$$\eta_{A} = \eta_{B} \tag{6}$$

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

$$\Delta\Omega_{\mathbf{A}} = \Delta\Omega_{\mathbf{B}} \tag{7}$$

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 Bader<sup>9</sup>). 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  $\Omega_i = E_i - (N_i - N_i^{\circ})\mu_i$ . In equilibrium at the final, equalized chemical potential  $\mu$ , 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 chargetransfer equilibration shows this; one finds  $\mu = (S_A \mu_A + S_B \mu_B)/(S_A \mu_B)$ 

$$\Delta\Omega_{\rm A} = -\frac{1}{2}S_{\rm A}(\mu - \mu_{\rm A})^2 = -\frac{(\mu_{\rm B} - \mu_{\rm A})^2}{4} \frac{\eta_{\rm A}}{(\eta_{\rm A} + \eta_{\rm B})^2}$$
(8)

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

The argument is that  $\Omega_A$  and  $\Omega_B$  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.

Acknowledgment. Financial support from the National Science Foundation is gratefully acknowledged.

(9) For example, Sec. III in the following: Bader, R. F. W.; Nguyen-Dang,

(11) P.K.C. and R.G.P.

## (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 = Si, Ge, Sn, and Pb, R = 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. To date, the only synthetic derivatives of this important class of compounds are represented by one [3] prismane  $[M = Ge, R = bis(trimethylsilyl)methyl]^2$  and two [4] prismanes (M = Si, R = tert-butyldimethylsilyl; M = Sn, R= 2,6-diethylphenyl).<sup>3,4</sup> Herein, we report the successful isolation

(2) Sekiguchi, A.; Kabuto, C.; Sakurai, H. Angew. Chem., Int. Ed. Engl. 1989, 28, 55.

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 = Sn, R =2,6-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)cyclotristannane (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 proposed<sup>4</sup> that perstanna[n] prismanes are products generated by the thermal bimolecular disproportionation of the highly reactive diorganostannylene 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 stannylene monomer 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  $[RSn]_{2n}$  formulation.<sup>9,10</sup> Due to restricted rotation about the tin-carbon bonds in 1, the <sup>1</sup>H 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

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.

<sup>(1) (</sup>a) Nagase, S.; Kudo, T.; Aoki, M. J. Chem. Soc., Chem. Commun. 1985, 1121. (b) Clabo, D. A., Jr.; Schaefer, H. F., III. J. Am. Chem. Soc. 1986, 108, 4344. (c) Sax, A. F.; Kalcher, J. J. Chem. Soc., Chem. Commun. 1987, 809. (d) Nagase, S.; Nakano, M.; Kudo, T. J. Chem. Soc., Chem. Commun. 1987, 60. (e) Sax, A. F.; Kalcher, J.; Janoschek, R. J. Comput. Chem. 1988, 9, 564. (f) Nagase, S.; Nakano, M. Angew. Chem., Int. Ed. Engl. 1988, 27, 1081. (g) Nagase, S. Angew. Chem., Int. Ed. Engl. 1989, 28, 329. (h) Nagase, S. Polyhedron, in press.

<sup>(3)</sup> Matsumoto, H.; Higuchi, K.; Hoshino, Y.; Koike, H.; Naoi, Y.; Nagai,

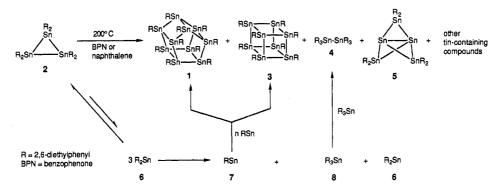
<sup>Y. J. Chem. Soc., Chem. Commun. 1988, 1083.
(4) Sita, L. R.; Kinoshita, I. Organometallics 1990, 9, 2865.
(5) Masamune, S.; Sita, L. R.; Williams, D. J. J. Am. Chem. Soc. 1983,</sup> 105, 630.

<sup>(6) (</sup>a) Sita, L. R.; Bickerstaff, R. D. J. Am. Chem. Soc. 1989, 111, 6454. (b) Sita, L. R.; Kinoshita, I. J. Am. Chem. Soc. 1990, 112, 8839

<sup>(7)</sup> Masamune, S.; Sita, L. R. J. Am. Chem. Soc. 1985, 107, 6390.

<sup>(8)</sup> Veith, M.; Recktenwald, O. *Top. Curr. Chem.* **1982**, *104*, 1. (9) Anal. Calcd for 1: C, 47.68; H, 5.20. Found: C, 47.39; H, 5.00. <sup>1</sup>H NMR (500 MHz, toluene- $d_8$ , 40 °C):  $\delta$  (ppm) 0.84 (t, 6 H), 2.92 (q, 4 H), 6.94 (d, 2 H), and 7.08 (t, 1 H). <sup>119</sup>Sn NMR (186.5 MHz, toluene- $d_8$ ,  $\delta$  reference to external Me<sub>4</sub>Sn):  $\delta$  (ppm) -21.3 [ $^1J(^{119}\text{Sn}^{-117}\text{Sn})$  = 693 Hz,  $^2J(^{119}\text{Sn}^{-117}\text{Sn})$  = 1224 Hz between tin atoms in different five-membered rings;  $^1J(^{119}\text{Sn}^{-117}\text{Sn})$  = 3312 Hz,  $^2J(^{119}\text{Sn}^{-117}\text{Sn})$  = 90 Hz between tin atoms within the same five-membered rings]. <sup>12</sup> UV (hexane):  $\lambda$  270 ( $\epsilon$  83 600), 350 nm (6100).

<sup>(10)</sup> Detailed information is supplied in the supplementary material.



for aryl group rotation in 3 is <-80 °C. As revealed by <sup>119</sup>Sn NMR spectroscopy, the single resonance observed for 19 is 66 ppm upfield from that of 3, and this is opposite to the downfield <sup>13</sup>C chemical shift of  $[HC]_{10}$  relative to  $[HC]_{8}$ . In addition, the expected  $^{3}J(^{119}Sn-^{117}Sn)$  coupling satellites  $^{12}$  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.<sup>13</sup> 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 [HSn]<sub>10</sub> should be more stable than [HSn]<sub>8</sub>.<sup>14</sup> 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 tintin-bonded molecular framework of 1 is composed of two fivemembered rings which are held together by five inter-ring bonds. The mean tin-tin bond length of 2.856 (2) Å within the fivemembered 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  $[HM]_8$  and  $[HM]_{10}$  (M = C, 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,  $[RSn]_{2n}$ , where n = 4and 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.

Acknowledgment. We thank Dr. Cynthia Day of Crystalytics Co. for the crystallographic analysis of 1 and the National Science Foundation (Grant CHE-9001462) for support of this work. Acknowledgment is also made to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research.

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(1H)-one (TIBO) and -thione derivatives have been found to be highly effective inhibitors of the reverse transcriptase (RTase) of HIV-1, the principal etiological agent of AIDS. One of the derivatives, coded R82913 (C<sub>16</sub>H<sub>20</sub>N<sub>3</sub>SCl; Figure 1), has an IC<sub>50</sub> 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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<sup>(12)</sup> Ordering of "J(119Sn-117Sn) values was made according to the approximate relative intensities of each coupling satellite to the main signal and on the basis that |<sup>2</sup>J(<sup>119</sup>Sn-<sup>117</sup>Sn)| is larger than |<sup>1</sup>J(<sup>119</sup>Sn-<sup>117</sup>Sn)| in cyclotetrastannanes; see: (a) Reference 7. (b) Puff, H.; Bach, C.; Schuh, W.; Zimmer, R. J. Organomet. Chem. 1986, 312, 313.

(13) Mitchell, T. N.; Reimann, W.; Nettelbeck, C. Organometallics 1985,

<sup>4. 1044.</sup> 

<sup>(14)</sup> The calculated HF/6-31G\* strain energy of cyclotetrastannane, [H<sub>2</sub>Sn]<sub>4</sub>, is 12.2 kcal mol<sup>-1</sup>, and using this value, the approximate strain energy of [HSn]<sub>8</sub> is 73.2 kcal mol<sup>-1</sup> and that of [HSn]<sub>10</sub> is 61.0 kcal mol<sup>-1</sup>; see: (a) Reference 1g. (b) Dailey, W. P. Tetrahedron Lett. 1987, 28, 5787.

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<sup>(1)</sup> Pauwels, R.; Andries, K.; Desmyter, J.; Schols, D.; Kukla, M. J.; Breslin, H. J.; Raeymaeckers, A.; van Gelder, J.; Woestenborghs, R.; Heykants, J.; Schellekens, K.; Janssen, M.; De Clercq, E.; Janssen, P. A. J. Nature (London) 1990, 343, 470-474.

<sup>(2)</sup> For an excellent recent review on the molecular targets of AIDS therapy, see: Mitsuya, H.; Yarchoan, R.; Broder, S. Science 1990, 249, 1533-1544.