parentheses) of skeletal atoms are as follows: 0.2674 (0.2144) for B; −0.1840 (0.9953) for C_2; −0.0295 (0.9285) for C_3; −0.0195 (1.0361) for C_{3a}; −0.1765 (1.0702) for C_4; and 0.2817 (1.7301 for 3pπ, and 1.9950 for 2pπ) for S. The HOMO–LUMO gap in **3** (0.409 au) is found to be larger than that in azulene (0.340 au). This corresponds well to the fact that **3** has no long wavelength absorption maxima in the visible region. These results clearly support the experimental data. As a whole, the thiophene moiety has positive charges and the borepine moiety has negative charges. The calculated dipole moment is 2.35 *D*, which has the reverse direction to that of azulene.

Acknowledgment. This work was supported by a Grant-in-Aid for Scientific Research on Priority Areas (No. 03214103) from the Ministry of Education, Science and Culture, Japan.

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closo-Silaboranes and *closo*-Carboranes: Contrasting Relative Stabilities and Breakdown of the Rule of Topological Charge Stabilization

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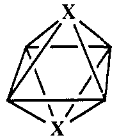
Despite their diagonal relationship in the periodic table and the many similarities between silicon and boron, studies of the chemistry of compounds involving both silicon and boron are only beginning to appear.[2,3] Since silicon is isoelectronic to carbon, a conceptually simple point of entry to the chemistry of boron and silicon is provided by the silaborane family of molecules, the silicon analogues of carboranes.[4] To our knowledge, there have been no reports to date of polyhedral boranes based on the octahedron and the pentagonal bipyramid in which one or more silicon atoms form a part of the polyhedra. In this paper, we use the concept of compatibility of orbitals in overlap[5] and ab initio molecular orbital calculations to predict the relative stabilities of positional isomers among the *closo*-silaboranes, **1c**–**6c**. The relative stabilities predicted by the orbital overlap model for the silaboranes emerge in the reverse order to those found in the corresponding *closo*-carboranes,[4,5a,6] and in the case of $Si_2B_4H_6$, the ordering is contrary to predictions based on the rule of topological charge stabilization.[6b] However, the ab initio calculations on the isomers of $Si_2B_4H_6$ and $Si_2B_5H_7$ support the qualitative orbital overlap predictions which now invite experimental verification.



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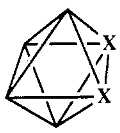

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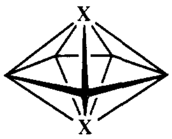

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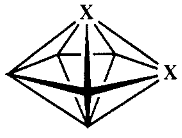

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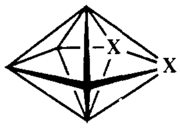

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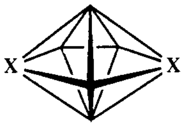

6

(a) X = BH^- (b) X = CH (c) X = SiH

There are several qualitative approaches available to rationalize and to predict the relative stabilities of positional isomers within a given polyhedral system. Carboranes form a well-studied group of compounds on which these methods can be tried. In one approach, Williams[7] suggested that the carbon atoms in dicarbacarboranes prefer to be as far apart as possible so as to minimize the repulsion between the negatively charged CH groups. The greater stability of 1,6-*closo*-$C_2B_4H_6$ (**1b**) over the 1,2-isomer (**2b**) could be explained on this basis. Extrapolation of this rule to the $Si_2B_4H_6$ system leads to the prediction that in this case also the 1,6-isomer (**1c**) should be favored over the 1,2-isomer (**2c**). In a second approach, Gimarc has used the rule of topological charge stabilization to explain the relative stabilities of *closo*-carboranes.[6b,8] According to this model, more electronegative atoms prefer to be located at sites of higher electron density while more electropositive elements prefer sites of lower electron density. The pattern of relative electron densities has normally been determined by calculations on a model isoelectronic, isostructural, homoatomic system. To apply this rule to polyhedral molecules where all the vertices are identical, the procedure which has been used previously involves applying a perturbation to the homoatomic system. For example, the positional preference for electronegative substituents in $B_6H_6^{2-}$ (**1a**) was obtained by calculating the charges on the atoms in a C_5N^- octahedron by the extended Hückel method.[6b] Since the unique carbon was calculated to have the greater negative charge, the 1,6-isomer of $C_2B_4H_6$ (**1b**) was predicted to be favored over the 1,2-isomer (**2b**), as found experimentally. We have performed similar calculations on C_5B^{3-}

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(1) (a) Australian National University. (b) University of Hyderabad.

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and C_5Si^{2-} in order to obtain the predictions of the topological charge stabilization model for the $Si_2B_4H_6$ system. In these cases, lower charges are found on the unique carbons, suggesting that the more electropositive silicon atoms should also be located in such positions, i.e., 1,6-$Si_2B_4H_6$ (**1c**) should be favored over 1,2-$Si_2B_4H_6$ (**2c**). Similarly, calculations of the charges in C_7^{2-} suggest that 1,7-$Si_2B_5H_7$ (**3c**) should be the preferred $Si_2B_5H_7$ isomer. The preference of 2,4-$C_2B_5H_7$ (**6b**) over 2,3-$C_2B_5H_7$ (**5b**) has been explained previously on the basis of the charges calculated for C_6N^- with N at position 2. We have similarly simulated an electropositive perturbation through calculations on C_6B^{3-} and C_6Si^{2-} with the heteroatom located within the five-membered ring. The resulting charges suggest that, for the $Si_2B_5H_7$ system also, the 2,4-isomer (**6c**) should be the favored structure.

A third qualitative approach involves the idea of the compatibility of orbitals in overlap, used previously to explain the relative stabilities of polyhedral carboranes.[5a,9] These polyhedral molecules may be considered to be composed of rings and caps, formed by the interaction of the π orbitals of the ring with the p-orbitals of the cap. We have shown that the B_4H_4 ring requires a capping group with less diffuse orbitals than BH (e.g., CH) to have optimum ring–cap orbital overlap. Thus, the interaction of two CH groups from either side of the B_4H_4 ring leads to the 1,6-isomer (**1b**) of $C_2B_4H_6$, which is favored over the 1,2-isomer (**2b**).[5a] SiH groups have more diffuse orbitals than CH or BH so that 1,6-$Si_2B_4H_6$ (**1c**), obtained from the interaction of two SiH groups with the B_4H_4 ring, should be relatively less favorable. The B_5H_5 ring, on the other hand, requires a capping group with more diffuse orbitals than BH itself (e.g., SiH). Therefore, 1,7-$Si_2B_5H_7$, obtained by the interaction of two SiH groups with the larger B_5H_5 ring, might be expected to be the preferred isomer of this system. Other isomers of $Si_2B_5H_7$ in which the SiH groups are removed from the apical positions should be progressively less favorable.

The predictions of the qualitative models of the relative stabilities of silaboranes may be summarized as follows. All three approaches suggest the 1,7-form (**3c**) to be the favored isomer of $Si_2B_5H_7$. For the $Si_2B_4H_6$ systems, Williams's rule and the rule of topological charge stabilization suggest a preference for 1,6-$Si_2B_4H_6$ (**1c**) over the 1,2-isomer (**2c**). On the other hand, arguments based on compatibility of orbitals in overlap suggest the opposite preference of **2c** over **1c**.

In order to resolve these conflicting qualitative predictions, and in order to obtain a more detailed characterization of the relevant silaboranes, standard ab initio molecular orbital calculations[10] were carried out using the GAUSSIAN 90 suite of programs.[11] The geometries of the silaborane isomers **1c**–**6c** and, for comparison purposes, the corresponding borane anions (**1a**, **3a**) and carboranes (**1b**–**6b**) were optimized at the HF/6-31G* level. Harmonic vibrational frequency calculations, also at HF/6-31G*, confirmed that the optimized structures are located at minima on their respective potential energy surfaces. Electron correlation was incorporated through calculations at the MP2/6-31G* level on the HF/6-31G* geometries. Table I gives the total and relative energies for all species. The relative energies of carboranes from the current study are consistent with previous values obtained at somewhat lower levels of theory.[6a] Optimized geometrical parameters are given in the supplementary material.

The calculated order of stabilities for the silaborane isomers are exactly the reverse of the ordering for the carboranes. Thus, whereas *trans*-1,6-$C_2B_4H_6$ (**1b**) is more stable than *cis*-1,2-$C_2B_4H_6$ (**2b**) by 40 kJ mol^{-1}, *cis*-1,2-$Si_2B_4H_6$ (**2c**) is more stable than *trans*-1,6-$Si_2B_4H_6$ (**1c**) by 46 kJ mol^{-1}. The reversal of stability ordering is even more striking for the $X_2B_5H_7$ isomers. Among the $C_2B_5H_7$ carboranes, the 2,4-isomer (**6b**) is the most stable, with the energies of the other isomers increasing in the order **6b** < **5b** < **4b** < **3b**. For the $Si_2B_5H_7$ silaboranes, the preferred isomer is the trans-1,7 form (**3c**). The structure with one SiH group and one BH group bridging the five-membered ring (**4c**) is less stable than **3c** by 17 kJ mol^{-1}, while the 2,3- and 2,4-isomers lie 87 and 113 kJ mol^{-1}, respectively, above **3c**. Thus, the stability ordering for the silaboranes is **3c** < **4c** < **5c** < **6c**. The ab initio results are consistent with all the qualitative predictions concerning the preferred isomer of $Si_2B_5H_7$, but in the case of the $Si_2B_4H_6$ system, they support the prediction of the orbital overlap model over that of the other qualitative approaches.

Table I. Calculated Total Energies and Relative Energies of Borane Anions (**1a** and **3a**), Carboranes (**1b**–**6b**), and Silaboranes (**1c**–**6c**)[a]

		total energy, hartrees		relative energy, kJ mol^{-1}
molecule	symmetry	HF/6-31G*	MP2/6-31G*	MP2/6-31G*
1a	O_h	−151.427 64	−151.990 58	
3a	D_{5h}	−176.722 73	−177.380 01	
1b	D_{4h}	−177.946 22	−178.562 02	0
2b	C_{2v}	−177.936 21	−178.546 92	40
3b	D_{5h}	−203.116 38	−203.836 01	283
4b	C_s	−203.170 70	−203.876 06	178
5b	C_{2v}	−203.214 93	−203.916 88	71
6b	C_{2v}	−203.245 12	−203.943 78	0
1c	D_{4h}	−679.965 41	−680.501 35	46
2c	C_{2v}	−679.983 20	−680.518 95	0
3c	D_{5h}	−705.275 37	−705.899 73	0
4c	C_s	−705.265 19	−705.893 38	17
5c	C_{2v}	−705.239 27	−705.866 62	87
6c	C_{2v}	−705.238 20	−705.856 85	113

[a] HF/6-31G* optimized geometries.

The relative energies of the $C_2B_5H_7$ isomers span a range of almost 283 kJ mol^{-1}, and only the lowest energy isomer is known experimentally.[12] For the $Si_2B_5H_7$ system, the spread of relative energies is much smaller (113 kJ mol^{-1}). These results suggest the possibility that several of the $Si_2B_5H_7$ isomers may be experimentally accessible.

The calculated energies for the formal reactions 1–3 provide measures of the relative preferences among BH^-, CH, and SiH caps for four- and five-membered boron rings. The preference

$$\mathbf{1b} + \mathbf{3a} \rightarrow \mathbf{1a} + \mathbf{3b} \qquad \Delta E = +72 \text{ kJ mol}^{-1} \qquad (1)$$

$$\mathbf{1b} + \mathbf{3c} \rightarrow \mathbf{1c} + \mathbf{3b} \qquad \Delta E = +78 \text{ kJ mol}^{-1} \qquad (2)$$

$$\mathbf{1a} + \mathbf{3c} \rightarrow \mathbf{1c} + \mathbf{3a} \qquad \Delta E = +6 \text{ kJ mol}^{-1} \qquad (3)$$

of CH for the smaller ring is seen in the large energies of reactions 1 and 2. There is greater similarity between BH^- and SiH, as seen by the energy of reaction 3. The small positive value indicates a very slight preference for silicon to cap a larger ring. The greater similarity of SiH and BH^- (compared with CH and BH^-) is also seen in the smaller range of relative energies calculated for the silaboranes than for the corresponding carboranes.

We conclude from this study that the relative isomer stabilities in $X_2B_4H_6$ and $X_2B_5H_7$ systems are reversed in going from the *closo*-carboranes (X = C) to the *closo*-silaboranes (X = Si). The topological charge stabilization model does not predict this reversal for the $Si_2B_4H_6$ system, nor for isomers **5c** and **6c** of the $Si_2B_5H_7$ system. The greater similarity between boron and silicon should make silaboranes based on pentagonal bipyramids more accessible than the corresponding carboranes. We hope that our theoretical predictions will stimulate experimental investigations in this area.

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computers of the Australian National University Supercomputing Facility.

Supplementary Material Available: Table of Cartesian coordinates of the 14 isomeric structures **1a**, **3a**, **1b**–**6b**, and **1c**–**6c** optimized at the 6-31G* level (7 pages). This supplementary material is provided in the archival edition of the journal, which is available in many libraries. Alternatively, ordering information is given on any current masthead page.

Formation of Tungsten–Carbyne and Tungsten–Oxo–Allyl Complexes on Reaction of $WCl_2(PR_3)_4$ with Unsaturated Silanes

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Reactions of the tungsten(II) complex $WCl_2(PMePh_2)_4$ (**1a**) show a high propensity to form metal–ligand multiple bonds, and this provides the driving force for a number of interesting transformations. Alcohols are deoxygenated to hydrocarbons,[2] epoxides to alkenes,[3] and CO_2 to CO,[4] all with the production of tungsten(IV) oxo compounds; imido, sulfido,[4] phosphinidine,[5] and alkylidene complexes[6] are formed in related reactions. This report describes reaction of **1a** and $WCl_2(PMe_3)_4$ (**1b**) with (allyloxy)trimethylsilane to give rare examples of oxo–allyl complexes[7] and remarkable reactions of **1b** with vinyl- and allylsilane reagents which rearrange to give tungsten carbyne compounds.[8]

Reactions of **1** require significant initial binding of the substrate to the tungsten center. This is a primary reason why deoxygenation of simple alcohols by **1a** is slow and why deoxygenation of ethers such as Et_2O or $MeOSiMe_3$, while thermodynamically favorable,[9] does not occur. Addition of a potential tungsten binding site to the substrate, however, can circumvent this kinetic barrier.[10] For instance, allyl alcohol and 1-buten-4-ol are rapidly deoxygenated by **1a** to give alkenes and $W(O)Cl_2(PMePh_2)_3$ because the alkene function acts as a "tether" to bring the oxygen close to the metal.[2]

Use of a "tether" allows extension of this chemistry to silyl ethers. For example, 0.45 mL of (allyloxy)trimethylsilane reacts with 0.50 g of **1b** in 50 mL of toluene to give an orange solution after heating of the solution at 65 °C overnight. Subsequent workup[11] gives the tungsten–oxo–allyl complex **2b** in 74% yield. **1a** also reacts with (allyloxy)trimethylsilane to give a tungsten–oxo–allyl complex $W(O)(\eta^3\text{-}C_3H_5)(PMePh_2)_2Cl$ (**2a**) (eq 1). The

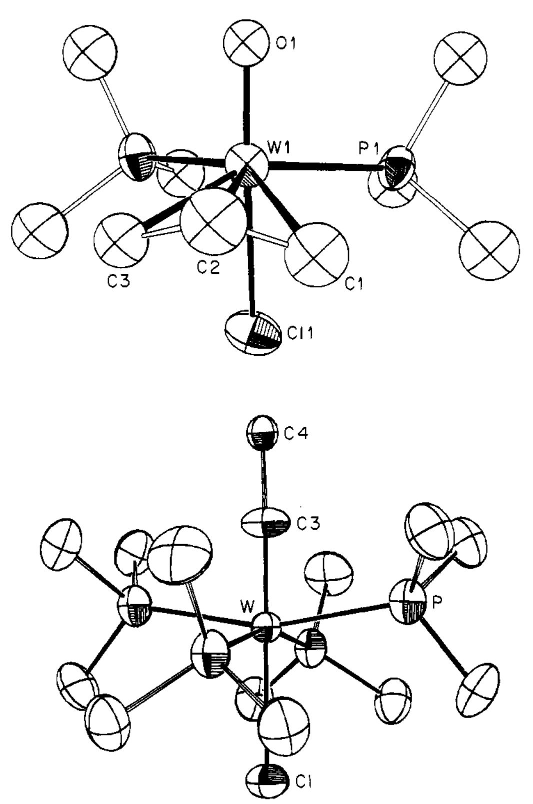

Figure 1. ORTEP drawings of $W(O)(\eta^3\text{-}C_3H_5)Cl(PMe_3)_2$ (**2b**; top) and $W(\equiv CCH_3)(PMe_3)_4Cl$ (**3**; bottom) with 40% probability thermal ellipsoids. Selected bond distances (Å) and angles (deg) for **2b**: W–Cl1 2.639 (9), W–P1 2.483 (9), W–P2 2.491 (9), W–C1 2.29 (4), W–C2 2.25 (4), W–C3 2.31 (3), O1–W–P1 93.5 (8), O1–W–P2 90.8 (8), O1–W–Cl1 161.8 (9), O1–W–C1 114.4 (13), O1–W–C2 102.6 (14), O1–W–C3 111.0 (11), P1–W–P2 102.4 (3), C1–C2–C3 127 (4). For **3**: W–P 2.464 (2), W–Cl 2.589 (15), W–C3 1.76 (4), P–W–Cl 80.75 (9), P–W–C3 99.25 (9), W–C3–C4 176 (3), P–W–P′ 161.51 (18), P–W–P″ 91.48 (9).


(1)

$$WCl_2L_4 + Me_3SiOCH_2CH{=}CH_2 \longrightarrow W(O)(\eta^3\text{-}C_3H_5)L_2Cl + Me_3SiCl \quad (1)$$

1a,b **2a,b**

tungsten abstracts the oxygen atom and retains the organic fragment; the silicon removes a chloride. The formation of the strong W≡O multiple bond and the η^3-allyl provide the driving force for cleavage of the Si–O bond.[12] The X-ray crystal structure of the PMe_3 derivative **2b** (Figure 1)[13] shows a pseudooctahedral complex (the η^3-allyl ligand occupying two sites), with a short tungsten–oxo distance of 1.651 (17) Å.[14] The allyl ligand lies cis to the oxo, as expected for a ligand with π-acceptor orbitals,[4] and the W–C distances are typical for tungsten η^3-allyl compounds.[15] NMR data for **2a** and **2b** are consistent with similar

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(11) The solution was reduced to 7 mL, cooled at −76 °C, filtered, and dried in vacuo to give 0.15 g of orange **2b**; a second crop from toluene/pentane gave an overall yield of 74%. Anal. Calcd for $WClP_2OC_9H_{23}$: O, 3.73; C, 25.23; H, 5.41; Found: O, 3.58; C, 25.68; H, 5.43.

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(13) Crystal data (CAD4) for **2b**: $P2_12_12_1$ (orthorhombic setting), $a = 8.661$ (1) Å, $b = 10.834$ (1) Å, $c = 16.890$ (2) Å, $Z = 4$, $V = 1584.9$ (6) Å^3, $\mu = 77.93$ cm^{-1}; 77 parameters were refined using 992 unique data ($I > 2\sigma_I$) to $R = 6.6\%$, $R_w = 7.8\%$, GOF = 1.420. For **3**: $I\bar{4}2m$ (tetragonal setting), $a = 9.6854$ (13) Å, $c = 12.5307$ (14) Å, $Z = 2$, $V = 1175.5$ (4) Å^3, $\mu = 53.97$ cm^{-1}; 38 parameters were refined using 427 unique data ($I > 3\sigma_I$) to $R = 3.8\%$, $R_w = 5.1\%$, GOF = 1.288; the CCH_3 and Cl are disordered because of the S_4 site symmetry.

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