OL000346E **Supporting Information**

Supporting Information for Unusually Short Distances Between the Carbonyl Oxygen and the Tin Atom in RCOSMR'3 (M = Ge, Sn, Pb): the Importance of Intramolecular $n_O \rightarrow \sigma^*_{MS}$ Orbital Interactions

Kazuyasu Tani, Shinzi Kato,* Takahiro Kanda, and Satoshi Inagaki*

Department of Chemistry, Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifu 501-1193, Japan

Experimental section

IR spectra were recorded on a Perkin-Elmer FT-IR 1640 spectrophotometer. ^1H, ^{13}C, and ^{119}Sn NMR were recorded on a JEOL JNM-α400 instrument at 400, 100, and 149 MHz, respectively. $CDCl_3$ was employed as a solvent with tetramethylsilane as internal standard for ^1H NMR. $CDCl_3$ was used as an internal standard for ^{13}C NMR. Me_4Sn was used as an external standard for ^{119}Sn NMR. Elemental analyses were performed by the Elemental Analysis Center of Kyoto University. All solvents were dried and distilled prior to use. Ph_3GeCl, Ph_3SnCl, and Ph_3PbCl are of commercial grade were obtained from Aldrich.

S-Triphenylgermanium 4-methylbenzenecarbothioate (**1**)

To a solution of Ph_3GeCl (0.340 g, 1.00 mmol) in ether (15 mL), potassium 4-methylthiobenzoate (0.191 g, 1.00 mmol) was added and the mixture was stirred at 20° C for 1 h. After addition of CH_2Cl_2 (100 mL), the mixture was washed with water (3 x 90 mL), followed by drying over $MgSO_4$. The solvents were removed under reduced pressure (30° C/2.7 kPa). The resulting residue was dissolved into a mixed solvent of CH_2Cl_2 (4 mL) and hexane (3 mL) and allowed to stand in a refrigerator (-20 °C) for 24 h to give **1c** as colorless crystals (0.367 g, 85%); mp 110–112 °C; IR (KBr) 1651 (C=O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H, CH_3), 7.06 (d, J = 8.1 Hz, 2H), 7.25–7.30 (m, 9H), 7.57–7.60 (m, 6H), 7.84 (d, J = 8.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6 (CH_3), 128.5, 128.6, 129.0, 129.8, 134.8, 134.9, 135.7, 144.2, 191.7 (C=O); Anal. Calcd for $C_{26}H_{22}GeOS$: C, 68.62; H, 4.87. Found: C, 68.59; H, 4.87.

S-Triphenyltin 4-methylbenzenecarbothioate (**2**)

Colorless crystals (83%): mp 234–235 °C; IR (KBr) 1621 (C=O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.37 (s, 3H, CH_3), 7.11 (d, J = 7.9 Hz, 2H), 7.35–7.37 (m, 9H), 7.64–7.73 (m, 6H), 7.95 (d, J = 7.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6 (CH_3), 128.8, 129.0, 129.1, 130.0, 135.1, 136.8, 138.1, 144.3, 196.0 (C=O); ^{119}Sn NMR (149 MHz, $CDCl_3$) δ -97.7 ($^1J_{C-Sn}$ = 594 Hz); Anal. Calcd for $C_{26}H_{22}OSSn$: C, 62.31; H, 4.42. Found: C, 62.21; H, 4.39.

S-Triphenyllead 4-methylbenzenecarbothioate (**3**)

Colorless crystals (91%): mp 106–107 °C; IR (KBr) 1618 (C=O) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H, CH_3), 7.12 (d, J = 7.9 Hz, 2H), 7.31 (t, J = 7.5 Hz, 3H), 7.44 (t, J = 7.5 Hz, 6H), 7.76 (d, J = 7.5 Hz, 6H), 7.99 (d, J = 7.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5 (CH_3), 128.8, 129.0, 129.3, 130.0, 136.0, 137.0, 143.6, 154.0 ($^1J_{C-Pb}$ = 545 Hz), 196.4 (C=O); Anal. Calcd for $C_{26}H_{22}OPbS$: C, 52.96; H, 3.76. Found: C, 53.00; H, 3.80.

X-Ray Structural Analysis. The measurements were carried out on a Rigaku AFC7R four-circle diffractometer with graphite-monochromated Mo Kα radiation (λ= 0.71069 Å). A Rigaku XR-TCS-2-050 temperature controller was used for low temperature measurement. All of the structures were solved and refined using the teXsan® crystallographic software package on an IRIS Indigo computer. The crystals were cut from the grown crystals. The crystals were mounted on a glass fiber. The cell dimensions were determined from a least-squares refinement of the setting diffractometer angles for 25 automatically centered reflections. Three standard reflections were measured every 150 reflections and showed no significant intensity variations during the data collection. Lorentz and polarization corrections were applied to the data, and empirical absorption corrections [DIFABS (**2**) and Ψ-scans (**1** and **3**)] were also applied. The structures were solved by direct methods using SHELXS86 and expanded using DIRDIF94. Scattering factors for neutral atoms were from Cromer and Waber, and anomalous dispersion was used. The function minimized was $\Sigma w(|F_{obs}|-|F_{calc}|)^2$, and the weighting scheme employed was $w = [\sigma^2(F_o) + p^2(F_o)^2/4]^{-1}$. A full- matrix least-squares refinement was executed with non-hydrogen atoms being anisotropic. The final least square cycle included fixed hydrogen atoms at calculated positions of which each

isotropic thermal parameter was set to 1.2 times of that of the connecting atom. Positional parameters, anisotropic displacement parameters and bond lengths and angles of **1**, **2**, and **3** are summarized in Tables S1 to S12.

Preparation of single crystals. *S*-Triphenylgermanium 4-methylbenzenecarbothioate **1** (0.100 g) was single-crystallized from dichloromethane (0.6 mL), ether (0.2 mL) and hexane (0.8 mL) at 25 °C for 1 day. *S*-Triphenyltin 4-methylbenzenecarbothioate **2** (0.071 g) was single-crystallized from dichloromethane (0.5 mL), ether (0.2 mL) and hexane (0.5 mL) at 25 °C for 1 day. *S*-Triphenyltlead 4-methylbenzenecarbothioate **3** (0.166 g) was single-crystallized from dichloromethane (1.2 mL) and hexane (2.0 mL) at 25 °C for 1 day.

Crystal data for **1** at 193 K: $C_{26}H_{22}GeOS$, M = 455.11, triclinic, space group $P\ \bar{1}$ (#2), a = 9.372(5) Å, b = 16.024(2) Å, c = 7.873(2) Å, α = 91.27(2)°, β = 112.32(3)°, γ = 94.08(3)°, V = 1089.4(7) Å^3, Z = 2, D_C = 1.387 g cm^{-3}, $\mu(Mo\text{-}K\alpha)$ = 15.15 cm^{-1}, 5327 reflections measured, 5016 unique (R_{int} = 0.029), 3746 reflections observed [I > 2σ(I)], R = 0.034, Rw = 0.038.

Crystal data for **2** at 296 K: $C_{26}H_{22}OSSn$, M = 501.21, triclinic, space group $P\ \bar{1}$ (#2), a = 9.6152(4) Å, b = 16.3582(6) Å, c = 7.7772(4) Å, α = 92.171(4)°, β = 110.186(3)°, γ = 92.483(3)°, V = 1145.22(9) Å^3, Z = 2, D_C = 1.453 g cm^{-3}, $\mu(Mo\text{-}K\alpha)$ = 12.20 cm^{-1}, 5562 reflections measured, 5247 unique (R_{int} = 0.012), 4520 reflections observed [I > 2σ(I)], R = 0.031, Rw = 0.037.

Crystal data for **3** at 193 K: $C_{26}H_{22}OPbS$, M = 589.72, triclinic, space group $P\ \bar{1}$ (#2), a = 9.6581(9) Å, b = 16.102(1) Å, c = 7.7097(5) Å, α = 92.521(7)°, β = 109.511(6)°, γ = 91.951(8)°, V = 1127.5(2) Å^3, Z = 2, D_C = 1.737 g cm^{-3}, $\mu(Mo\text{-}K\alpha)$ = 76.01 cm^{-1}, 5469 reflections measured, 5157 unique (R_{int} = 0.013), 4319 reflections observed [I > 2σ(I)], R = 0.034, Rw = 0.035.

Table S1. Positional parameters and B(eq) for 4-$CH_3C_6H_4COSGePh_3$ **1**

atom	x	y	z	B(eq)
Ge(1)	0.75500(3)	0.71436(2)	0.31275(4)	0.02859(8)
S(11)	0.68412(9)	0.83294(5)	0.40633(10)	0.0387(2)
O(11)	0.9312(2)	0.7985(1)	0.6864(3)	0.0394(6)
C(11)	0.8222(3)	0.8408(2)	0.6387(4)	0.0323(7)
C(12)	0.7923(3)	0.8998(2)	0.7665(4)	0.0327(7)
C(13)	0.8818(3)	0.8984(2)	0.9532(4)	0.0344(8)
C(14)	0.8569(4)	0.9513(2)	1.0771(4)	0.0393(8)
C(15)	0.7465(4)	1.0083(2)	1.0218(4)	0.0420(9)
C(16)	0.6583(4)	1.0100(2)	0.8362(5)	0.0501(10)
C(17)	0.6807(4)	0.9566(2)	0.7103(4)	0.0449(9)
C(18)	0.7255(4)	1.0672(2)	1.1591(5)	0.061(1)
C(21)	0.9429(3)	0.7307(2)	0.2633(4)	0.0303(7)
C(22)	1.0698(3)	0.7844(2)	0.3690(4)	0.0400(8)
C(23)	1.1990(3)	0.7937(2)	0.3216(4)	0.0500(9)
C(24)	1.2033(3)	0.7499(2)	0.1731(4)	0.0480(10)
C(25)	1.0775(4)	0.6957(2)	0.0672(4)	0.0465(10)
C(26)	0.9484(3)	0.6863(2)	0.1129(4)	0.0375(8)
C(31)	0.5805(3)	0.6888(2)	0.0812(4)	0.0308(7)
C(32)	0.5513(3)	0.7450(2)	-0.0577(4)	0.0403(8)
C(33)	0.4279(4)	0.7296(2)	-0.2234(4)	0.0510(10)
C(34)	0.3315(4)	0.6571(2)	-0.2538(4)	0.0521(10)
C(35)	0.3582(4)	0.6008(2)	-0.1195(5)	0.0501(10)
C(36)	0.4823(3)	0.6163(2)	0.0475(4)	0.0392(8)
C(41)	0.7628(3)	0.6307(2)	0.4888(4)	0.0312(7)
C(42)	0.8867(4)	0.5825(2)	0.5548(5)	0.0453(9)
C(43)	0.8904(4)	0.5220(2)	0.6802(5)	0.053(1)
C(44)	0.7723(4)	0.5095(2)	0.7386(4)	0.0469(9)
C(45)	0.6490(4)	0.5575(2)	0.6760(5)	0.052(1)
C(46)	0.6439(4)	0.6175(2)	0.5510(4)	0.0442(9)
H(11)	0.9572	0.8613	0.9910	0.0262
H(12)	0.9172	0.9474	1.1995	0.0235
H(13)	0.5765	1.0489	0.7865	0.0600
H(14)	0.6175	0.9533	0.5886	0.0404
H(15)	0.7880	1.1209	1.1790	0.0911
H(16)	0.7634	1.0465	1.2843	0.0788
H(17)	0.6267	1.0847	1.1134	0.0851
H(21)	1.0698	0.8165	0.4706	0.0490
H(22)	1.2796	0.8314	0.3946	0.0610
H(23)	1.2960	0.7548	0.1448	0.0632
H(24)	1.0767	0.6623	-0.0431	0.0499
H(25)	0.8623	0.6505	0.0379	0.0365
H(31)	0.6152	0.7913	-0.0307	0.0379
H(32)	0.4051	0.7696	-0.3169	0.0673
H(33)	0.2506	0.6476	-0.3663	0.0567
H(34)	0.2934	0.5501	-0.1424	0.0456
H(35)	0.5002	0.5788	0.1362	0.0240
H(41)	0.9710	0.5892	0.5169	0.0663
H(42)	0.9741	0.4888	0.7173	0.0530
H(43)	0.7731	0.4696	0.8202	0.0534
H(44)	0.5579	0.5477	0.7089	0.0777
H(45)	0.5530	0.6477	0.5025	0.0526

Table S2. Anisotropic Displacement Parameters for 4-$CH_3C_6H_4COSGePh_3$ **1**

atom	U11	U22	U33	U12	U13	U23
Ge(1)	0.0267(2)	0.0314(2)	0.0266(2)	0.0018(1)	0.0091(1)	0.0037(1)
S(11)	0.0420(4)	0.0381(4)	0.0304(4)	0.0110(3)	0.0064(3)	0.0023(3)
O(11)	0.038(1)	0.046(1)	0.034(1)	0.0118(10)	0.0112(9)	0.0032(9)
C(11)	0.034(1)	0.032(1)	0.031(1)	0.000(1)	0.013(1)	0.004(1)
C(12)	0.032(1)	0.029(1)	0.037(1)	0.000(1)	0.013(1)	0.003(1)

C(13)	0.035(1)	0.033(2)	0.035(1)	0.001(1)	0.013(1)	0.006(1)
C(14)	0.045(2)	0.040(2)	0.031(1)	-0.005(1)	0.015(1)	-0.001(1)
C(15)	0.043(2)	0.035(2)	0.052(2)	-0.008(1)	0.025(2)	-0.009(1)
C(16)	0.047(2)	0.045(2)	0.053(2)	0.014(2)	0.013(2)	-0.002(2)
C(17)	0.044(2)	0.045(2)	0.039(2)	0.012(1)	0.007(1)	0.000(1)
C(18)	0.066(2)	0.056(2)	0.066(2)	-0.001(2)	0.033(2)	-0.020(2)
C(21)	0.028(1)	0.034(1)	0.029(1)	0.007(1)	0.010(1)	0.012(1)
C(22)	0.036(2)	0.056(2)	0.026(1)	-0.003(1)	0.010(1)	0.007(1)
C(23)	0.030(2)	0.075(2)	0.039(2)	-0.005(2)	0.007(1)	0.018(2)
C(24)	0.032(2)	0.071(2)	0.049(2)	0.013(2)	0.022(1)	0.026(2)
C(25)	0.051(2)	0.055(2)	0.046(2)	0.022(2)	0.028(2)	0.016(2)
C(26)	0.038(2)	0.034(2)	0.042(2)	0.006(1)	0.016(1)	0.006(1)
C(31)	0.024(1)	0.038(2)	0.029(1)	0.003(1)	0.010(1)	0.000(1)
C(32)	0.040(2)	0.037(2)	0.036(2)	-0.001(1)	0.006(1)	0.003(1)
C(33)	0.053(2)	0.053(2)	0.035(2)	0.009(2)	0.003(2)	0.005(1)
C(34)	0.033(2)	0.070(2)	0.040(2)	0.008(2)	-0.001(1)	-0.010(2)
C(35)	0.036(2)	0.054(2)	0.054(2)	-0.013(2)	0.015(2)	-0.014(2)
C(36)	0.039(2)	0.041(2)	0.039(2)	-0.002(1)	0.018(1)	0.000(1)
C(41)	0.033(1)	0.031(1)	0.029(1)	0.001(1)	0.012(1)	0.002(1)
C(42)	0.038(2)	0.049(2)	0.054(2)	0.008(1)	0.022(2)	0.016(2)
C(43)	0.052(2)	0.050(2)	0.058(2)	0.017(2)	0.018(2)	0.022(2)
C(44)	0.064(2)	0.039(2)	0.042(2)	0.005(2)	0.025(2)	0.013(1)
C(45)	0.061(2)	0.052(2)	0.059(2)	0.007(2)	0.040(2)	0.014(2)
C(46)	0.043(2)	0.051(2)	0.046(2)	0.011(1)	0.025(1)	0.013(1)

Table S3. Bond Lengths for 4-$CH_3C_6H_4COSGePh_3$ **1**

atom	atom	distance	atom	atom	distance
Ge(1)	S(11)	2.2547(8)	C(24)	C(25)	1.383(5)
Ge(1)	O(11)	3.003(2)	C(24)	H(23)	0.974
Ge(1)	C(21)	1.944(3)	C(25)	C(26)	1.386(4)
Ge(1)	C(31)	1.942(3)	C(25)	H(24)	1.008
Ge(1)	C(41)	1.934(3)	C(26)	H(25)	0.941
S(11)	C(11)	1.790(3)	C(31)	C(32)	1.390(4)
O(11)	C(11)	1.209(3)	C(31)	C(36)	1.385(4)
C(11)	C(12)	1.481(4)	C(32)	C(33)	1.378(4)
C(12)	C(13)	1.390(4)	C(32)	H(31)	0.888
C(12)	C(17)	1.385(4)	C(33)	C(34)	1.377(5)
C(13)	C(14)	1.375(4)	C(33)	H(32)	0.960
C(13)	H(11)	0.922	C(34)	C(35)	1.367(5)
C(14)	C(15)	1.380(4)	C(34)	H(33)	0.922
C(14)	H(12)	0.920	C(35)	C(36)	1.387(4)
C(15)	C(16)	1.380(4)	C(35)	H(34)	0.950
C(15)	C(18)	1.496(4)	C(36)	H(35)	0.906
C(16)	C(17)	1.380(4)	C(41)	C(42)	1.379(4)
C(16)	H(13)	0.990	C(41)	C(46)	1.383(4)
C(17)	H(14)	0.913	C(42)	C(43)	1.392(4)
C(18)	H(15)	0.980	C(42)	H(41)	0.945
C(18)	H(16)	0.986	C(43)	C(44)	1.355(5)
C(18)	H(17)	0.924	C(43)	H(42)	0.936
C(21)	C(22)	1.385(4)	C(44)	C(45)	1.371(5)
C(21)	C(26)	1.388(4)	C(44)	H(43)	0.915
C(22)	C(23)	1.395(4)	C(45)	C(46)	1.382(4)
C(22)	H(21)	0.941	C(45)	H(44)	0.985
C(23)	C(24)	1.366(5)	C(46)	H(45)	0.961
C(23)	H(22)	0.925			

Table S4. Bond Angles for 4-$CH_3C_6H_4COSGePh_3$ **1**

atom	atom	atom	angle	atom	atom	atom	angle
S(11)	Ge(1)	O(11)	7.80(4)	C(24)	C(23)	H(22)	22.4
S(11)	Ge(1)	C(21)	13.71(9)	C(23)	C(24)	C(25)	19.6(3)
S(11)	Ge(1)	C(31)	9.89(9)	C(23)	C(24)	H(23)	20.3
S(11)	Ge(1)	C(41)	08.11(8)	C(25)	C(24)	H(23)	20.1
O(11)	Ge(1)	C(21)	8.16(9)	C(24)	C(25)	C(26)	19.8(3)
O(11)	Ge(1)	C(31)	56.76(9)	C(24)	C(25)	H(24)	21.8
O(11)	Ge(1)	C(41)	3.65(9)	C(26)	C(25)	H(24)	18.4
C(21)	Ge(1)	C(31)	08.7(1)	C(21)	C(26)	C(25)	21.0(3)
C(21)	Ge(1)	C(41)	14.0(1)	C(21)	C(26)	H(25)	19.9
C(31)	Ge(1)	C(41)	11.6(1)	C(25)	C(26)	H(25)	19.1
Ge(1)	S(11)	C(11)	8.25(10)	Ge(1)	C(31)	C(32)	19.4(2)
Ge(1)	O(11)	C(11)	1.8(2)	Ge(1)	C(31)	C(36)	22.7(2)
S(11)	C(11)	O(11)	20.8(2)	C(32)	C(31)	C(36)	17.9(3)
S(11)	C(11)	C(12)	16.2(2)	C(31)	C(32)	C(33)	21.3(3)
O(11)	C(11)	C(12)	23.0(2)	C(31)	C(32)	H(31)	15.6
C(11)	C(12)	C(13)	18.1(2)	C(33)	C(32)	H(31)	23.1
C(11)	C(12)	C(17)	23.7(3)	C(32)	C(33)	C(34)	19.9(3)
C(13)	C(12)	C(17)	18.2(3)	C(32)	C(33)	H(32)	21.1
C(12)	C(13)	C(14)	20.2(3)	C(34)	C(33)	H(32)	19.0
C(12)	C(13)	H(11)	18.5	C(33)	C(34)	C(35)	19.9(3)
C(14)	C(13)	H(11)	21.3	C(33)	C(34)	H(33)	18.4
C(13)	C(14)	C(15)	21.9(3)	C(35)	C(34)	H(33)	21.6
C(13)	C(14)	H(12)	17.3	C(34)	C(35)	C(36)	20.3(3)
C(15)	C(14)	H(12)	20.8	C(34)	C(35)	H(34)	19.6
C(14)	C(15)	C(16)	17.9(3)	C(36)	C(35)	H(34)	20.1
C(14)	C(15)	C(18)	20.8(3)	C(31)	C(36)	C(35)	20.8(3)
C(16)	C(15)	C(18)	21.4(3)	C(31)	C(36)	H(35)	19.0
C(15)	C(16)	C(17)	20.9(3)	C(35)	C(36)	H(35)	20.2
C(15)	C(16)	H(13)	22.4	Ge(1)	C(41)	C(42)	20.9(2)
C(17)	C(16)	H(13)	16.6	Ge(1)	C(41)	C(46)	20.8(2)
C(12)	C(17)	C(16)	20.9(3)	C(42)	C(41)	C(46)	18.3(3)
C(12)	C(17)	H(14)	16.7	C(41)	C(42)	C(43)	20.3(3)
C(16)	C(17)	H(14)	22.1	C(41)	C(42)	H(41)	21.6
C(15)	C(18)	H(15)	13.5	C(43)	C(42)	H(41)	18.0
C(15)	C(18)	H(16)	12.7	C(42)	C(43)	C(44)	20.5(3)
C(15)	C(18)	H(17)	10.3	C(42)	C(43)	H(42)	17.7
H(15)	C(18)	H(16)	01.2	C(44)	C(43)	H(42)	21.7
H(15)	C(18)	H(17)	00.8	C(43)	C(44)	C(45)	19.9(3)
H(16)	C(18)	H(17)	17.4	C(43)	C(44)	H(43)	21.3
Ge(1)	C(21)	C(22)	23.5(2)	C(45)	C(44)	H(43)	18.8
Ge(1)	C(21)	C(26)	17.7(2)	C(44)	C(45)	C(46)	20.0(3)
C(22)	C(21)	C(26)	18.8(3)	C(44)	C(45)	H(44)	22.3
C(21)	C(22)	C(23)	19.8(3)	C(46)	C(45)	H(44)	17.5
C(21)	C(22)	H(21)	21.4	C(41)	C(46)	C(45)	20.8(3)
C(23)	C(22)	H(21)	18.8	C(41)	C(46)	H(45)	20.5
C(22)	C(23)	C(24)	21.0(3)	C(45)	C(46)	H(45)	18.6
C(22)	C(23)	H(22)	16.6				

Table S5. Positional parameters and B(eq) for 4-$CH_3C_6H_4COSSnPh_3$ **2**

atom	x	y	z	B(eq)
Sn(1)	0.75709(2)	0.21520(1)	0.31156(3)	0.05308(7)
S(11)	0.6584(1)	0.33639(6)	0.4108(1)	0.0711(3)
O(11)	0.9093(2)	0.3058(2)	0.6599(3)	0.0701(7)
C(11)	0.8020(3)	0.3462(2)	0.6289(4)	0.0564(9)
C(12)	0.7811(3)	0.4040(2)	0.7694(4)	0.0560(9)
C(13)	0.8787(4)	0.4027(2)	0.9487(4)	0.0613(9)
C(14)	0.8617(4)	0.4546(2)	1.0841(5)	0.071(1)
C(15)	0.7514(4)	0.5086(2)	1.0453(6)	0.077(1)
C(16)	0.6556(5)	0.5102(2)	0.8667(6)	0.089(1)

C(17)	0.6685(4)	0.4586(2)	0.7297(5)	0.078(1)
C(18)	0.7387(6)	0.5678(3)	1.1941(7)	0.112(2)
C(21)	0.9554(3)	0.2363(2)	0.2515(4)	0.0537(8)
C(22)	1.0757(4)	0.2868(2)	0.3602(4)	0.069(1)
C(23)	1.2007(4)	0.2986(3)	0.3103(5)	0.083(1)
C(24)	1.2073(4)	0.2585(3)	0.1544(6)	0.083(1)
C(25)	1.0898(4)	0.2084(3)	0.0465(5)	0.079(1)
C(26)	0.9641(4)	0.1973(2)	0.0943(5)	0.067(1)
C(31)	0.5774(3)	0.1860(2)	0.0592(4)	0.0557(8)
C(32)	0.5491(4)	0.2405(2)	-0.0795(5)	0.074(1)
C(33)	0.4315(5)	0.2254(3)	-0.2432(5)	0.089(1)
C(34)	0.3414(4)	0.1558(3)	-0.2711(6)	0.090(1)
C(35)	0.3681(4)	0.1015(3)	-0.1354(6)	0.089(1)
C(36)	0.4843(4)	0.1168(2)	0.0301(5)	0.071(1)
C(41)	0.7729(3)	0.1235(2)	0.5024(4)	0.0534(8)
C(42)	0.9022(4)	0.0833(3)	0.5755(6)	0.082(1)
C(43)	0.9121(5)	0.0227(3)	0.6981(6)	0.094(2)
C(44)	0.7958(5)	0.0018(2)	0.7505(5)	0.083(1)
C(45)	0.6687(5)	0.0419(3)	0.6825(7)	0.100(2)
C(46)	0.6555(4)	0.1022(3)	0.5583(5)	0.079(1)
H(11)	0.9633	0.3674	0.9840	0.0973
H(12)	0.9315	0.4459	1.2006	0.0973
H(13)	0.5739	0.5510	0.8341	0.0973
H(14)	0.5831	0.4626	0.5925	0.0973
H(15)	0.7604	0.5407	1.3058	0.0973
H(16)	0.8075	0.6135	1.2118	0.1261
H(17)	0.6409	0.5859	1.1586	0.1261
H(21)	1.0603	0.3204	0.4655	0.0973
H(22)	1.2942	0.3422	0.4025	0.0973
H(23)	1.3031	0.2639	0.1061	0.0973
H(24)	1.0930	0.1775	-0.0747	0.0973
H(25)	0.8667	0.1586	0.0095	0.0973
H(31)	0.6069	0.2976	-0.0723	0.0973
H(32)	0.4238	0.2673	-0.3447	0.0973
H(33)	0.2489	0.1595	-0.3987	0.0973
H(34)	0.2992	0.0571	-0.1718	0.0253
H(35)	0.5044	0.0779	0.1254	0.1191
H(41)	0.9928	0.1144	0.5386	0.0973
H(42)	1.0038	-0.0041	0.7478	0.1102
H(43)	0.7949	-0.0560	0.8359	0.0973
H(44)	0.5867	0.0281	0.7201	0.1163
H(45)	0.5553	0.1360	0.5060	0.0973

Table S6. Anisotropic Displacement Parameters for 4-$CH_3C_6H_4COSSnPh_3$ **2**

atom	U11	U22	U33	U12	U13	U23
Sn(1)	0.0522(1)	0.0544(1)	0.0526(1)	0.00243(8)	0.01838(9)	0.00361(9)
S(11)	0.0753(5)	0.0676(6)	0.0623(5)	0.0198(4)	0.0124(4)	-0.0001(4)
O(11)	0.065(1)	0.077(2)	0.068(1)	0.021(1)	0.022(1)	-0.002(1)
C(11)	0.065(2)	0.049(2)	0.057(2)	0.003(1)	0.024(1)	0.005(1)
C(12)	0.064(2)	0.044(2)	0.064(2)	0.001(1)	0.027(1)	0.001(1)
C(13)	0.068(2)	0.053(2)	0.064(2)	0.002(1)	0.024(2)	0.002(1)
C(14)	0.086(2)	0.059(2)	0.066(2)	-0.006(2)	0.026(2)	-0.006(2)
C(15)	0.089(3)	0.055(2)	0.097(3)	-0.007(2)	0.046(2)	-0.016(2)
C(16)	0.098(3)	0.064(2)	0.103(3)	0.031(2)	0.031(2)	-0.008(2)
C(17)	0.088(3)	0.065(2)	0.076(2)	0.025(2)	0.020(2)	0.000(2)
C(18)	0.129(4)	0.091(3)	0.125(4)	-0.004(3)	0.063(3)	-0.044(3)
C(21)	0.052(2)	0.055(2)	0.054(2)	0.007(1)	0.018(1)	0.011(1)
C(22)	0.059(2)	0.091(3)	0.054(2)	-0.003(2)	0.018(1)	0.005(2)
C(23)	0.054(2)	0.116(3)	0.072(2)	-0.010(2)	0.014(2)	0.017(2)
C(24)	0.065(2)	0.112(3)	0.087(3)	0.022(2)	0.040(2)	0.029(2)
C(25)	0.084(3)	0.082(3)	0.084(2)	0.026(2)	0.045(2)	0.007(2)
C(26)	0.070(2)	0.061(2)	0.073(2)	0.009(2)	0.031(2)	0.001(2)
C(31)	0.051(2)	0.061(2)	0.055(2)	0.004(1)	0.019(1)	-0.001(1)

C(32)	0.077(2)	0.072(2)	0.066(2)	0.000(2)	0.015(2)	0.007(2)
C(33)	0.088(3)	0.100(3)	0.066(2)	0.016(2)	0.009(2)	0.009(2)
C(34)	0.065(2)	0.115(4)	0.076(3)	0.013(2)	0.007(2)	-0.020(2)
C(35)	0.063(2)	0.091(3)	0.107(3)	-0.020(2)	0.028(2)	-0.033(3)
C(36)	0.066(2)	0.070(2)	0.077(2)	-0.008(2)	0.029(2)	-0.006(2)
C(41)	0.059(2)	0.049(2)	0.055(2)	0.002(1)	0.024(1)	-0.001(1)
C(42)	0.064(2)	0.089(3)	0.096(3)	0.011(2)	0.031(2)	0.026(2)
C(43)	0.090(3)	0.092(3)	0.102(3)	0.034(2)	0.030(2)	0.034(3)
C(44)	0.123(3)	0.061(2)	0.072(2)	0.008(2)	0.041(2)	0.014(2)
C(45)	0.115(3)	0.103(3)	0.108(3)	0.008(3)	0.071(3)	0.033(3)
C(46)	0.076(2)	0.089(3)	0.090(3)	0.021(2)	0.046(2)	0.025(2)

Table S7. Bond Lengths for 4-$CH_3C_6H_4COSSnPh_3$ **2**

atom	atom	distance	atom	atom	distance
Sn(1)	S(11)	2.4453(9)	C(24)	C(25)	1.366(6)
Sn(1)	O(11)	2.907(2)	C(24)	H(23)	1.109
Sn(1)	C(21)	2.131(3)	C(25)	C(26)	1.388(5)
Sn(1)	C(31)	2.141(3)	C(25)	H(24)	1.064
Sn(1)	C(41)	2.123(3)	C(26)	H(25)	1.097
S(11)	C(11)	1.775(3)	C(31)	C(32)	1.387(4)
O(11)	C(11)	1.208(4)	C(31)	C(36)	1.375(4)
C(11)	C(12)	1.490(4)	C(32)	C(33)	1.385(5)
C(12)	C(13)	1.388(4)	C(32)	H(31)	1.056
C(12)	C(17)	1.391(4)	C(33)	C(34)	1.364(6)
C(13)	C(14)	1.385(5)	C(33)	H(32)	1.050
C(13)	H(11)	0.986	C(34)	C(35)	1.368(6)
C(14)	C(15)	1.370(5)	C(34)	H(33)	1.086
C(14)	H(12)	0.943	C(35)	C(36)	1.388(5)
C(15)	C(16)	1.379(6)	C(35)	H(34)	0.928
C(15)	C(18)	1.521(5)	C(36)	H(35)	0.969
C(16)	C(17)	1.377(5)	C(41)	C(42)	1.383(4)
C(16)	H(13)	1.023	C(41)	C(46)	1.379(4)
C(17)	H(14)	1.106	C(42)	C(43)	1.385(5)
C(18)	H(15)	0.952	C(42)	H(41)	1.116
C(18)	H(16)	0.950	C(43)	C(44)	1.350(6)
C(18)	H(17)	0.949	C(43)	H(42)	0.965
C(21)	C(22)	1.388(4)	C(44)	C(45)	1.361(6)
C(21)	C(26)	1.387(4)	C(44)	H(43)	1.178
C(22)	C(23)	1.393(5)	C(45)	C(46)	1.387(5)
C(22)	H(21)	1.025	C(45)	H(44)	0.952
C(23)	C(24)	1.379(6)	C(46)	H(45)	1.091
C(23)	H(22)	1.137			

Table S8. Bond Angles for 4-$CH_3C_6H_4COSSnPh_3$ **2**

atom	atom	atom	angle	atom	atom	atom	angle
S(11)	Sn(1)	O(11)	57.43(5)	C(24)	C(23)	H(22)	122.6
S(11)	Sn(1)	C(21)	115.86(9)	C(23)	C(24)	C(25)	119.9(3)
S(11)	Sn(1)	C(31)	97.84(8)	C(23)	C(24)	H(23)	124.6
S(11)	Sn(1)	C(41)	108.75(8)	C(25)	C(24)	H(23)	115.4
O(11)	Sn(1)	C(21)	86.90(9)	C(24)	C(25)	C(26)	120.1(3)
O(11)	Sn(1)	C(31)	155.16(9)	C(24)	C(25)	H(24)	120.7
O(11)	Sn(1)	C(41)	77.97(9)	C(26)	C(25)	H(24)	119.1
C(21)	Sn(1)	C(31)	108.5(1)	C(21)	C(26)	C(25)	121.0(3)
C(21)	Sn(1)	C(41)	113.4(1)	C(21)	C(26)	H(25)	116.9
C(31)	Sn(1)	C(41)	111.5(1)	C(25)	C(26)	H(25)	122.1
Sn(1)	S(11)	C(11)	93.5(1)	Sn(1)	C(31)	C(32)	119.1(2)
Sn(1)	O(11)	C(11)	87.9(2)	Sn(1)	C(31)	C(36)	122.9(2)
S(11)	C(11)	O(11)	120.3(2)	C(32)	C(31)	C(36)	118.0(3)
S(11)	C(11)	C(12)	117.0(2)	C(31)	C(32)	C(33)	121.2(4)

O(11)	C(11)	C(12)	122.7(3)	C(31)	C(32)	H(31)	125.9
C(11)	C(12)	C(13)	118.0(3)	C(33)	C(32)	H(31)	112.8
C(11)	C(12)	C(17)	123.3(3)	C(32)	C(33)	C(34)	120.2(4)
C(13)	C(12)	C(17)	118.7(3)	C(32)	C(33)	H(32)	116.0
C(12)	C(13)	C(14)	119.8(3)	C(34)	C(33)	H(32)	123.6
C(12)	C(13)	H(11)	122.4	C(33)	C(34)	C(35)	119.2(4)
C(14)	C(13)	H(11)	117.7	C(33)	C(34)	H(33)	108.5
C(13)	C(14)	C(15)	121.6(3)	C(35)	C(34)	H(33)	131.7
C(13)	C(14)	H(12)	111.6	C(34)	C(35)	C(36)	120.9(4)
C(15)	C(14)	H(12)	126.8	C(34)	C(35)	H(34)	110.5
C(14)	C(15)	C(16)	118.4(3)	C(36)	C(35)	H(34)	128.5
C(14)	C(15)	C(18)	120.8(4)	C(31)	C(36)	C(35)	120.5(4)
C(16)	C(15)	C(18)	120.8(4)	C(31)	C(36)	H(35)	118.5
C(15)	C(16)	C(17)	121.3(3)	C(35)	C(36)	H(35)	121.0
C(15)	C(16)	H(13)	119.7	Sn(1)	C(41)	C(42)	120.9(2)
C(17)	C(16)	H(13)	119.0	Sn(1)	C(41)	C(46)	121.4(2)
C(12)	C(17)	C(16)	120.1(3)	C(42)	C(41)	C(46)	117.7(3)
C(12)	C(17)	H(14)	124.1	C(41)	C(42)	C(43)	121.0(3)
C(16)	C(17)	H(14)	115.8	C(41)	C(42)	H(41)	109.5
C(15)	C(18)	H(15)	109.4	C(43)	C(42)	H(41)	128.7
C(15)	C(18)	H(16)	109.6	C(42)	C(43)	C(44)	120.7(4)
C(15)	C(18)	H(17)	109.6	C(42)	C(43)	H(42)	119.3
H(15)	C(18)	H(16)	109.3	C(44)	C(43)	H(42)	120.0
H(15)	C(18)	H(17)	109.4	C(43)	C(44)	C(45)	119.0(3)
H(16)	C(18)	H(17)	109.6	C(43)	C(44)	H(43)	121.8
Sn(1)	C(21)	C(22)	123.7(2)	C(45)	C(44)	H(43)	118.6
Sn(1)	C(21)	C(26)	117.9(2)	C(44)	C(45)	C(46)	121.3(4)
C(22)	C(21)	C(26)	118.3(3)	C(44)	C(45)	H(44)	119.6
C(21)	C(22)	C(23)	120.4(3)	C(46)	C(45)	H(44)	119.1
C(21)	C(22)	H(21)	116.2	C(41)	C(46)	C(45)	120.2(4)
C(23)	C(22)	H(21)	122.9	C(41)	C(46)	H(45)	117.9
C(22)	C(23)	C(24)	120.2(4)	C(45)	C(46)	H(45)	121.9
C(22)	C(23)	H(22)	117.2				

Table S9. Positional parameters and B(eq) for 4-$CH_3C_6H_4COSPbPh_3$ **3**

atom	x	y	z	B(eq)
Pb(1)	0.25976(2)	0.21148(1)	-0.20086(3)	0.04467(7)
S(11)	0.1574(2)	0.3383(1)	-0.0887(2)	0.0580(5)
O(11)	0.4114(4)	0.3093(3)	0.1553(5)	0.056(1)
C(11)	0.3015(7)	0.3494(4)	0.1264(8)	0.049(2)
C(12)	0.2806(6)	0.4060(3)	0.2719(8)	0.046(2)
C(13)	0.3793(6)	0.4061(4)	0.4486(8)	0.050(2)
C(14)	0.3632(7)	0.4561(4)	0.5890(8)	0.056(2)
C(15)	0.2486(8)	0.5098(4)	0.5562(10)	0.063(2)
C(16)	0.1490(8)	0.5106(4)	0.376(1)	0.069(2)
C(17)	0.1644(8)	0.4586(4)	0.2370(9)	0.061(2)
C(18)	0.2387(9)	0.5676(5)	0.710(1)	0.084(3)
C(21)	0.4643(6)	0.2362(3)	-0.2616(7)	0.045(2)
C(22)	0.5791(7)	0.2876(4)	-0.1513(8)	0.055(2)
C(23)	0.7023(7)	0.3005(5)	-0.2010(9)	0.065(2)
C(24)	0.7115(7)	0.2631(5)	-0.3600(10)	0.064(2)
C(25)	0.5973(8)	0.2131(4)	-0.4717(9)	0.060(2)
C(26)	0.4718(7)	0.1993(4)	-0.4237(8)	0.054(2)
C(31)	0.0734(6)	0.1845(4)	-0.4605(7)	0.044(2)
C(32)	0.0492(7)	0.2398(4)	-0.6001(8)	0.055(2)
C(33)	-0.0658(8)	0.2253(5)	-0.7628(9)	0.066(2)
C(34)	-0.1594(7)	0.1545(5)	-0.7892(10)	0.070(2)
C(35)	-0.1371(7)	0.0999(4)	-0.652(1)	0.065(2)
C(36)	-0.0205(7)	0.1139(4)	-0.4854(9)	0.055(2)
C(41)	0.2760(6)	0.1175(3)	0.0032(7)	0.044(2)
C(42)	0.4057(7)	0.0795(4)	0.0826(9)	0.058(2)
C(43)	0.4139(8)	0.0194(5)	0.2079(10)	0.071(2)
C(44)	0.2942(8)	-0.0021(4)	0.2556(9)	0.063(2)

C(45)	0.1692(8)	0.0380(5)	0.1838(10)	0.070(2)
C(46)	0.1566(7)	0.0971(4)	0.0541(9)	0.060(2)
H(11)	0.4625	0.3692	0.4745	0.0581
H(12)	0.4331	0.4546	0.7150	0.0643
H(13)	0.0682	0.5492	0.3498	0.0788
H(14)	0.0944	0.4611	0.1075	0.0834
H(15)	0.3015	0.6169	0.7263	0.0923
H(16)	0.1398	0.5849	0.6862	0.0923
H(17)	0.2672	0.5414	0.8261	0.0923
H(21)	0.5716	0.3159	-0.0379	0.0636
H(22)	0.7912	0.3354	-0.1239	0.0834
H(23)	0.8192	0.2826	-0.3803	0.0834
H(24)	0.6038	0.1854	-0.5843	0.0699
H(25)	0.3930	0.1574	-0.5116	0.0834
H(31)	0.1166	0.2893	-0.5807	0.0637
H(32)	-0.0772	0.2637	-0.8849	0.0834
H(33)	-0.2407	0.1445	-0.9062	0.0792
H(34)	-0.2211	0.0550	-0.6649	0.0834
H(35)	-0.0043	0.0764	-0.3867	0.0641
H(41)	0.4996	0.0967	0.0450	0.0834
H(42)	0.5059	-0.0091	0.2625	0.0798
H(43)	0.3014	-0.0512	0.3425	0.0834
H(44)	0.0847	0.0232	0.2223	0.0783
H(45)	0.0644	0.1264	0.0019	0.0681

Table S10. Anisotropic Displacement Parameters for 4-$CH_3C_6H_4COSPbPh_3$ **3**

atom	U11	U22	U33	U12	U13	U23
Pb(1)	0.0447(1)	0.0474(1)	0.0417(1)	0.00090(9)	0.01405(9)	0.00625(8)
S(11)	0.0596(10)	0.0584(10)	0.0491(8)	0.0141(8)	0.0081(7)	0.0031(7)
O(11)	0.051(2)	0.067(3)	0.050(2)	0.012(2)	0.016(2)	0.000(2)
C(11)	0.052(3)	0.049(3)	0.048(3)	0.000(3)	0.020(3)	0.009(3)
C(12)	0.052(3)	0.038(3)	0.048(3)	-0.003(3)	0.018(3)	0.002(2)
C(13)	0.052(3)	0.043(3)	0.052(3)	0.001(3)	0.015(3)	0.005(3)
C(14)	0.065(4)	0.051(4)	0.049(3)	-0.008(3)	0.018(3)	-0.003(3)
C(15)	0.077(5)	0.044(3)	0.072(4)	-0.003(3)	0.033(4)	-0.007(3)
C(16)	0.077(5)	0.051(4)	0.077(5)	0.016(3)	0.024(4)	-0.004(3)
C(17)	0.070(4)	0.052(4)	0.055(4)	0.008(3)	0.014(3)	0.001(3)
C(18)	0.097(6)	0.069(5)	0.086(5)	-0.001(4)	0.037(5)	-0.026(4)
C(21)	0.045(3)	0.048(3)	0.041(3)	0.003(3)	0.014(2)	0.005(2)
C(22)	0.050(3)	0.072(4)	0.040(3)	-0.005(3)	0.010(3)	0.005(3)
C(23)	0.044(3)	0.092(5)	0.053(4)	-0.007(3)	0.005(3)	0.016(4)
C(24)	0.052(4)	0.082(5)	0.064(4)	0.015(3)	0.023(3)	0.025(4)
C(25)	0.069(4)	0.062(4)	0.059(4)	0.018(3)	0.031(3)	0.007(3)
C(26)	0.053(4)	0.055(4)	0.053(4)	0.005(3)	0.017(3)	0.000(3)
C(31)	0.039(3)	0.051(3)	0.040(3)	0.001(2)	0.011(2)	-0.002(2)
C(32)	0.058(4)	0.051(4)	0.053(4)	-0.003(3)	0.014(3)	0.007(3)
C(33)	0.062(4)	0.074(5)	0.050(4)	0.012(4)	0.004(3)	0.006(3)
C(34)	0.049(4)	0.093(6)	0.058(4)	0.008(4)	0.006(3)	-0.015(4)
C(35)	0.046(4)	0.071(5)	0.076(5)	-0.013(3)	0.022(3)	-0.019(4)
C(36)	0.055(4)	0.051(4)	0.065(4)	0.001(3)	0.028(3)	0.005(3)
C(41)	0.048(3)	0.045(3)	0.042(3)	0.005(3)	0.019(3)	0.004(2)
C(42)	0.048(3)	0.066(4)	0.062(4)	0.005(3)	0.022(3)	0.012(3)
C(43)	0.068(5)	0.076(5)	0.068(4)	0.020(4)	0.017(4)	0.023(4)
C(44)	0.085(5)	0.052(4)	0.054(4)	0.004(4)	0.026(4)	0.012(3)
C(45)	0.083(5)	0.072(5)	0.073(5)	0.006(4)	0.048(4)	0.020(4)
C(46)	0.062(4)	0.061(4)	0.067(4)	0.010(3)	0.030(3)	0.013(3)

Table S11. Bond Lengths for 4-$CH_3C_6H_4COSPbPh_3$ **3**

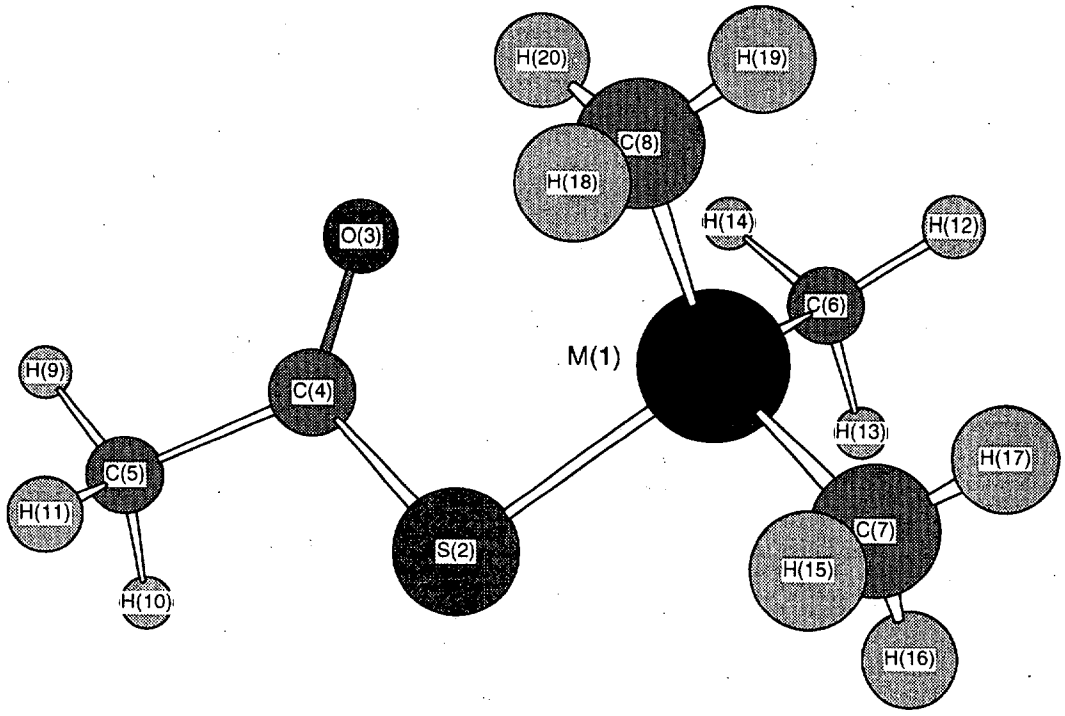
atom	atom	distance	atom	atom	distance
Pb(1)	S(11)	2.539(2)	C(24)	C(25)	1.360(9)
Pb(1)	O(11)	2.990(4)	C(24)	H(23)	1.139
Pb(1)	C(21)	2.205(5)	C(25)	C(26)	1.395(9)
Pb(1)	C(31)	2.213(5)	C(25)	H(24)	0.980
Pb(1)	C(41)	2.202(5)	C(26)	H(25)	1.036
S(11)	C(11)	1.770(6)	C(31)	C(32)	1.392(8)
O(11)	C(11)	1.222(7)	C(31)	C(36)	1.395(8)
C(11)	C(12)	1.485(8)	C(32)	C(33)	1.373(8)
C(12)	C(13)	1.378(8)	C(32)	H(31)	0.986
C(12)	C(17)	1.390(8)	C(33)	C(34)	1.394(10)
C(13)	C(14)	1.374(8)	C(33)	H(32)	1.126
C(13)	H(11)	0.987	C(34)	C(35)	1.373(10)
C(14)	C(15)	1.391(9)	C(34)	H(33)	0.981
C(14)	H(12)	0.982	C(35)	C(36)	1.399(9)
C(15)	C(16)	1.400(9)	C(35)	H(34)	1.044
C(15)	C(18)	1.503(9)	C(36)	H(35)	0.967
C(16)	C(17)	1.383(9)	C(41)	C(42)	1.375(8)
C(16)	H(13)	0.988	C(41)	C(46)	1.371(8)
C(17)	H(14)	1.005	C(42)	C(43)	1.383(9)
C(18)	H(15)	0.960	C(42)	H(41)	1.072
C(18)	H(16)	0.964	C(43)	C(44)	1.363(10)
C(18)	H(17)	0.967	C(43)	H(42)	0.987
C(21)	C(22)	1.372(8)	C(44)	C(45)	1.349(9)
C(21)	C(26)	1.385(8)	C(44)	H(43)	1.047
C(22)	C(23)	1.378(9)	C(45)	C(46)	1.390(9)
C(22)	H(21)	0.993	C(45)	H(44)	0.983
C(23)	C(24)	1.373(10)	C(46)	H(45)	0.990
C(23)	H(22)	1.001			

Table S12. Bond Angles for 4-$CH_3C_6H_4COSPbPh_3$ **3**

atom	atom	atom	angle	atom	atom	atom	angle
S(11)	Pb(1)	O(11)	55.77(8)	C(24)	C(23)	H(22)	115.6
S(11)	Pb(1)	C(21)	115.0(2)	C(23)	C(24)	C(25)	119.9(6)
S(11)	Pb(1)	C(31)	96.9(1)	C(23)	C(24)	H(23)	110.9
S(11)	Pb(1)	C(41)	106.2(1)	C(25)	C(24)	H(23)	129.1
O(11)	Pb(1)	C(21)	85.6(2)	C(24)	C(25)	C(26)	120.0(6)
O(11)	Pb(1)	C(31)	152.6(2)	C(24)	C(25)	H(24)	120.3
O(11)	Pb(1)	C(41)	77.8(2)	C(26)	C(25)	H(24)	119.7
C(21)	Pb(1)	C(31)	110.0(2)	C(21)	C(26)	C(25)	119.8(6)
C(21)	Pb(1)	C(41)	114.4(2)	C(21)	C(26)	H(25)	125.0
C(31)	Pb(1)	C(41)	113.2(2)	C(25)	C(26)	H(25)	115.1
Pb(1)	S(11)	C(11)	94.1(2)	Pb(1)	C(31)	C(32)	119.0(4)
Pb(1)	O(11)	C(11)	88.4(3)	Pb(1)	C(31)	C(36)	121.3(4)
S(11)	C(11)	O(11)	120.8(5)	C(32)	C(31)	C(36)	119.7(5)
S(11)	C(11)	C(12)	117.5(4)	C(31)	C(32)	C(33)	120.7(6)
O(11)	C(11)	C(12)	121.6(5)	C(31)	C(32)	H(31)	118.8
C(11)	C(12)	C(13)	118.9(5)	C(33)	C(32)	H(31)	120.5
C(11)	C(12)	C(17)	122.5(5)	C(32)	C(33)	C(34)	119.9(6)
C(13)	C(12)	C(17)	118.6(5)	C(32)	C(33)	H(32)	121.6
C(12)	C(13)	C(14)	121.2(6)	C(34)	C(33)	H(32)	117.8
C(12)	C(13)	H(11)	119.1	C(33)	C(34)	C(35)	119.9(6)
C(14)	C(13)	H(11)	119.7	C(33)	C(34)	H(33)	119.3
C(13)	C(14)	C(15)	121.0(6)	C(35)	C(34)	H(33)	120.9
C(13)	C(14)	H(12)	120.4	C(34)	C(35)	C(36)	120.8(6)
C(15)	C(14)	H(12)	118.6	C(34)	C(35)	H(34)	117.4
C(14)	C(15)	C(16)	118.0(6)	C(36)	C(35)	H(34)	120.7
C(14)	C(15)	C(18)	120.0(7)	C(31)	C(36)	C(35)	119.0(6)
C(16)	C(15)	C(18)	122.0(6)	C(31)	C(36)	H(35)	119.2
C(15)	C(16)	C(17)	120.5(6)	C(35)	C(36)	H(35)	121.8
C(15)	C(16)	H(13)	119.1	Pb(1)	C(41)	C(42)	120.7(4)

C(17)	C(16)	H(13)	120.4	Pb(1)	C(41)	C(46)	120.0(4)
C(12)	C(17)	C(16)	120.8(6)	C(42)	C(41)	C(46)	119.3(5)
C(12)	C(17)	H(14)	119.3	C(41)	C(42)	C(43)	120.2(6)
C(16)	C(17)	H(14)	119.9	C(41)	C(42)	H(41)	119.1
C(15)	C(18)	H(15)	111.7	C(43)	C(42)	H(41)	120.7
C(15)	C(18)	H(16)	111.5	C(42)	C(43)	C(44)	120.5(6)
C(15)	C(18)	H(17)	111.7	C(42)	C(43)	H(42)	120.5
H(15)	C(18)	H(16)	107.5	C(44)	C(43)	H(42)	119.1
H(15)	C(18)	H(17)	107.2	C(43)	C(44)	C(45)	119.1(6)
H(16)	C(18)	H(17)	106.9	C(43)	C(44)	H(43)	118.6
Pb(1)	C(21)	C(22)	123.4(4)	C(45)	C(44)	H(43)	122.3
Pb(1)	C(21)	C(26)	116.8(4)	C(44)	C(45)	C(46)	121.6(6)
C(22)	C(21)	C(26)	119.8(5)	C(44)	C(45)	H(44)	118.3
C(21)	C(22)	C(23)	119.6(6)	C(46)	C(45)	H(44)	120.0
C(21)	C(22)	H(21)	119.6	C(41)	C(46)	C(45)	119.1(6)
C(23)	C(22)	H(21)	120.8	C(41)	C(46)	H(45)	119.6
C(22)	C(23)	C(24)	120.9(6)	C(45)	C(46)	H(45)	121.2
C(22)	C(23)	H(22)	123.4				

Calculation Method. Gaussian 98 was used as source program for ab initio MO calculations and NBO deletion analysis. Geometries of model compounds $CH_3COSM(CH_3)_3$ (**1'**; M = Ge, **2'**; M = Sn, **3'**; M = Pb) were optimized at the B3LYP/LANL2DZ+p. The d-polarization function for ECP basis set of all atoms except for H are taken from* Huzinaga, S.; Andzelm, J.; Klobukowski, M.; Raszio-Andzelm, Y.; Sakai, Y.; Tatewaki, H. *Gaussian basis sets for molecu;ar calculations*; Elsevier: Amsterdam, 1984. NBO analyses were performed on the optimized conformations using the same basis sets. Calculated coordinates for all conformers are listed.



Z-matrix orientation for $CH_3COSGe(CH_3)_3$ **1'**

Ge	1.032045	-0.046979	-0.000117
S	-0.931741	1.175027	-0.000264
O	-1.829069	-1.357552	0.000702
C	-2.140404	-0.180892	0.000347
C	-3.585058	0.300509	0.000322
C	1.120120	-1.130613	1.636112
C	2.397030	1.374814	-0.000826
C	1.119657	-1.131818	-1.635570
H	-4.255972	-0.565345	0.001162
H	-3.774490	0.922347	0.885299
H	-3.774873	0.920871	-0.885614
H	2.080105	-1.664577	1.682857
H	1.032771	-0.497123	2.527873
H	0.307275	-1.865419	1.641599
H	2.305340	2.010316	-0.891123
H	2.305662	2.010881	0.889100
H	3.402573	0.930776	-0.000867
H	1.032022	-0.498993	-2.527774
H	2.079643	-1.665788	-1.682206
H	0.306830	-1.866650	-1.640268

Calculated Distance matrix (angstroms) for $CH_3COSGe(CH_3)_3$ **1'**

		1	2	3	4	5
1	Ge	0.000000				
2	S	2.312954	0.000000			
3	O	3.146995	2.686849	0.000000		
4	C	3.175274	1.816420	1.217152	0.000000	
5	C	4.630161	2.793720	2.415091	1.522751	0.000000
6	C	1.964501	3.493399	3.379909	3.769445	5.182916
7	C	1.970959	3.334761	5.032468	4.796721	6.077788
8	C	1.964499	3.493421	3.379841	3.769414	5.182861
9	H	5.313363	3.752254	2.552930	2.150217	1.095367
10	H	4.982603	2.988192	3.124918	2.161137	1.098067
11	H	4.982700	2.988618	3.124567	2.161087	1.098072
12	H	2.558799	4.468497	4.266796	4.779629	6.227886
13	H	2.567755	3.612045	3.913702	4.069082	5.324385
14	H	2.554848	3.670856	2.741247	3.394477	4.747135
15	H	2.578301	3.459773	5.406591	5.035946	6.197976
16	H	2.578293	3.459826	5.406625	5.035996	6.198055
17	H	2.564256	4.341191	5.710212	5.653353	7.015998
18	H	2.567755	3.612065	3.913586	4.069013	5.324275
19	H	2.558794	4.468511	4.266757	4.779613	6.227846
20	H	2.554845	3.670895	2.741173	3.394459	4.747094

		6	7	8	9	10
6	C	0.000000				
7	C	3.253802	0.000000			
8	C	3.271682	3.253809	0.000000		
9	H	5.647562	6.930127	5.647758	0.000000	
10	H	5.360557	6.251208	5.875972	1.796316	0.000000
11	H	5.876108	6.251504	5.360260	1.796292	1.770914
12	H	1.099488	3.489001	3.495461	6.646975	6.450159
13	H	1.097350	3.429237	4.212439	5.861717	5.274723
14	H	1.095759	4.190912	3.455137	5.020403	5.000443
15	H	4.202035	1.097679	3.439920	7.104999	6.426794
16	H	3.439843	1.097678	4.202038	7.104957	6.176825
17	H	3.484052	1.099221	3.484000	7.803313	7.231569
18	H	4.212440	3.429266	1.097349	5.861979	6.063978
19	H	3.495473	3.488987	1.099487	6.647159	6.896477
20	H	3.455120	4.190918	1.095759	5.020642	5.551051

		11	12	13	14	15
11	H	0.000000				
12	H	6.896546	0.000000			

13	H	6.064325	1.781547	0.000000		
14	H	5.551049	1.784647	1.784393	0.000000	
15	H	6.177047	4.492320	4.426761	5.042645	0.000000
16	H	6.427335	3.766951	3.255136	4.425552	1.780223
17	H	7.231778	3.364477	3.748251	4.482998	1.778168
18	H	5.274367	4.492936	5.055647	4.447027	3.255241
19	H	6.449862	3.365063	4.492937	3.772111	3.767027
20	H	5.000008	3.772068	4.447021	3.281867	4.425622

		16	17	18	19	20
16	H	0.000000				
17	H	1.778168	0.000000			
18	H	4.426811	3.748201	0.000000		
19	H	4.492282	3.364400	1.781546	0.000000	
20	H	5.042646	4.482951	1.784392	1.784649	0.000000

Calculated Interatomic angles for $CH_3COSGe(CH_3)_3$ **1'**

Ge1-S2-O3= 77.6172	Ge1-S2-C4= 99.821	S2-C4-O3=123.4659
Ge1-S2-C5=129.8653	S2-O3-C5= 66.153	S2-C4-C5=113.2842
O3-C4-C5=123.25	S2-Ge1-C6=109.2414	S2-Ge1-C7=101.9394
C6-Ge1-C7=111.5408	S2-Ge1-C8=109.2426	C6-Ge1-C8=112.7544
C7-Ge1-C8=111.5413	S2-O3-H9= 91.4319	S2-C4-H9=142.0135
O3-C4-H9= 94.5207	S2-C5-H9=146.0125	O3-C5-H9= 84.4136
C4-C5-H9=109.341	Ge1-S2-H10=139.7311	O3-S2-H10= 66.5764
S2-C4-H10= 97.019	O3-C4-H10=133.3771	S2-C5-H10= 89.2404
O3-C5-H10=120.9371	C4-C5-H10=110.0404	S2-H10-H9=100.3208
O3-H9-H10= 90.1306	C4-H9-H10= 65.6939	H9-C5-H10=109.9598
Ge1-S2-H11=139.7113	O3-S2-H11= 66.5615	S2-C4-H11= 97.0395
O3-C4-H11=133.3487	S2-C5-H11= 89.2641	O3-C5-H11=120.9092
C4-C5-H11=110.0362	S2-H11-H9=100.3061	O3-H9-H11= 90.1175
C4-H9-H11= 65.6925	H9-C5-H11=109.9574	S2-H10-H11= 72.7778
C4-H11-H10= 65.8141	H10-C5-H11=107.4867	H9-H11-H10= 60.4671
S2-Ge1-H12=132.9841	Ge1-C6-H12=110.0258	C7-Ge1-H12= 99.9393
C8-Ge1-H12=100.3808	S2-Ge1-H13= 95.3318	Ge1-C6-H13=110.7841
C7-Ge1-H13= 97.2743	C8-Ge1-H13=136.2854	Ge1-H12-H13= 69.935
H12-C6-H13=108.3795	S2-Ge1-H14= 97.7718	Ge1-H14-O3= 72.8165
S2-O3-H14= 85.0994	C4-O3-H14=112.2485	C5-O3-H14=133.9423
Ge1-C6-H14=109.9266	O3-H14-C6=116.8002	C7-Ge1-H14=135.2463
C8-Ge1-H14= 98.8912	H9-O3-H14=142.9627	Ge1-H14-H12= 69.693
O3-H14-H12=140.0996	H12-C6-H14=108.7721	Ge1-H14-H13= 70.0033
O3-H14-H13=118.171	H13-C6-H14=108.9055	H12-H13-H14= 60.0622
S2-Ge1-H15= 89.8686	C6-Ge1-H15=134.8969	Ge1-C7-H15=111.1052
C8-Ge1-H15= 97.5223	H12-Ge1-H15=121.9679	H13-Ge1-H15=118.6834
H14-Ge1-H15=158.4497	S2-Ge1-H16= 89.8705	C6-Ge1-H16= 97.5195
Ge1-C7-H16=111.1046	C8-Ge1-H16=134.8977	H12-Ge1-H16= 94.3242
H13-Ge1-H16= 78.4768	H14-Ge1-H16=119.1176	Ge1-H16-H15= 69.8043
H15-C7-H16=108.3686	S2-Ge1-H17=125.6929	C6-Ge1-H17= 99.737
Ge1-C7-H17=110.0064	C8-Ge1-H17= 99.735	H12-Ge1-H17= 82.1022
H13-Ge1-H17= 93.8343	H14-Ge1-H17=122.265	Ge1-H17-H15= 70.1961
H15-C7-H17=108.0745	Ge1-H17-H16= 70.1958	H16-C7-H17=108.0745
H15-H17-H16= 60.0765	S2-Ge1-H18= 95.3324	C6-Ge1-H18=136.2853
C7-Ge1-H18= 97.2754	Ge1-C8-H18=110.7843	H12-Ge1-H18=122.4232
H13-Ge1-H18=159.7646	H14-Ge1-H18=120.4813	H15-Ge1-H18= 78.4797
H16-Ge1-H18=118.6858	H17-Ge1-H18= 93.8327	S2-Ge1-H19=132.9852
C6-Ge1-H19=100.3814	C7-Ge1-H19= 99.9389	Ge1-C8-H19=110.0256
H12-Ge1-H19= 82.2263	H13-Ge1-H19=122.4235	H14-Ge1-H19= 95.0643
H15-Ge1-H19= 94.3266	H16-Ge1-H19=121.9666	H17-Ge1-H19= 82.1001
Ge1-H19-H18= 69.9352	H18-C8-H19=108.3796	S2-Ge1-H20= 97.7732
Ge1-H20-O3= 72.8178	S2-O3-H20= 85.1019	C4-O3-H20=112.2519
C5-O3-H20=133.944	C6-Ge1-H20= 98.8906	C7-Ge1-H20=135.2468
Ge1-C8-H20=109.9265	O3-H20-C8=116.8004	H9-O3-H20=142.9839
H12-Ge1-H20= 95.0628	H13-Ge1-H20=120.4811	H14-Ge1-H20= 79.9245
H14-O3-H20= 73.5418	H15-Ge1-H20=119.1205	H16-Ge1-H20=158.451
H17-Ge1-H20=122.2629	Ge1-H20-H18= 70.0034	O3-H20-H18=118.1686
H18-C8-H20=108.9055	Ge1-H20-H19= 69.6928	O3-H20-H19=140.1021
H19-C8-H20=108.7723	H19-H18-H20= 60.0623	

Z-matrix orientation for $CH_3COSSn(CH_3)_3$ **2'**

Sn	0.885674	-0.047421	-0.000024
S	-1.229262	1.278355	0.000255
O	-1.900692	-1.306755	-0.000215
C	-2.323698	-0.160819	0.000007
C	-3.807665	0.175587	0.000117
C	0.983475	-1.207687	1.794144
C	2.363106	1.511970	0.000261
C	0.983431	-1.206967	-1.794661
H	-4.391985	-0.750873	-0.000219
H	-4.056256	0.775614	0.885457
H	-4.056265	0.776283	-0.884764
H	1.970060	-1.681743	1.889019
H	0.818795	-0.571342	2.672530
H	0.213325	-1.986359	1.770654
H	2.262274	2.146755	-0.889400
H	2.262315	2.146404	0.890178
H	3.373860	1.081090	0.000152
H	0.819045	-0.570217	-2.672810
H	1.969905	-1.681244	-1.889590
H	0.213076	-1.985448	-1.771599

Calculated Distance matrix (angstroms) for $CH_3COSSn(CH_3)_3$ **2'**

		1	2	3	4	5
1	Sn	0.000000				
2	S	2.496124	0.000000			
3	O	3.057737	2.670882	0.000000		
4	C	3.211375	1.808040	1.221518	0.000000	
5	C	4.698634	2.804329	2.415344	1.521619	0.000000
6	C	2.138883	3.780826	3.398228	3.905413	5.299717
7	C	2.148141	3.599956	5.111280	4.976380	6.313821
8	C	2.138885	3.780815	3.398258	3.905428	5.299744
9	H	5.324333	3.757736	2.552557	2.150808	1.095334
10	H	5.087645	3.004700	3.125241	2.159325	1.098024
11	H	5.087633	3.004543	3.125375	2.159344	1.098022
12	H	2.723120	4.750292	4.323487	4.931322	6.356078
13	H	2.724245	3.841480	3.883299	4.145621	5.394796
14	H	2.710504	3.984184	2.840229	3.592252	4.896648
15	H	2.738691	3.706269	5.481575	5.210286	6.443672
16	H	2.738699	3.706289	5.481581	5.210297	6.443678
17	H	2.732144	4.607347	5.789879	5.831338	7.238386
18	H	2.724250	3.841622	3.883583	4.145889	5.395110
19	H	2.723122	4.750306	4.323366	4.931257	6.356031
20	H	2.710500	3.983995	2.840148	3.592086	4.896469

		6	7	8	9	10
6	C	0.000000				
7	C	3.538070	0.000000			
8	C	3.588805	3.538060	0.000000		
9	H	5.685418	7.124024	5.685344	0.000000	
10	H	5.491637	6.521809	6.042524	1.796468	0.000000
11	H	6.042488	6.521720	5.491787	1.796477	1.770221
12	H	1.098673	3.731179	3.842961	6.701594	6.585000
13	H	1.097095	3.723722	4.515189	5.859014	5.364144
14	H	1.095450	4.471482	3.729878	5.086383	5.161529
15	H	4.482078	1.097550	3.701674	7.312048	6.704772
16	H	3.701691	1.097550	4.482076	7.312094	6.465557
17	H	3.764419	1.098763	3.764401	7.979000	7.488905
18	H	4.515206	3.723565	1.097095	5.859199	6.183937
19	H	3.842811	3.731322	1.098673	6.701415	7.074719
20	H	3.730006	4.471471	1.095450	5.086113	5.736776

		11	12	13	14	15

11	H	0.000000				
12	H	7.074769	0.000000			
13	H	6.183579	1.781093	0.000000		
14	H	5.736970	1.786875	1.783886	0.000000	
15	H	6.465458	4.739452	4.707338	5.325102	0.000000
16	H	6.704633	3.967091	3.556216	4.696097	1.779578
17	H	7.488841	3.629286	4.049752	4.746883	1.778361
18	H	5.364589	4.834316	5.345340	4.702842	3.556037
19	H	6.585122	3.778608	4.834240	4.071370	3.967296
20	H	5.161483	4.071775	4.702858	3.542253	4.696018
		16	17	18	19	20
16	H	0.000000				
17	H	1.778362	0.000000			
18	H	4.707222	4.049521	0.000000		
19	H	4.739568	3.629422	1.781094	0.000000	
20	H	5.325095	4.746927	1.783889	1.786872	0.000000

Calculated Interatomic angles for $CH_3COSSn(CH_3)_3$ **2'**

Sn1-S2-O3= 72.4776	Sn1-S2-C4= 95.1695	S2-C4-O3=122.4875
Sn1-S2-C5=124.7618	S2-O3-C5= 66.7008	S2-C4-C5=114.4789
O3-C4-C5=123.0336	S2-Sn1-C6=109.0728	S2-Sn1-C7=101.3719
C6-Sn1-C7=111.2371	S2-Sn1-C8=109.0723	C6-Sn1-C8=114.0575
C7-Sn1-C8=111.2366	S2-O3-H9= 91.9813	S2-C4-H9=143.1743
O3-C4-H9= 94.3382	S2-C5-H9=145.3958	O3-C5-H9= 84.3808
C4-C5-H9=109.467	Sn1-S2-H10=135.1001	O3-S2-H10= 66.5209
S2-C4-H10= 98.0728	O3-C4-H10=133.2171	S2-C5-H10= 89.6121
O3-C5-H10=120.9461	C4-C5-H10=109.9785	S2-H10-H9= 99.9483
O3-H9-H10= 90.1517	C4-H9-H10= 65.6144	H9-C5-H10=109.9794
Sn1-S2-H11=135.1076	O3-S2-H11= 66.5266	S2-C4-H11= 98.0651
O3-C4-H11=133.2279	S2-C5-H11= 89.6034	O3-C5-H11=120.9567
C4-C5-H11=109.9802	S2-H11-H9= 99.9537	O3-H9-H11= 90.1567
C4-H9-H11= 65.6149	H9-C5-H11=109.9804	S2-H11-H10= 72.8723
C4-H10-H11= 65.802	H10-C5-H11=107.4322	H9-H10-H11= 60.4825
S2-Sn1-H12=131.0026	Sn1-C6-H12=110.3381	C7-Sn1-H12= 99.3057
C8-Sn1-H12=103.7974	S2-Sn1-H13= 94.6596	Sn1-C6-H13=110.4936
C7-Sn1-H13= 98.9958	C8-Sn1-H13=136.054	Sn1-H12-H13= 70.9496
H12-C6-H13=108.4165	S2-Sn1-H14= 99.7702	Sn1-H14-O3= 66.8061
S2-O3-H14= 92.5432	C4-O3-H14=118.8234	C5-O3-H14=137.2579
Sn1-C6-H14=109.6006	O3-H14-C6=111.5042	C7-Sn1-H14=133.6145
C8-Sn1-H14= 99.8841	H9-O3-H14=141.1287	Sn1-H14-H12= 71.1832
O3-H14-H12=137.0769	H12-C6-H14=109.0544	Sn1-H14-H13= 71.2556
O3-H14-H13=112.2128	H13-C6-H14=108.9011	H12-H13-H14= 60.1628
S2-Sn1-H15= 90.0225	C6-Sn1-H15=133.1596	Sn1-C7-H15=110.8889
C8-Sn1-H15= 97.9835	H12-Sn1-H15=120.3947	H13-Sn1-H15=119.0127
H14-Sn1-H15=155.4976	S2-Sn1-H16= 90.0229	C6-Sn1-H16= 97.9839
Sn1-C7-H16=110.8894	C8-Sn1-H16=133.159	H12-Sn1-H16= 93.159
H13-Sn1-H16= 81.2292	H14-Sn1-H16=119.0366	Sn1-H15-H16= 71.041
H15-C7-H16=108.3297	S2-Sn1-H17=123.5213	C6-Sn1-H17=100.5077
Sn1-C7-H17=110.3657	C8-Sn1-H17=100.507	H12-Sn1-H17= 83.4077
H13-Sn1-H17= 95.8389	H14-Sn1-H17=121.4218	Sn1-H17-H15= 71.2303
H15-C7-H17=108.1338	Sn1-H17-H16= 71.2305	H16-C7-H17=108.1339
H15-H17-H16= 60.0453	S2-Sn1-H18= 94.6641	C6-Sn1-H18=136.0549
C7-Sn1-H18= 98.9899	Sn1-C8-H18=110.4939	H12-Sn1-H18=125.1112
H13-Sn1-H18=157.6662	H14-Sn1-H18=119.84	H15-Sn1-H18= 81.2243
H16-Sn1-H18=119.0074	H17-Sn1-H18= 95.8315	S2-Sn1-H19=131.0033
C6-Sn1-H19=103.7916	C7-Sn1-H19= 99.311	Sn1-C8-H19=110.3381
H12-Sn1-H19= 87.8635	H13-Sn1-H19=125.1079	H14-Sn1-H19= 97.0578
H15-Sn1-H19= 93.1654	H16-Sn1-H19=120.3992	H17-Sn1-H19= 83.4115
Sn1-H19-H18= 70.9497	H18-C8-H19=108.4165	S2-Sn1-H20= 99.7638
Sn1-H20-O3= 66.8073	S2-O3-H20= 92.5393	C4-O3-H20=118.8175
C5-O3-H20=137.2517	C6-Sn1-H20= 99.889	C7-Sn1-H20=133.614
Sn1-C8-H20=109.6003	O3-H20-C8=111.5115	H9-O3-H20=141.1164
H12-Sn1-H20= 97.0708	H13-Sn1-H20=119.841	H14-Sn1-H20= 81.6016
H14-O3-H20= 77.1582	H15-Sn1-H20=119.0337	H16-Sn1-H20=155.4965
H17-Sn1-H20=121.4238	Sn1-H20-H18= 71.2559	O3-H20-H18=112.2297
H18-C8-H20=108.9013	Sn1-H20-H19= 71.1834	O3-H20-H19=137.074

H19-C8-H20=109.0541 H19-H18-H20= 60.1626

Z-matrix orientation for $CH_3COSPb(CH_3)_3$ **3'**

Pb	-0.718624	-0.042995	-0.000106
S	1.469393	1.300978	0.000421
O	2.134024	-1.290333	0.000662
C	2.553264	-0.141920	0.000564
C	4.039751	0.191264	0.000123
C	-0.760835	-1.220360	-1.852118
C	-2.214315	1.578701	-0.000295
C	-0.761646	-1.220655	1.851692
H	4.621490	-0.736980	0.003974
H	4.290772	0.786975	-0.887385
H	4.290260	0.794439	0.882672
H	0.068128	-1.934118	-1.822143
H	-1.715429	-1.756089	-1.929905
H	-0.646176	-0.553103	-2.713719
H	-2.090507	2.201841	0.893155
H	-2.090141	2.201986	-0.893593
H	-3.224715	1.149794	-0.000536
H	-0.646970	-0.553574	2.713428
H	-1.716430	-1.756091	1.929170
H	0.067109	-1.934655	1.821784

Calculated Distance matrix (angstroms) for $CH_3COSPb(CH_3)_3$ **3'**

		1	2	3	4	5
1	Pb	0.000000				
2	S	2.567816	0.000000			
3	O	3.113431	2.675187	0.000000		
4	C	3.273384	1.804641	1.222545	0.000000	
5	C	4.764138	2.799680	2.413903	1.523370	0.000000
6	C	2.194976	3.842260	3.437716	3.946988	5.335645
7	C	2.206125	3.694162	5.209549	5.068565	6.406117
8	C	2.194970	3.842314	3.437452	3.947022	5.336220
9	H	5.385021	3.753532	2.548274	2.152131	1.095478
10	H	5.154626	3.002096	3.123364	2.161072	1.097977
11	H	5.154562	2.998706	3.126271	2.161489	1.097937
12	H	2.741376	3.968769	2.829311	3.565128	4.859187
13	H	2.766303	4.818184	4.331547	4.955198	6.374895
14	H	2.762093	3.908939	3.954855	4.215783	5.465980
15	H	2.778357	3.779076	5.553241	5.277741	6.513064
16	H	2.778366	3.779068	5.553337	5.277748	6.512858
17	H	2.775471	4.696542	5.888150	5.920606	7.327432
18	H	2.762081	3.908806	3.954218	4.215517	5.466458
19	H	2.766301	4.818216	4.331520	4.955336	6.375503
20	H	2.741357	3.969016	2.829094	3.565349	4.860028

		6	7	8	9	10
6	C	0.000000				
7	C	3.657403	0.000000			
8	C	3.703811	3.657390	0.000000		
9	H	5.713856	7.217383	5.711931	0.000000	
10	H	5.520764	6.612860	6.087697	1.796200	0.000000
11	H	6.087039	6.610914	5.524614	1.796404	1.770073
12	H	1.094316	4.568213	3.833356	5.049846	5.109682
13	H	1.097409	3.884984	3.936606	6.703358	6.605185
14	H	1.095781	3.790293	4.615403	5.930259	5.431828
15	H	4.584323	1.096306	3.794489	7.380936	6.774429
16	H	3.794507	1.096306	4.584318	7.381676	6.535927
17	H	3.888019	1.097665	3.887993	8.069874	7.576324
18	H	4.615385	3.790443	1.095781	5.927179	6.256535
19	H	3.936789	3.884786	1.097409	6.701805	7.105395
20	H	3.833179	4.568209	1.094315	5.047895	5.708433

		11	12	13	14	15
11	H	0.000000				
12	H	5.708541	0.000000			
13	H	7.105214	1.795656	0.000000		
14	H	6.254462	1.792301	1.790208	0.000000	
15	H	6.534147	5.398028	4.876019	4.762914	0.000000
16	H	6.770954	4.756857	4.108615	3.603944	1.786748
17	H	7.575037	4.865345	3.800601	4.112188	1.786593
18	H	5.435535	4.794650	4.914080	5.427147	3.604095
19	H	6.609136	4.157966	3.859074	4.914168	4.108344
20	H	5.115163	3.643927	4.157462	4.794606	4.756917

		16	17	18	19	20
16	H	0.000000				
17	H	1.786594	0.000000			
18	H	4.763030	4.112400	0.000000		
19	H	4.875862	3.800376	1.790210	0.000000	
20	H	5.398037	4.865263	1.792295	1.795669	0.000000

Calculated Interatomic angles for $CH_3COSPb(CH_3)_3$ **3'**

Pb1-S2-O3= 72.8254	Pb1-S2-C4= 95.353	S2-C4-O3=123.0318
Pb1-S2-C5=125.0884	S2-O3-C5= 66.5223	S2-C4-C5=114.2795
O3-C4-C5=122.6887	S2-Pb1-C6=107.2956	S2-Pb1-C7=101.1254
C6-Pb1-C7=112.4071	S2-Pb1-C8=107.298	C6-Pb1-C8=115.0665
C7-Pb1-C8=112.4067	S2-O3-H9= 91.8438	S2-C4-H9=142.9643
O3-C4-H9= 94.0038	S2-C5-H9=145.4267	O3-C5-H9= 84.2126
C4-C5-H9=109.442	Pb1-S2-H10=135.3266	O3-S2-H10= 66.4651
S2-C4-H10= 98.0006	O3-C4-H10=132.8055	S2-C5-H10= 89.7094
O3-C5-H10=120.9092	C4-C5-H10=109.9978	S2-H10-H9= 99.8778
O3-H9-H10= 90.2214	C4-H9-H10= 65.6494	H9-C5-H10=109.9478
Pb1-S2-H11=135.4966	O3-S2-H11= 66.5869	S2-C4-H11= 97.8348
O3-C4-H11=133.0376	S2-C5-H11= 89.5206	O3-C5-H11=121.1407
C4-C5-H11=110.033	S2-H11-H9= 99.9938	O3-H9-H11= 90.3305
C4-H9-H11= 65.661	H9-C5-H11=109.9693	S2-H11-H10= 72.949
C4-H10-H11= 65.8391	H10-C5-H11=107.4285	H9-H10-H11= 60.4876
S2-Pb1-H12= 96.6989	Pb1-H12-O3= 67.9377	S2-O3-H12= 92.2318
C4-O3-H12=117.6512	C5-O3-H12=135.7232	Pb1-C6-H12=108.1905
O3-H12-C6=114.9834	C7-Pb1-H12=134.5564	C8-Pb1-H12=101.3169
H9-O3-H12=139.7294	S2-Pb1-H13=129.1466	Pb1-C6-H13=109.7787
C7-Pb1-H13=102.1728	C8-Pb1-H13=104.4315	Pb1-H12-H13= 71.7258
O3-H12-H13=137.8474	H12-C6-H13=110.0273	S2-Pb1-H14= 94.2732
Pb1-C6-H14=109.56	C7-Pb1-H14= 98.8273	C8-Pb1-H14=136.9095
Pb1-H12-H14= 71.6213	O3-H12-H14=115.8593	H12-C6-H14=109.8431
Pb1-H14-H13= 71.2334	H13-C6-H14=109.4238	H12-H14-H13= 60.1626
S2-Pb1-H15= 89.8734	C6-Pb1-H15=134.0404	Pb1-C7-H15=109.9494
C8-Pb1-H15= 98.7764	H12-Pb1-H15=155.8913	H13-Pb1-H15=123.1419
H14-Pb1-H15=118.557	S2-Pb1-H16= 89.8729	C6-Pb1-H16= 98.7767
Pb1-C7-H16=109.95	C8-Pb1-H16=134.0399	H12-Pb1-H16=119.0347
H13-Pb1-H16= 95.6335	H14-Pb1-H16= 81.1547	Pb1-H15-H16= 71.2438
H15-C7-H16=109.154	S2-Pb1-H17=122.9876	C6-Pb1-H17=102.2997
Pb1-C7-H17=109.6845	C8-Pb1-H17=102.2989	H12-Pb1-H17=123.7453
H13-Pb1-H17= 86.5984	H14-Pb1-H17= 95.9062	Pb1-H17-H15= 71.3227
H15-C7-H17=109.0402	Pb1-H17-H16= 71.323	H16-C7-H17=109.0403
H15-H17-H16= 60.0057	S2-Pb1-H18= 94.2693	C6-Pb1-H18=136.9087
C7-Pb1-H18= 98.833	Pb1-C8-H18=109.5596	H12-Pb1-H18=121.1979
H13-Pb1-H18=125.4661	H14-Pb1-H18=158.4912	H15-Pb1-H18= 81.1591
H16-Pb1-H18=118.5618	H17-Pb1-H18= 95.913	S2-Pb1-H19=129.1483
C6-Pb1-H19=104.4385	C7-Pb1-H19=102.1654	Pb1-C8-H19=109.7789
H12-Pb1-H19= 98.0392	H13-Pb1-H19= 88.4559	H14-Pb1-H19=125.4697
H15-Pb1-H19= 95.6255	H16-Pb1-H19=123.1349	H17-Pb1-H19= 86.5921
Pb1-H18-H19= 71.2336	H18-C8-H19=109.424	S2-Pb1-H20= 96.7074
Pb1-H20-O3= 67.941	S2-O3-H20= 92.244	C4-O3-H20=117.6797
C5-O3-H20=135.7842	C6-Pb1-H20=101.3107	C7-Pb1-H20=134.5573
Pb1-C8-H20=108.1896	O3-H20-C8=114.9795	H9-O3-H20=139.6211
H12-Pb1-H20= 83.3061	H12-O3-H20= 80.1792	H13-Pb1-H20= 98.0237
H14-Pb1-H20=121.1964	H15-Pb1-H20=119.0382	H16-Pb1-H20=155.8931
H17-Pb1-H20=123.7424	Pb1-H20-H18= 71.6215	O3-H20-H18=115.8377

H18-C8-H20=109.8427 Pb1-H20-H19= 71.7261 O3-H20-H19=137.8598
H19-C8-H20=110.0285 H19-H18-H20= 60.1631