yield) was isolated from the first fraction. By the same sequence, the Gulf of California *B. neritina* (12.5 kg) afforded 12.3 mg (9.8×10^{-5}% yield) and the Gulf of Sagami collection (5 kg) provided 1.0 mg (2×10^{-5}% yield) of bryostatin 4.

When necessary, bryostatin 4 was brought to analytical purity by repeating the HPLC sequence. A pure specimen ($C_{46}H_{70}O_{17}$, mol wt 894) was obtained as a colorless amorphous powder (PS ED_{50}, 6.7×10^{-4}, T/C 162 at 46 μg/kg) melting at 198–200 °C: MS (SP-SIMS)[4], with lithium iodide in sulfolane, *m/z* 901 $[M + Li]^+$, 883 $[M + Li - 18]^+$, and 799 $[M + Li - 102]^+$, with sodium iodide in sulfolane, *m/z* 917 $[M + Na]^+$, 899 $[M + Na - 18]^+$, 829 $[M + Na - 88]^+$, and 815 $[M + Na - 102]^+$, and with silver tetrafluoroborate in sulfolane, *m/z* 1001 and 1003 $[M + Ag^{107}$ and $Ag^{109}]^+$, 983 and 985 $[M + Ag - 18]^+$, 913 and 915 $[M + Ag - 88]^+$, and 899 and 901 $[M + Ag - 102]^+$; $[\alpha]^{27}{}_D$ +93.6° (*c* 0.032, CH_3OH); UV (CH_3OH) λ_{max} 228 (ϵ 36 500); IR (KBr) 3470, 2980–2945, 1740, 1725, 1660–1645, 1440, 1390, 1370, 1290, 1240, 1170, 1100, 1080, 1050, and 1000 cm^{-1}. The 400-MHz ^1H NMR data have been displayed in Table I in comparison with bryostatin 1, and the ^{13}C NMR assignments accompany structure **3**. Because of the unequivocal spectral evidence and exceptional value of bryostatin 4, elemental analyses were not performed.

Acid-Catalyzed Hydrolysis of Bryostatin 4. A specimen of bryostatin 4 (**3**, 1.0 mg) in 0.5 mL of 1% hydrochloric acid in methanol was hydrolyzed for 24 h at room temperature. The mixture (0.9 mg) obtained by extraction with methylene chloride, washing with water, and drying was separated by HPLC reversed phase (C-18) column chromatography with methanol–water (from 1:1 to 9:1) to furnish C-7 des-ester **4a** (0.72 mg) and C-20 des-ester **4b** (0.100 mg). The C-7 des-ester **4a** ($C_{41}H_{62}O_{16}$) was obtained as an amorphous powder from aqueous methanol: MS (SP-SIMS)[4] using sodium iodide in sulfolane, *m/z* 833 $[M + Na]^+$, 815 $[M + Na - 18]^+$, and 727 $[M + Na - 88]^+$; IR (KBr) 3475, 3420, 2975–2950, 1740, 1720, 1640, 1615, 1440, 1380, 1290, 1240, 1165, 1095, 1080, 1050, and 870 cm^{-1}. Analogously the C-20 des-ester **4b** ($C_{42}H_{64}O_{16}$) was obtained as an amorphous solid from aqueous methanol: MS (SP-SIMS) with sodium iodide in sulfolane, *m/z* 847 $[M + Na]^+$, 829 $[M + Na - 18]^+$, and 727 $[M + Na - 102]^+$.

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Registry No. 3, 91523-82-9; **4a**, 91523-83-0; **4b**, 91549-41-6.

MNDO Calculations for Compounds Containing Tin[1]

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Abstract: The MNDO parametric SCF–MO treatment has been parametrized for tin. Calculations are reported for a number of compounds of tin. The results are comparable with those for the third-period elements.

The MNDO semiempirical SCF–MO method[3,4] is now established[5] as a practical procedure for studying chemical behavior, giving results comparable[6] with those from quite good ab initio models (e.g., 4-31G) while requiring only one-thousandth as much computer time. Parameters are currently available for hydrogen,[4] for the second-period elements beryllium,[7] boron,[8] carbon,[4] nitrogen,[4] oxygen,[4] and fluorine,[9] for the third-period elements aluminum,[10] silicon,[11] phosphorus,[11] sulfur,[12] and chlorine,[13] and for bromine[14] and iodine.[15] Since MNDO currently uses an s,p basis set without d AOs, calculations are confined to compounds involving only normal group valencies. Schleyer et al.[16] have also reported extensive MNDO calculations for compounds containing lithium, but the parameters for lithium have not yet been published.

Table I. MNDO Parameters for Tin

optimized parameters	value	derived parameters	value
U_{ss}	-40.851802^a	E_{heat}	72.2^b
U_{pp}	-28.560249^a	E_{el}	-92.3241020^a
ζ_s	2.080380^c	D_1	1.5697766^d
ζ_p	1.937106^c	D_2	1.3262292^d
β_s	-3.235147^a	AM	0.3601617^d
β_p	-4.290416^a	AD	0.3219998^d
A_{1p}	1.800814^e	AQ	0.3713827^d
G_{ss}	9.800000^a		
G_{pp}	7.300000^a		
G_{sp}	8.300000^a		
G_{p2}	6.500000^a		
H_{sp}	1.300000^a		

[a] In eV. [b] In kcal/mol at 298 K (heat of atomization). [c] Atomic units (Bohrs). [d] In atomic units. [e] In Å^{-1}.

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(1) Part 68 of the series Ground States of Molecules. For Part 67 see: Dewar, M. J. S.; Healy, E. F.; Stewart, J. J. P. *J. Comput. Chem.* **1984**, *4*, 358.

(2) On sabbatical leave from St. Michael's College, Winooski, VT 05404.

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Table II. Calculated Heats of Formation (ΔH_f), First Ionization Energies (I_1), and Dipole Moments (μ) (Asterisks Denote Molecules Used in the Basis Set for Parametrization)

	ΔH_f, kcal/mol		I_1, eV		μ, D	
compd	calcd	obsd	calcd	obsd	calcd	obsd
SnH	49	49a	6.99		2.35	
SnF	−20.44	−9[a]	7.06	7.04[a]	4.64	
SnCl	−5.6	16[a]	7.35		4.55	
SnBr	16.1	24[a]	7.38		4.65	
SnI	36.6	36[a]	7.52		3.80	
SnF_2	−114.6	−116[a]	12.6		6.85	
$SnCl_2$	−82.2	−56.4[a]	11.7	10.1[a]	6.06	
$SnBr_2$	−38.1	−29[a]	11.0		5.60	
SnI_2	5.7	2[a]	10.0		4.65	
SnH_4*	31.9	38.9[b]	12.0	9.2[c]	0.00	
$SnCl_4$*	−100.8	−112[d]	13.3	11.9[e]	0.01	
$SnBr_4$	−30.5	−75[d]	12.2	11.0[f]	0.00	
$SnH_2(CH_3)_2$*	5.8	21[g]	11.2		0.66	0.78[h]
$SnCl_2(CH_3)_2$*	−68.6	−71[i]			5.34	4.41[h]
$SnH(CH_3)_3$*	−4.5	5.2[g]			0.44	0.67[h]
$SnCl(CH_3)_3$*	−44.2	−46.4[j]	11.0	9.88[k]	3.53	3.50[l]
$SnBr(CH_3)_3$*	−23.8	−33.6[m]	10.8	9.60[k]	3.75	3.45[l]
$SnI(CH_3)_3$	−8.6	−19.7[j]	10.4		2.24	3.37[l]
$Sn(CH_3)_3$(*i*-Pr)	−20.5	−11.2[n]	10.4		0.03	
$Sn(CH_3)_3$(*t*-Bu)	−15.8	−16[n]	10.2	8.4[o]	0.01	
$Sn(CH_3)_3Ph$	20.2	25.0[m]	9.3		0.66	0.51[p]
$Sn(CH_3)_3$(CH2Ph)	13.3	21.1[n]	9.0		0.03	
$Sn(CH_3)_3$(CHCH2)	9.2	21.7[n]	9.9		0.50	0.45[q]
$Sn(CH_3)_3NMe_2$*	3.4	−4.3[j]	9.0		2.04	
$Sn(CH_3)_3OH$	−48.2	−75.8[j]	10.3		2.96	
$Sn(CH_3)OC_2H_5$*	−48.6	−63.1[j]	10.2		3.08	
$Sn(CH_3)_4$*	−16.4	−4.6[n]	10.9	8.8[j]	0.00	
$Sn(C_2H_5)_2H_2$	−2.6	10.2[g]	10.8		0.57	
$Sn(C_2H_5)_4$	−31.8	−10.7[n]	10.4		0.10	
$Sn_2(CH_3)_6$	−22.0	−6.4[n]	8.9		0.01	

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Table III. Calculated (Observed) Geometrical Parameters

molecule	bond lengths, Å calcd (obsd)	bond angles, deg calcd (obsd)	ref
SnH_4	SnH 1.586 (1.701)		*a*
$SnCl(CH_3)_3$	SnCl 2.319 (2.354)	ClSnC 105.2	*b*
	SnC 2.066 (2.108)		
$SnCl_2(CH_3)_2$	SnCl 2.307 (2.327)	ClSnCl 106.2	*b*
	SnC 2.076 (2.109)	ClSnC 108.5	
$SnCl_4$	SnCl 2.285 (2.280)		*c*
$SnBr(CH_3)_3$	SnBr 2.42 (2.49)	BrSnC 105.9	*d*
	SnC 2.06 (2.17)		
$SnI(CH_3)_3$	SnI 2.55 (2.72)	ISnC 108.5	*d*
	SnC 2.07		
$SnH(CH_3)_3$	SnH 1.589 (1.705)	HSnC 107.9 (111.5)	*e*
	SnC 2.061 (2.147)	CSnC 111.0 (107.5)	
$SnH_2(CH_3)_2$	SnH 1.587 (1.680)	HSnC 109.2 (108.0)	*b*
	SnC 2.058 (2.150)	CSnC 112.5 (104.8)	
$Sn(CH_3)_4$	SnC 2.064 (2.134)	CSnC 109.28	*f*
$SnBr_4$	SnBr 2.38 (2.44)		*g*
$SnBr_2$	SnBr 2.35 (2.51)	BrSnBr 101.9 (100)	*h*
SnI_2	SnI 2.50 (2.70)	ISnI 104.8 (103)	*h*

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In our continuing program of improving and extending the scope of MNDO, the elements of group 4B were an obvious target. Recent work[17] here has shown that d AOs are not needed to explain the chemical behavior of silicon, suggesting that the standard form of MNDO, without d AOs, should be equally applicable to the other group 4B elements. Apart from their chemical interest, availability of MNDO parameters should provide a good test of a recently developed[18] program for solid-state calculations, using MNDO, given that these elements include an insulator (diamond), two semiconductors (silicon and germanium), and two metals (tin and lead). Most of them also exist in different allotropic forms.

We decided to start with tin, for three reasons: first, because organotin chemistry is not only interesting and varied but is also playing an increasing role in organic synthesis; second, because tin is a metal and MNDO parameters are as yet available for only two metals; and third, as a test of the applicability of the MNDO formalism to elements of later periods. While the results for bromine[14] and iodine[15] were satisfactory, univalent elements cannot exhibit the variety of geometries and types of bonding that polyatomic ones can.

Procedure

Parameters were determined by a least-squares optimization procedure which involved minimizing the sum (Y) of the squares of the weighted errors in the heats of formation, dipole moments, geometries, and ionization potentials for the molecules in the parametrization basis set. The direction of fastest descent was determined by using the first and second derivatives of the parameters with respect to Y. The derivatives involved were calculated analytically, with the exception of the derivatives involving the dipole moments, for which the derivatives were evaluated by finite difference. The resulting method ran between 300 and 2000 times faster than the original nonderivative method.[3]

Results and Discussion

Table I shows the final parameters for tin, in the notation used previously.[3-15] They present no unexpected features.

Table II shows the heats of formation (ΔH_f), first ionization energies (I_1, derived by using Koopmans' theorem), and dipole moments (μ) for 30 tin-containing molecules, including the interesting diatomic molecules of tin. The molecules included in the basis set for parametrization are indicated by asterisks. Experimental values are included for comparison whenever they are available.

The mean absolute error in ΔH_f is 11.4 kcal/mol with a few molecules accounting for a large part of the average error. The results for tin are thus about the same as those[10-13] for compounds of the third-period elements. The values for compounds containing more electronegative atoms are systematically too positive, while those for compounds containing less electronegative atoms are too negative. The largest error is for stannic bromide. It should be noted that measured heats of formation are scarce for tin compounds. Those reported may moreover be subject to considerable experimental error.[19] Here, as elsewhere, the lack of accurate thermochemical data is not only deplorable in itself but is also a serious obstacle to any kind of theoretical calculation, given that the only way to assess the value of *any* current procedure, ab initio

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or semiempirical, is by comparisons with experiment.

The calculated ionization energies are systematically too large. The mean error in I_1 for the 24 molecules in Table II for which there are experimental data is 1.30 eV. A similar error was found in MNDO calculations for compounds of the third-period elements, in particular chlorine,[13] and was attributed to neglect of interactions between the inner electrons and valence electrons in MNDO, due to use of the core approximation. However, attempts to correct the calculated values for tin in the way used successfully for chlorine[13] failed.

As usual, dipole moments are well reproduced. The average absolute error for the eight molecules in Table II for which data are available is only 0.39 D.

Table III compares the calculated geometries with experiment. While bond angles involving tin are reproduced fairly nicely, the errors in bond lengths are greater than those for compounds of third-period elements[10-13] and much greater than for the "organic" elements, C, H, N, and O.[4] While bonds involving tin are generally too short by ca 0.1 Å, this should not be serious because the bonds are so long. Underestimation of the lengths of bonds to tin should not greatly alter the geometry of the rest of the molecule. The most serious errors are found in molecules of the type R_2SnX_2.

The calculated charge distributions usually show tin to have a formal charge of ca 1^+, regardless of the attached ligands.

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Registry No. Tin, 7440-31-5.

Aspects of Organotin Chemistry[1]

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Abstract: MNDO has been applied with success to four topics of current interest in organotin chemistry, leading to satisfactory interpretations of the mechanism for hydrostannylation, the structures of sandwich and half-sandwich cyclopentadienyltin compounds, the possibility of multiple bonding by tin in distannene or dimethylmethylenestannane, and the geometry of the trimethylstannyl radical.

Organotin chemistry has been increasingly studied in recent years, partly because of the growing use of organotin compounds in synthesis and partly because of the current renaissance of non-transition-metal inorganic chemistry. Since MNDO parameters for tin are now available,[1] we decided to study four topics of current interest in the organotin area, partly in the hope of resolving uncertainties and partly to check the ability of MNDO to deal with an element from the fifth period. The topics studied were (a) the mechanism of hydrostannylation; (b) sandwich and half-sandwich cyclopentadienyltin compounds; (c) the ability of tin to form multiple bonds as in distannene or dimethylmethylstannane; and (d) the structure of the trimethyltin radical.

Procedure

The calculations were carried out by using the standard MNDO method and parameters,[3] as implemented in the MOPAC[4] package of computer programs. Geometries were optimized by the derivative procedures included in MOPAC, with no assumptions other than symmetry in cases where symmetry was deliberately enforced. Radicals were calculated by the spin-unrestricted (UHF)[5a] version of MNDO (UMNDO). Transition states were located by the reaction coordinate method[5b] or by a new procedure recently developed here[6] and refined by minimizing the scalar gradient of the energy.[7] All stationary points were characterized by calculating force constants.[7] Options for all these procedures are included in MOPAC.

Applications

A. Hydrostannylation. One of the most important methods for forming tin–carbon bonds is the hydrostannylation of olefins;[8-12]

$$\underset{\mathbf{1},\ R = CH_3}{R_3SnH} \quad + \quad \underset{\mathbf{2},\ R' = H}{R'_2CCR'_2} \rightarrow \underset{\mathbf{3},\ R = CH_3;\ R' = H}{R_3SnCR'_2CR'_2H} \qquad (1)$$

While a polar mechanism may be involved in the case of olefins carrying a strongly electron withdrawing substituent,[13] most of these reactions seem to be radical chain processes involving the following propagation steps;[8-12]

$$\underset{\mathbf{4},\ R = CH_3}{R_3Sn\cdot} \quad + \quad \mathbf{2} \quad \rightleftarrows \quad \underset{\mathbf{5},\ R = CH_3;\ R' = H}{R_3SnCR'_2CR'_2\cdot} \qquad (2)$$

$$\mathbf{5} + \mathbf{1} \rightarrow \mathbf{4} + \mathbf{3} \qquad (3)$$

The first step has been shown[14,15] to be reversible as indicated in

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(1) Part 69 of the series Ground States of Molecules. For Part 68 see: Dewar, M. J. S.; Grady, G. L.; Stewart, J. P. *J. Am. Chem. Soc.*, preceding paper in this issue.

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