

$$\eta_A = \eta_B \quad (6)$$

Minimization of $\Delta\Omega_B$ with respect to η_B at fixed η_A gives the same result. The HSAB principle! Under these conditions

$$\Delta\Omega_A = \Delta\Omega_B \quad (7)$$

If this equation were assumed, it would imply eq 6.

In the molecule AB, A and B are open systems (as first pointed out by Richard Bader⁹). This means that the natural thermodynamic quantity for an atom (or other subunit) in a molecule is not the energy E but the *grand potential* $\Omega_i = E_i - (N_i - N_i^0)\mu_i$. In equilibrium at the final, equalized chemical potential μ , the grand potentials of both A and B prefer to be as negative as possible. This implies in turn that $\Delta\Omega_A$ and $\Delta\Omega_B$ in eq 5 prefer to be as negative as possible, for these $\Delta\Omega$'s are just the grand potential changes. An elementary calculation on the charge-transfer equilibration shows this; one finds $\mu = (S_A\mu_A + S_B\mu_B)/(S_A + S_B)$ and

$$\Delta\Omega_A = -\frac{1}{2}S_A(\mu - \mu_A)^2 = -\frac{(\mu_B - \mu_A)^2}{4} \frac{\eta_A}{(\eta_A + \eta_B)^2} \quad (8)$$

and similarly with $\Delta\Omega_B$, verifying eq 5.

The argument is that Ω_A and Ω_B separately like to be as negative as possible. This has the HSAB principle as a consequence, and also the equity principle of eq 7. There is a dictum in economics called the Pareto principle: Efficiency is highest when partners are both well satisfied.¹⁰ So it appears to be in chemistry, and that is the HSAB principle.

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(9) For example, Sec. III in the following: Bader, R. F. W.; Nguyen-Dang, T. T. *Adv. Quantum Chem.* **1981**, *14*, 63-124.

(10) See, for example, pp 747-748 and especially Fig. 31-2 of the following: Samuelson, P. A.; Nordhaus, W. D. *Economics*, 13th ed.; McGraw-Hill: New York, 1989.

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(12) H.L. and R.G.P.

Decakis(2,6-diethylphenyl)decastanna[5]prismane: Characterization and Molecular Structure

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The theoretical structures presented by the family of heavy-atom group IVA [n]prismanes, $[RM]_{2n}$, where $M = \text{Si, Ge, Sn, and Pb}$, $R = \text{H}$, and $n = 2-6$, respectively, all possess severe $M-M-R$ and $M-M-M$ bond-angle distortions due to the unique geometrical constraints imposed upon the $M-M$ -bonded networks in these molecular frameworks.¹ To date, the only synthetic derivatives of this important class of compounds are represented by one [3]prismane [$M = \text{Ge}$, $R = \text{bis(trimethylsilyl)methyl}$]² and two [4]prismanes ($M = \text{Si}$, $R = \text{tert-butyl-dimethylsilyl}$; $M = \text{Sn}$, $R = 2,6\text{-diethylphenyl}$).^{3,4} Herein, we report the successful isolation

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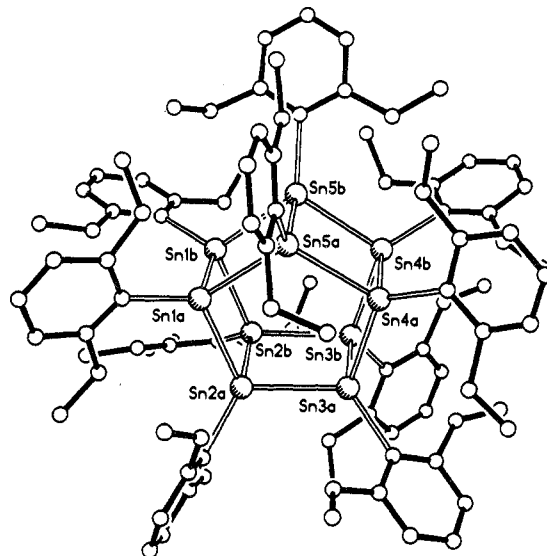


Figure 1. Molecular structure of **1**. Tin and carbon atoms are represented by large and small spheres, respectively, of arbitrarily chosen size. Hydrogen atoms have been omitted for purposes of clarity. For a complete listing of bond lengths and angles, see the supplementary material.

and characterization, including crystallographic analysis, of the titled first heavy-atom [5]prismane derivative **1** ($M = \text{Sn}$, $R = 2,6\text{-diethylphenyl}$), which is prepared through a novel process.

Preparation and Characterization. Thermolysis of a 1:1 mixture (w/w) of benzophenone and hexakis(2,6-diethylphenyl)cyclo-tristannane (**2**)⁵ at 200 °C for 20 min provides **1** and octakis-(2,6-diethylphenyl)octastanna[4]prismane (**3**)⁴ in a 2.3:1 ratio for a combined yield of 12% along with small amounts of hexakis-(2,6-diethylphenyl)distannane (**4**),⁶ hexakis(2,6-diethylphenyl)-pentastanna[1.1.1]propellane (**5**)⁶ (5%), recovered **2** (12%), and other tin-containing compounds (Scheme I). In contrast, substitution of naphthalene for benzophenone provides, under identical conditions, a large quantity of recovered **2** (51%), larger amounts of **4** and **5** (27%), and only traces of **1** and **3** (<2-3%). Concerning the role of benzophenone in providing higher yields of **1** and **3**, we have previously proposed⁴ that perstanna[n]prismanes are products generated by the thermal bimolecular disproportionation of the highly reactive diorganostannylenes **6**, which is in thermal equilibrium with **2**,⁷ to produce the monovalent and trivalent tin species, **7** and **8**, respectively, followed by oligomerization of **7** according to Scheme I. In this mechanism, benzophenone, acting as the solvent, might serve to stabilize the stannylenes **6** relative to **2** through Lewis acid-base complexation,⁸ thereby leading to higher concentrations of **7**, and hence to **1** and **3**.

Orange microcrystalline **1** was isolated through chromatography on silica gel using a 4:1 hexane/toluene solvent mixture as the eluant, and chemical analysis and spectroscopic data are fully consistent with the $[R\text{Sn}]_{2n}$ formulation.^{9,10} Due to restricted rotation about the tin-carbon bonds in **1**, the ¹H NMR spectrum is temperature-dependent with a coalescence temperature, T_c , being observed for this process at -30 °C. In contrast, the T_c value

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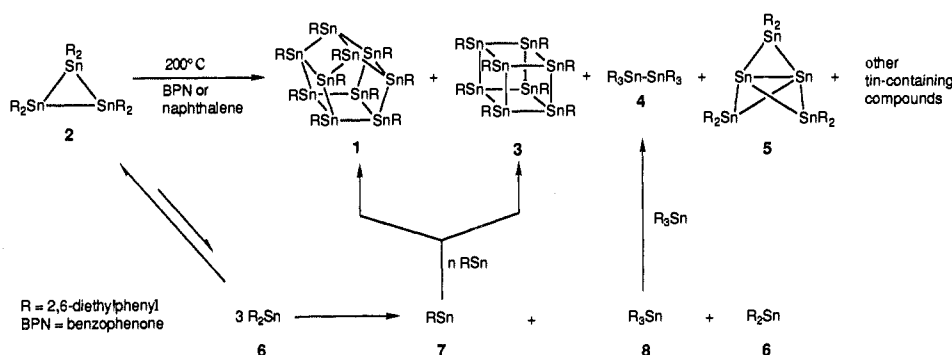
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(9) Anal. Calcd for **1**: C, 47.68; H, 5.20. Found: C, 47.39; H, 5.00. ¹H NMR (500 MHz, toluene-*d*₃, 40 °C): δ (ppm) 0.84 (t, 6 H), 2.92 (q, 4 H), 6.94 (d, 2 H), and 7.08 (t, 1 H). ¹¹⁹Sn NMR (186.5 MHz, toluene-*d*₃, δ reference to external Me₄Sn): δ (ppm) -21.3 [$^1J(^{119}\text{Sn}-^{117}\text{Sn}) = 693 \text{ Hz}$, $^2J(^{119}\text{Sn}-^{117}\text{Sn}) = 1224 \text{ Hz}$ between tin atoms in different five-membered rings; $^1J(^{119}\text{Sn}-^{117}\text{Sn}) = 3312 \text{ Hz}$, $^2J(^{119}\text{Sn}-^{117}\text{Sn}) = 90 \text{ Hz}$ between tin atoms within the same five-membered rings].¹² UV (hexane): λ 270 (ϵ 83600), 350 nm (6100).

(10) Detailed information is supplied in the supplementary material.

Scheme I



for aryl group rotation in **3** is < -80 °C. As revealed by ^{119}Sn NMR spectroscopy, the single resonance observed for **1** is 66 ppm upfield from that of **3**, and this is opposite to the downfield ^{13}C chemical shift of $[\text{HC}]_{10}$ relative to $[\text{HC}]_8$.¹¹ In addition, the expected $^3J(^{119}\text{Sn}-^{117}\text{Sn})$ coupling satellites¹² are not observed for either **1** or **3**, and on the basis of the Karplus correlation between dihedral angle and vicinal coupling constants, it is assumed that the magnitudes of these tin-tin coupling constants are near 0 due to the 90° dihedral angle in both molecular frameworks.¹³ Finally, the electronic spectra of **1** and **3** in hexane are remarkably different from each other, with no well-defined maxima being observed for the former.^{9,10}

Concerning the relative stabilities of the two perstanna[n]prismanes, heating of solutions of pure **1** or **3** in toluene at 200 °C shows no interconversion between the two species, and while both compounds are relatively stable at this temperature, **3** was observed to decompose to a greater extent than **1**, which remains unchanged, as determined by ^1H NMR spectroscopy. This increased stability of **1** over **3** is in keeping with the prediction that $[\text{HSn}]_{10}$ should be more stable than $[\text{HSn}]_8$.¹⁴ Finally, a solution of **1** in methylcyclohexane remained unchanged upon photolysis at room temperature using a Hanovia high-pressure lamp.

Crystallographic Analysis.¹⁰ As shown in Figure 1, the tin-tin-bonded molecular framework of **1** is composed of two five-membered rings which are held together by five inter-ring bonds. The mean tin-tin bond length of 2.856 (2) Å within the five-membered rings is identical with the value found for the mean inter-ring tin-tin bond length, and this value can be compared with the mean tin-tin bond length in **3**, which is 2.854 (2) Å. The average bond angles within the five-membered and four-membered rings of **1** are 108.0 (1)° and 90.0 (1)°, respectively, and both of these are exactly the values of the geometric ideals. For Sn-Sn-C bond angles in **3**, the average value is 125.1 (4)°, and in **1**, the average value for this angle for tin atoms on adjacent five-membered rings is 124.1 (4)° while it is 119.0 (4)° for tin atoms within the same five-membered ring. Surprisingly, all three of these mean bond angles are in very close agreement with those calculated for $[\text{HM}]_8$ and $[\text{HM}]_{10}$ ($M = \text{C}, \text{Si}$), even in spite of the steric interactions between adjacent 2,6-diethylphenyl ligands in the perstanna[n]prismanes.^{1h,15}

In conclusion, perstanna[n]prismanes, $[\text{RSn}]_{2n}$, where $n = 4$ and 5 , have been shown to be isolable compounds when the steric demands of the organic ligand are sufficient to kinetically stabilize these structures. In the present study, the 2,6-diethylphenyl ligand

appears to be the ideal choice for stabilization of **1** and **2**; however, by carefully modelling the steric requirements, other perstanna[n]prismanes, where $n = 2, 3$, or 6 , should be accessible from the appropriate stannylene precursors.

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Supplementary Material Available: Detailed information concerning the spectroscopic and crystallographic analysis of **1**, including listings of atomic coordinates and temperature factors, bond lengths, bond angles, and anisotropic temperature factors (30 pages). Ordering information is given on any current masthead page.

Molecular Structure of a Potent HIV-1 Inhibitor Belonging to the TIBO Family

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A series of tricyclic tetrahydroimidazo[4,5,1-*jk*]benzodiazepin-2(1*H*)-one (TIBO) and -thione derivatives have been found to be highly effective inhibitors of the reverse transcriptase (RTase) of HIV-1, the principal etiologic agent of AIDS.¹ One of the derivatives, coded R82913 ($\text{C}_{16}\text{H}_{20}\text{N}_3\text{S}$; Figure 1), has an IC_{50} of 1.5 nM for the growth inhibition of HIV-1/HIV-IIIb. The extraordinary potency of this compound, together with its relatively low cytotoxicity, gives it a selectivity index 3 times greater than that of AZT (3'-azido-2',3'-dideoxythymidine), at present the only drug approved for the treatment of AIDS.² It would be of great interest to investigate the structure of these compounds to gain insight on their unusual specificity toward RTase. The crystal structures of a number of nucleoside derivatives with anti-AIDS activity have been determined. These

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