Supporting Information

A Comparison of the Flexibility of Eight-Membered Tetrasiloxane and Stannasiloxane Rings: A Crystallographic and Computational Study†

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Crystallography

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Table 1a. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) **for 1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	5081(1)	3085(1)	-46(1)	49(1)
Si(1)	3225(2)	4946(1)	1013(1)	47(1)
O(3)	1494(6)	4790(4)	502(3)	105(2)
Si(1')	4611(7)	4959(5)	1415(4)	47(2)
O(3')	6280(20)	4851(17)	1964(14)	110(9)
O(1)	4345(4)	4044(2)	749(2)	79(1)
O(2)	3967(5)	6051(2)	848(2)	96(1)
C(1)	6969(6)	2237(4)	655(3)	71(1)
C(2)	6301(8)	1624(6)	1323(4)	127(3)
C(3)	8121(9)	3010(5)	1061(5)	145(3)
C(4)	7729(8)	1541(6)	70(4)	138(3)
C(11)	3101(6)	2328(5)	-738(3)	84(2)
C(12)	3691(7)	1650(6)	-1384(4)	134(3)
C(13)	2042(9)	3145(5)	-1179(5)	153(4)
C(14)	2250(8)	1709(6)	-125(4)	141(3)
C(21)	3056(6)	4838(3)	2156(3)	64(1)
C(22)	2628(10)	3699(6)	2354(4)	159(3)
C(23)	1995(13)	5635(7)	2445(5)	226(6)
C(24)	4549(12)	5062(5)	2648(5)	160(4)

Table 2a. Bond lengths [A] and angles [deg] for 1.

Sn(1)-O(1)	1.936(3)
Sn(1)-O(2)#1	1.953(3)
Sn(1)-C(11)	2.163(5)
Sn(1)-C(1)	2.170(5)
Si(1)-O(2)	1.592(3)
Si(1)-O(1)	1.596(3)
Si(1)-O(3)	1.634(5)
Si(1)-C(21)	1.874(4)
O(3)-H(3)	0.90(7)
Si(1')-O(1)	1.594(7)
Si(1')-O(3')	1.61(2)
Si(1')-O(2)	1.735(7)
Si(1')-C(21)	1.897(7)
O(2)-Sn(1)#1	1.953(3)
C(1)-C(2)	1.501(7)
C(1)-C(3)	1.503(7)
C(1)-C(4)	1.503(8)
C(11)-C(12)	1.491(7)
C(11)-C(13)	1.517(8)
C(11)-C(14)	1.520(8)
C(21)-C(24)	1.463(10)
C(21)-C(23)	1.481(8)
C(21)-C(22)	1.552(8)
O(1)-Sn(1)-O(2)#1	105.65(15)
O(1)-Sn(1)-C(11)	109.53(17)
O(2)#1-Sn(1)-C(11)	106.0(2)
O(1)-Sn(1)-C(1)	104.68(17)
O(2)#1-Sn(1)-C(1)	106.77(18)
C(11)-Sn(1)-C(1)	123.0(2)
O(2)-Si(1)-O(1)	109.8(2)
O(2)-Si(1)-O(3)	112.6(2)
O(1)-Si(1)-O(3)	108.6(2)
O(2)-Si(1)-C(21)	107.9(2)
O(1)-Si(1)-C(21)	108.9(2)
O(3)-Si(1)-C(21)	108.9(3)
H(3)-O(3)-Si(1)	84(5)
O(1)-Si(1')-O(3')	111.2(9)
O(1)-Si(1')-O(2)	103.1(4)
O(3')-Si(1')-O(2)	125.1(9)
O(1)-Si(1')-C(21)	107.9(4)
O(3')-Si(1')-C(21)	107.1(9)
O(2)-Si(1')-C(21)	101.2(4)
Si(1')-O(1)-Si(1)	47.8(2)
Si(1')-O(1)-Sn(1)	152.2(3)
Si(1)-O(1)-Sn(1)	153.0(2)
Si(1)-O(2)-Si(1')	45.5(2)
Si(1)-O(2)-Sn(1)#1	145.5(2)
Si(1')-O(2)-Sn(1)#1	132.7(3)
C(2)-C(1)-C(3)	108.6(5)
C(2)-C(1)-C(4)	111.6(6)
C(3)-C(1)-C(4)	111.0(6)
C(2)-C(1)-Sn(1)	108.4(4)
C(3)-C(1)-Sn(1)	108.4(4)
C(4)-C(1)-Sn(1)	108.8(4)
C(12)-C(11)-C(13)	108.0(6)
C(12)-C(11)-C(14)	112.0(6)
C(13)-C(11)-C(14)	111.2(6)
C(12)-C(11)-Sn(1)	108.5(4)
C(13)-C(11)-Sn(1)	109.2(4)
C(14)-C(11)-Sn(1)	107.8(4)
C(24)-C(21)-C(23)	103.1(6)
C(24)-C(21)-C(22)	106.7(5)
C(23)-C(21)-C(22)	114.8(6)
C(24)-C(21)-Si(1)	111.3(4)
C(23)-C(21)-Si(1)	112.1(4)
C(22)-C(21)-Si(1)	108.6(4)
C(24)-C(21)-Si(1')	72.0(5)
C(23)-C(21)-Si(1')	130.1(5)
C(22)-C(21)-Si(1')	114.0(4)
Si(1)-C(21)-Si(1')	40.1(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 3a. Anisotropic displacement parameters (A^2 x 10^3) **for 1.**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sn(1)	61(1)	38(1)	47(1)	0(1)	7(1)	1(1)
Si(1)	50(1)	48(1)	43(1)	2(1)	10(1)	2(1)
O(3)	74(3)	163(6)	73(3)	6(3)	-5(3)	-15(3)
Si(1')	54(4)	43(3)	44(3)	5(3)	9(3)	5(3)
O(3')	50(11)	200(30)	82(14)	50(14)	-3(10)	22(12)
O(1)	110(3)	67(2)	63(2)	-9(2)	21(2)	22(2)
O(2)	167(4)	52(2)	75(2)	10(2)	41(2)	-16(2)
C(1)	58(3)	82(4)	69(3)	7(3)	-3(3)	10(3)
C(2)	118(5)	155(6)	109(5)	77(5)	21(4)	31(5)
C(3)	114(6)	160(8)	145(7)	13(5)	-63(5)	-32(5)
C(4)	125(6)	178(7)	113(5)	4(5)	18(5)	85(6)
C(11)	69(4)	99(4)	81(4)	-33(3)	-1(3)	5(3)
C(12)	105(5)	157(7)	140(6)	-97(5)	5(4)	-24(5)
C(13)	111(6)	189(9)	144(7)	-43(6)	-50(5)	47(6)
C(14)	98(5)	179(8)	149(7)	-12(6)	24(5)	-73(5)
C(21)	69(3)	76(4)	49(3)	7(2)	18(2)	5(3)
C(22)	221(9)	167(8)	96(5)	51(5)	52(5)	-58(7)
C(23)	293(13)	280(13)	122(7)	13(9)	103(8)	152(12)
C(24)	183(9)	205(11)	83(5)	27(5)	-25(5)	-33(7)

Table 4a. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) **for 1.**

	x	y	z	U(eq)
H(3)	1150(100)	5080(40)	960(50)	120(30)
H(2A)	7128	1264	1652	209(8)
H(2B)	5556	1130	1072	209(8)
H(2C)	5790	2088	1673	209(8)
H(3A)	7637	3404	1468	209(8)
H(3B)	8446	3473	646	209(8)
H(3C)	9016	2649	1327	209(8)
H(4A)	8515	1124	380	209(8)
H(4B)	8205	1958	-326	209(8)
H(4C)	6952	1096	-218	209(8)
H(12A)	4349	1117	-1118	209(8)
H(12B)	4283	2061	-1734	209(8)
H(12C)	2822	1335	-1715	209(8)
H(13A)	2610	3529	-1557	209(8)
H(13B)	1687	3612	-776	209(8)
H(13C)	1157	2812	-1483	209(8)
H(14A)	1380	1349	-420	209(8)
H(14B)	1876	2173	274	209(8)
H(14C)	2955	1213	157	209(8)
H(22A)	3562	3284	2420	209(8)
H(22B)	1923	3426	1904	209(8)
H(22C)	2135	3682	2858	209(8)
H(23A)	2023	5598	3040	209(8)
H(23B)	947	5510	2195	209(8)
H(23C)	2328	6313	2288	209(8)
H(24A)	4946	5716	2477	209(8)
H(24B)	5285	4521	2564	209(8)
H(24C)	4396	5094	3227	209(8)

Table 5a. Least-squares plane (x,y,z in crystal coordinates) and deviations from that (* indicates atom used to define plane) **for 1**.

7.1150 (0.0093) x + 0.4204 (0.0080) y + 7.5418 (0.0273) z = 3.7677 (0.0060)

*	0.0589 (0.0016)	O1
*	-0.0577 (0.0016)	Sn1
*	-0.0589 (0.0016)	O1_$1
*	0.0577 (0.0016)	Sn1_$1
*	-0.0513 (0.0014)	O2
*	0.0513 (0.0014)	O2_$1
	-0.5010 (0.0046)	Si1_a
	0.5010 (0.0046)	Si1_$1a

Rms deviation of fitted atoms = 0.0561

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 1b. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) **for 2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	6242(1)	1714(1)	7921(1)	49(1)
Sn(2)	3106(1)	3379(1)	7055(1)	47(1)
Si(1)	3452(2)	1265(2)	8110(2)	51(1)
Si(2)	6040(2)	4121(2)	7351(2)	53(1)
Si(3)	8787(3)	2223(4)	9337(3)	99(1)
Si(4)	6552(5)	-388(3)	6799(4)	121(2)
Si(5)	897(3)	2635(3)	5322(3)	86(1)
Si(6)	2431(3)	5618(2)	7605(2)	67(1)
O(1)	4693(6)	1171(6)	7998(6)	72(2)
O(2)	3017(6)	2089(5)	7549(5)	69(2)
O(3)	4713(6)	4035(6)	7207(5)	67(2)
O(4)	6379(6)	3153(5)	7764(4)	61(2)
C(1)	7233(10)	1671(12)	9129(9)	89(4)
C(2)	8990(30)	3430(30)	10045(17)	270(20)
C(3)	9535(16)	1440(20)	9947(18)	226(18)
C(4)	9346(15)	2594(17)	8411(13)	134(8)
C(11)	6462(13)	950(10)	6811(8)	84(4)
C(12)	7940(30)	-400(20)	7410(30)	360(30)
C(13)	6720(40)	-820(30)	5770(30)	168(14)
C(14)	5460(30)	-1200(20)	7210(20)	112(9)
C(13')	5220(80)	-1080(70)	6110(60)	290(50)
C(14')	5890(40)	-1110(40)	7700(30)	123(15)
C(21)	2444(10)	-3(9)	7693(9)	77(4)
C(22)	2506(15)	-198(13)	6778(14)	125(7)
C(23)	2745(15)	-877(10)	8181(15)	138(8)
C(24)	1211(10)	-2(11)	7713(11)	106(5)
C(31)	3571(10)	1683(11)	9253(8)	75(3)
C(32)	2429(14)	1779(16)	9443(12)	131(7)
C(33)	4389(12)	2771(11)	9443(9)	96(4)
C(34)	4091(19)	1011(16)	9846(11)	147(8)
C(41)	2448(10)	2980(10)	5762(9)	80(4)
C(42)	419(19)	3820(20)	5250(18)	196(12)
C(43)	130(30)	1740(30)	5880(20)	131(11)
C(44)	630(30)	2290(30)	4190(20)	128(10)
C(43')	60(50)	2450(50)	6280(40)	160(20)
C(44')	520(60)	1160(50)	5200(40)	180(20)
C(51)	2381(13)	4263(10)	7788(10)	94(5)
C(52)	2976(15)	5985(12)	6646(11)	108(5)
C(53)	982(12)	5800(13)	7504(11)	109(5)
C(54)	3383(16)	6436(14)	8510(12)	125(6)
C(61)	6455(10)	4172(11)	6280(9)	80(4)
C(62)	7661(13)	4030(17)	6314(12)	133(7)
C(63)	5641(13)	3292(13)	5680(9)	98(4)
C(64)	6347(18)	5153(13)	5875(11)	129(7)
C(71)	6780(10)	5260(9)	8141(10)	78(4)
C(72)	8071(11)	5500(13)	8255(13)	126(7)
C(73)	6407(15)	6244(10)	7899(12)	119(6)
C(74)	6444(16)	5041(12)	8991(11)	113(5)

Table 2b. Bond lengths [A] and angles [deg] **for 2**.

Sn(1)-O(1)	1.923(7)
Sn(1)-O(4)	1.949(7)
Sn(1)-C(1)	2.119(13)
Sn(1)-C(11)	2.131(11)
Sn(2)-O(2)	1.942(7)
Sn(2)-O(3)	1.949(7)
Sn(2)-C(41)	2.098(14)
Sn(2)-C(51)	2.109(12)
Si(1)-O(2)	1.598(7)
Si(1)-O(1)	1.621(7)
Si(1)-C(31)	1.881(13)
Si(1)-C(21)	1.882(12)
Si(2)-O(3)	1.598(8)
Si(2)-O(4)	1.606(7)
Si(2)-C(71)	1.892(13)
Si(2)-C(61)	1.900(13)
Si(3)-C(3)	1.788(18)
Si(3)-C(4)	1.811(16)
Si(3)-C(1)	1.859(13)
Si(3)-C(2)	1.89(3)
Si(4)-C(14)	1.79(3)
Si(4)-C(13)	1.81(4)
Si(4)-C(13')	1.83(9)
Si(4)-C(12)	1.83(4)
Si(4)-C(11)	1.843(13)
Si(4)-C(14')	1.99(5)
Si(5)-C(43)	1.75(3)
Si(5)-C(44)	1.83(3)
Si(5)-C(42)	1.85(2)
Si(5)-C(41)	1.864(13)
Si(5)-C(44')	1.94(6)
Si(5)-C(43')	2.02(6)
Si(6)-C(54)	1.834(17)
Si(6)-C(52)	1.851(15)
Si(6)-C(53)	1.854(14)
Si(6)-C(51)	1.862(12)
C(21)-C(22)	1.51(2)
C(21)-C(23)	1.533(19)
C(21)-C(24)	1.541(17)
C(31)-C(34)	1.51(2)
C(31)-C(32)	1.542(19)
C(31)-C(33)	1.56(2)
C(61)-C(64)	1.531(18)
C(61)-C(63)	1.53(2)
C(61)-C(62)	1.549(19)
C(71)-C(72)	1.533(18)
C(71)-C(74)	1.53(2)
C(71)-C(73)	1.556(18)
O(1)-Sn(1)-O(4)	105.3(3)
O(1)-Sn(1)-C(1)	106.4(4)
O(4)-Sn(1)-C(1)	106.0(5)
O(1)-Sn(1)-C(11)	106.0(5)
O(4)-Sn(1)-C(11)	109.6(4)
C(1)-Sn(1)-C(11)	122.4(6)
O(2)-Sn(2)-O(3)	105.8(3)
O(2)-Sn(2)-C(41)	105.0(4)
O(3)-Sn(2)-C(41)	108.4(4)
O(2)-Sn(2)-C(51)	106.8(4)
O(3)-Sn(2)-C(51)	108.2(5)
C(41)-Sn(2)-C(51)	121.6(6)
O(2)-Si(1)-O(1)	112.4(4)
O(2)-Si(1)-C(31)	108.4(5)
O(1)-Si(1)-C(31)	107.2(5)
O(2)-Si(1)-C(21)	106.1(5)
O(1)-Si(1)-C(21)	106.4(5)
C(31)-Si(1)-C(21)	116.4(6)
O(3)-Si(2)-O(4)	112.6(4)
O(3)-Si(2)-C(71)	107.5(5)
O(4)-Si(2)-C(71)	106.0(5)
O(3)-Si(2)-C(61)	107.9(5)
O(4)-Si(2)-C(61)	107.3(5)
C(71)-Si(2)-C(61)	115.6(6)
C(3)-Si(3)-C(4)	113.0(10)
C(3)-Si(3)-C(1)	111.6(9)
C(4)-Si(3)-C(1)	114.7(8)
C(3)-Si(3)-C(2)	106.1(15)
C(4)-Si(3)-C(2)	107.4(13)
C(1)-Si(3)-C(2)	103.1(11)

Table 2b. Bond lengths [A] and angles [deg] **for 2**. (continued)

C(14)-Si(4)-C(13)	115.3(17)
C(14)-Si(4)-C(13')	58(3)
C(13)-Si(4)-C(13')	67(3)
C(14)-Si(4)-C(12)	110.5(16)
C(13)-Si(4)-C(12)	99.1(18)
C(13')-Si(4)-C(12)	149(3)
C(14)-Si(4)-C(11)	113.5(11)
C(13)-Si(4)-C(11)	109.9(14)
C(13')-Si(4)-C(11)	103(3)
C(12)-Si(4)-C(11)	107.4(11)
C(14)-Si(4)-C(14')	25.5(16)
C(13)-Si(4)-C(14')	133(2)
C(13')-Si(4)-C(14')	84(3)
C(12)-Si(4)-C(14')	88(2)
C(11)-Si(4)-C(14')	112.6(15)
C(43)-Si(5)-C(44)	114.4(16)
C(43)-Si(5)-C(42)	113.6(15)
C(44)-Si(5)-C(42)	96.5(14)
C(43)-Si(5)-C(41)	113.2(12)
C(44)-Si(5)-C(41)	109.7(12)
C(42)-Si(5)-C(41)	108.2(9)
C(43)-Si(5)-C(44')	49(2)
C(44)-Si(5)-C(44')	75(2)
C(42)-Si(5)-C(44')	149(2)
C(41)-Si(5)-C(44')	103(2)
C(43)-Si(5)-C(43')	35.4(19)
C(44)-Si(5)-C(43')	139(2)
C(42)-Si(5)-C(43')	83(2)
C(41)-Si(5)-C(43')	109.1(19)
C(44')-Si(5)-C(43')	84(3)
C(54)-Si(6)-C(52)	107.8(9)
C(54)-Si(6)-C(53)	110.1(8)
C(52)-Si(6)-C(53)	109.7(8)
C(54)-Si(6)-C(51)	108.6(8)
C(52)-Si(6)-C(51)	112.1(7)
C(53)-Si(6)-C(51)	108.4(7)
Si(1)-O(1)-Sn(1)	153.9(5)
Si(1)-O(2)-Sn(2)	157.1(5)
Si(2)-O(3)-Sn(2)	157.7(5)
Si(2)-O(4)-Sn(1)	156.6(5)
Si(3)-C(1)-Sn(1)	119.7(6)
Si(4)-C(11)-Sn(1)	120.4(7)
C(22)-C(21)-C(23)	109.1(14)
C(22)-C(21)-C(24)	107.3(13)
C(23)-C(21)-C(24)	108.6(12)
C(22)-C(21)-Si(1)	107.5(9)
C(23)-C(21)-Si(1)	112.2(11)
C(24)-C(21)-Si(1)	112.0(9)
C(34)-C(31)-C(32)	111.2(13)
C(34)-C(31)-C(33)	106.4(13)
C(32)-C(31)-C(33)	106.7(13)
C(34)-C(31)-Si(1)	112.7(12)
C(32)-C(31)-Si(1)	112.1(10)
C(33)-C(31)-Si(1)	107.4(8)
Si(5)-C(41)-Sn(2)	121.7(7)
Si(6)-C(51)-Sn(2)	121.1(6)
C(64)-C(61)-C(63)	106.3(12)
C(64)-C(61)-C(62)	109.6(13)
C(63)-C(61)-C(62)	106.7(14)
C(64)-C(61)-Si(2)	112.7(11)
C(63)-C(61)-Si(2)	108.5(8)
C(62)-C(61)-Si(2)	112.7(10)
C(72)-C(71)-C(74)	109.5(14)
C(72)-C(71)-C(73)	107.8(12)
C(74)-C(71)-C(73)	105.4(13)
C(72)-C(71)-Si(2)	112.4(10)
C(74)-C(71)-Si(2)	108.6(9)
C(73)-C(71)-Si(2)	112.8(10)

Symmetry transformations used to generate equivalent atoms:

Table 3b. Anisotropic displacement parameters (A^2 x 10^3) **for 2.**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sn(1)	49(1)	44(1)	66(1)	22(1)	24(1)	24(1)
Sn(2)	43(1)	42(1)	62(1)	22(1)	14(1)	19(1)
Si(1)	45(1)	40(1)	76(2)	26(1)	20(1)	17(1)
Si(2)	45(2)	46(2)	72(2)	27(1)	17(1)	13(1)
Si(3)	53(2)	155(4)	95(3)	59(3)	17(2)	31(2)
Si(4)	136(4)	71(3)	174(5)	-16(3)	72(4)	34(3)
Si(5)	58(2)	102(3)	92(3)	9(2)	-3(2)	20(2)
Si(6)	66(2)	55(2)	87(2)	13(2)	9(2)	31(2)
O(1)	51(4)	72(5)	102(6)	15(4)	30(4)	23(4)
O(2)	71(5)	51(4)	82(5)	28(4)	9(4)	13(4)
O(3)	53(4)	69(5)	78(5)	15(4)	15(4)	13(4)
O(4)	79(5)	46(4)	67(4)	23(3)	28(4)	20(3)
C(1)	65(8)	124(12)	88(9)	49(8)	21(7)	35(8)
C(2)	210(30)	390(50)	150(20)	-120(30)	10(20)	-30(30)
C(3)	93(14)	340(40)	290(30)	250(30)	62(17)	94(19)
C(4)	100(12)	184(19)	152(17)	93(15)	67(12)	54(13)
C(11)	116(11)	70(8)	81(9)	-1(7)	48(8)	30(7)
C(12)	200(30)	170(30)	770(110)	50(40)	200(50)	120(30)
C(21)	71(8)	48(6)	118(11)	15(7)	32(7)	13(6)
C(22)	98(12)	89(11)	176(19)	-30(12)	40(12)	-2(9)
C(23)	115(13)	45(8)	260(20)	50(11)	38(14)	16(8)
C(24)	46(7)	95(10)	164(15)	8(10)	21(8)	-6(7)
C(31)	68(7)	93(9)	70(8)	30(7)	23(6)	22(7)
C(32)	91(11)	180(19)	123(14)	-25(13)	52(10)	20(12)
C(33)	90(10)	109(11)	87(10)	-11(8)	5(7)	33(9)
C(34)	161(18)	174(19)	104(13)	87(14)	13(12)	38(15)
C(41)	60(7)	86(9)	107(10)	31(8)	26(7)	29(6)
C(42)	115(17)	230(30)	260(30)	80(30)	15(18)	80(18)
C(51)	119(11)	67(8)	133(12)	39(8)	77(10)	52(8)
C(52)	128(13)	84(10)	132(13)	59(10)	46(11)	39(9)
C(53)	77(9)	115(12)	135(14)	0(10)	-7(9)	48(9)
C(54)	116(13)	117(13)	132(15)	-20(11)	-5(11)	39(11)
C(61)	64(7)	93(9)	99(10)	54(8)	38(7)	26(7)
C(62)	77(10)	220(20)	120(14)	53(14)	51(10)	39(12)
C(63)	96(11)	129(13)	74(9)	16(9)	22(8)	32(10)
C(64)	173(18)	108(12)	113(13)	75(11)	52(12)	19(12)
C(71)	57(7)	44(6)	128(12)	14(7)	9(7)	10(5)
C(72)	55(8)	106(12)	189(19)	-19(12)	-13(10)	2(8)
C(73)	130(14)	54(8)	167(17)	11(9)	14(12)	28(8)
C(74)	134(14)	88(10)	117(13)	-3(9)	14(11)	39(10)

Table 4b. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) **for 2**.

	x	y	z	U(eq)
H(1A)	6935	2016	9537	169(9)
H(1B)	7107	962	9248	169(9)
H(2A)	8349	3368	10312	169(9)
H(2B)	9043	4001	9713	169(9)
H(2C)	9664	3525	10468	169(9)
H(3A)	9283	747	9691	169(9)
H(3B)	9392	1455	10509	169(9)
H(3C)	10331	1684	9970	169(9)
H(4A)	8947	3050	8128	169(9)
H(4B)	9252	1998	8035	169(9)
H(4C)	10135	2931	8577	169(9)
H(11A)	5840	982	6359	169(9)
H(11B)	7148	1346	6664	169(9)
H(12A)	7887	-1009	7698	169(9)
H(12B)	8210	186	7823	169(9)
H(12C)	8466	-375	7043	169(9)
H(13A)	6744	-1526	5763	169(9)
H(13B)	7410	-420	5651	169(9)
H(13C)	6092	-756	5348	169(9)
H(14A)	5553	-1886	7186	169(9)
H(14B)	4734	-1200	6871	169(9)
H(14C)	5496	-964	7780	169(9)
H(13D)	5374	-1387	5614	169(9)
H(13E)	4763	-612	5947	169(9)
H(13F)	4824	-1599	6404	169(9)
H(14D)	5962	-1799	7667	169(9)
H(14E)	5102	-1115	7614	169(9)
H(14F)	6278	-766	8237	169(9)
H(22A)	2299	338	6466	169(9)
H(22B)	1996	-840	6545	169(9)
H(22C)	3264	-215	6743	169(9)
H(23A)	2787	-723	8771	169(9)
H(23B)	3463	-959	8094	169(9)
H(23C)	2174	-1498	7982	169(9)
H(24A)	960	442	7316	169(9)
H(24B)	1166	233	8270	169(9)
H(24C)	738	-682	7566	169(9)
H(32A)	2048	2090	8995	169(9)
H(32B)	2559	2194	9965	169(9)
H(32C)	1970	1114	9488	169(9)
H(33A)	4366	3055	9990	169(9)
H(33B)	4159	3199	9023	169(9)
H(33C)	5145	2727	9432	169(9)
H(34A)	3611	331	9756	169(9)
H(34B)	4172	1277	10419	169(9)
H(34C)	4821	999	9737	169(9)
H(41A)	2782	3546	5469	169(9)
H(41B)	2732	2407	5602	169(9)
H(42A)	1054	4388	5250	169(9)
H(42B)	88	3931	5726	169(9)
H(42C)	-133	3771	4738	169(9)
H(43A)	626	1375	6185	169(9)
H(43B)	-464	1267	5486	169(9)
H(43C)	-188	2082	6262	169(9)
H(44A)	849	1664	4088	169(9)
H(44B)	1068	2820	3926	169(9)
H(44C)	-156	2191	3951	169(9)
H(43D)	582	2708	6806	169(9)
H(43E)	-278	1738	6297	169(9)
H(43F)	-517	2816	6200	169(9)
H(44D)	629	922	4665	169(9)
H(44E)	-255	896	5242	169(9)
H(44F)	1001	919	5644	169(9)
H(51A)	1591	3908	7726	169(9)
H(51B)	2736	4254	8373	169(9)
H(52A)	2590	5483	6183	169(9)
H(52B)	3772	6027	6745	169(9)
H(52C)	2850	6637	6511	169(9)
H(53A)	739	5693	8029	169(9)
H(53B)	475	5321	7066	169(9)
H(53C)	982	6482	7366	169(9)
H(54A)	4153	6488	8466	169(9)
H(54B)	3252	6145	9023	169(9)
H(54C)	3242	7102	8515	169(9)
H(62A)	8209	4638	6579	169(9)
H(62B)	7764	3898	5750	169(9)
H(62C)	7759	3464	6631	169(9)
H(63A)	5546	2677	5961	169(9)
H(63B)	5946	3198	5188	169(9)
H(63C)	4922	3448	5514	169(9)
H(64A)	6979	5703	6135	169(9)
H(64B)	5658	5311	5953	169(9)
H(64C)	6336	5059	5282	169(9)
H(72A)	8276	5561	7713	169(9)
H(72B)	8340	4959	8519	169(9)
H(72C)	8405	6129	8603	169(9)
H(73A)	6552	6398	7352	169(9)
H(73B)	6824	6802	8308	169(9)
H(73C)	5613	6140	7889	169(9)
H(74A)	6679	4452	9186	169(9)
H(74B)	5638	4917	8924	169(9)
H(74C)	6805	5618	9396	169(9)

Table 5b. Least-squares plane (x,y,z in crystal coordinates) and deviations from that (* indicates atom used to define plane) **for 2.**

- 1.0341 (0.0270) x + 5.3655 (0.0352) y + 14.2358 (0.0284) z = 11.5426 (0.0049)

*	0.0071	(0.0025)	Sn1
*	-0.0133	(0.0046)	O1
*	0.0134	(0.0047)	O2
*	-0.0073	(0.0025)	Sn2
	0.3946	(0.0097)	O3
	0.5089	(0.0098)	Si2
	0.5424	(0.0093)	O4
	0.3250	(0.0096)	Si1

Rms deviation of fitted atoms = 0.0107

Table 6a: HF/(v)TZPa Calculated Structures for **5**, **6**, **7**

Cyclo-[$H_2Si(OSnH_2O)_2SiH_2$] (**5**, D_{2h})

E = -888.822778644

Sn	2.505242	0.000000	0.000000
O	1.339658	1.538402	0.000000
Si	0.000000	2.443734	0.000000
O	-1.339658	1.538402	0.000000
Sn	-2.505242	0.000000	0.000000
O	-1.339658	-1.538402	0.000000
Si	0.000000	-2.443734	0.000000
O	1.339658	-1.538402	0.000000
H	3.397700	0.000000	1.439000
H	3.397700	0.000000	-1.439000
H	0.000000	3.292800	-1.205900
H	0.000000	3.292800	1.205900
H	-3.397700	0.000000	-1.439000
H	-3.397700	0.000000	1.439000
H	0.000000	-3.292800	-1.205900
H	0.000000	-3.292800	1.205900

Frequencies:
10, 15, 31, 34, 54, 71, 108, 216, 351, 360, 412, 424, 432, 460, 527, 529, 576, 576, 704, 744, 765, 776, 783, 790, 830, 830, 1020, 1052, 1075, 1085, 1087, 1091, 1102, 1134, 2027, 2028, 2050, 2051, 2310, 2311, 2340, 2343.
First 4 and 6th mode correspond to out of plane deformations.

Cyclo-[$(H_2SiO)_2(H_2SnO)_2$] (**6**, C_{2v})

E = -888.821427506

Si	0.000000	1.616000	2.477817
O	0.000000	0.000000	2.626293
Si	0.000000	-1.616000	2.477817
O	0.000000	-2.054300	0.927517
Sn	0.000000	-1.886800	-1.003683
O	0.000000	0.000000	-1.385173
Sn	0.000000	1.886800	-1.003683
O	0.000000	2.054300	0.927517
H	-1.206000	2.140000	3.139017
H	1.206000	2.140000	3.139017
H	-1.206000	-2.140000	3.139017
H	1.206000	-2.140000	3.139017
H	-1.436000	-2.576000	-1.583983
H	1.436000	-2.576000	-1.583983
H	-1.436000	2.576000	-1.583983
H	1.436000	2.576000	-1.583983

Frequencies:
9, 23, 46, 49, 58, 80, 110, 226, 305, 340, 383, 401, 455, 510, 542, 574, 581, 606, 682, 751, 753, 777, 789, 799, 823, 838, 919, 1004, 1065, 1077, 1092, 1098, 1122, 1209, 2014, 2016, 2037, 2042, 2327, 2331, 2353, 2362.
First 4 and 6th mode correspond to out of plane deformations.

Cyclo-[$H_2Si(OSiH_2O)_2SnH_2$] (**7**, C_{2v})

E = -1174.58734776

Sn	0.000000	0.000000	1.809438
O	0.000000	1.534818	0.632140
Si	0.000000	2.349429	-0.760374
O	0.000000	1.325580	-2.023766
Si	0.000000	0.000000	-2.953645
O	0.000000	-1.325580	-2.023766
Si	0.000000	-2.349429	-0.760374
O	0.000000	-1.534818	0.632140
H	-1.441352	0.000000	2.695433
H	1.441352	0.000000	2.695433
H	1.207583	3.184781	-0.845032
H	-1.207583	3.184781	-0.845032
H	1.208387	0.000000	-3.787563
H	-1.208387	0.000000	-3.787563
H	1.207583	-3.184781	-0.845032
H	-1.207583	-3.184781	-0.845032

Frequencies:
17, 39, 51, 53, 68, 86, 140, 314, 374, 396, 415, 466, 528, 571, 588, 627, 719, 745, 764, 786, 798, 816, 828, 834, 963, 1043, 1069, 1075, 1078, 1096, 1097, 1121, 1200, 1220, 2035, 2056, 2339, 2340, 2357, 2364, 2365, 2382.
First 4 and 6th mode correspond to out of plane deformations.

Table 6b: B3LYP/(v)TZb Calculated Structures for **4** and **5**

$(H_2SiO)_4$ (**4**, planar, D_{4h})
E = -1464.29829497

Si	-1.603415	1.603415	0.000000
Si	1.603415	1.603415	0.000000
Si	1.603415	-1.603415	0.000000
Si	-1.603415	-1.603415	0.000000
O	0.000000	1.901155	0.000000
O	1.901155	0.000000	0.000000
O	0.000000	-1.901155	0.000000
O	-1.901155	0.000000	0.000000
H	-2.189891	2.189891	1.224274
H	-2.189891	2.189891	-1.224274
H	2.189891	2.189891	1.224274
H	2.189891	2.189891	-1.224274
H	2.189891	-2.189891	1.224274
H	2.189891	-2.189891	-1.224274
H	-2.189891	-2.189891	1.224274
H	-2.189891	-2.189891	-1.224274

$(H_2SiO)_4$ (**4**, puckered, S_4)
E = -1464.29851355

O	1.324353	-1.324353	0.234359
Si	2.250756	-0.000867	-0.004888
O	1.324353	1.324353	-0.234359
Si	0.000867	2.250756	0.004888
O	-1.324353	1.324353	0.234359
Si	-2.250756	0.000867	-0.004888
O	-1.324353	-1.324353	-0.234359
Si	-0.000867	-2.250756	0.004888
H	3.072653	-0.191050	-1.219430
H	3.085618	0.187881	1.200975
H	-0.187881	3.085618	-1.200975
H	0.191050	3.072653	1.219430
H	-3.072653	0.191050	-1.219430
H	-3.085618	-0.187881	1.200975
H	-0.191050	-3.072653	1.219430
H	0.187881	-3.085618	-1.200975

Cyclo-$[H_2Si(OSnH_2O)_2SiH_2]$ (**5**, planar, D_{2h})
E = -891.895281853

Sn	2.505132	0.000000	0.000000
O	1.361140	1.575613	0.000000
Si	0.000000	2.464169	0.000000
O	-1.361140	1.575613	0.000000
Sn	-2.505132	0.000000	0.000000
O	-1.361140	-1.575613	0.000000
Si	0.000000	-2.464169	0.000000
O	1.361140	-1.575613	0.000000
H	3.377417	0.000000	1.459536
H	3.377417	0.000000	-1.459536
H	0.000000	3.313419	-1.220093
H	0.000000	3.313419	1.220093
H	-3.377417	0.000000	-1.459536
H	-3.377417	0.000000	1.459536
H	0.000000	-3.313419	-1.220093
H	0.000000	-3.313419	1.220093

Cyclo-$[H_2Si(OSnH_2O)_2SiH_2]$ (**5**, puckered, D_2)
E = -891.898595794

Sn	0.000000	2.420455	0.000000
O	1.479000	1.250000	0.535000
Si	2.384100	0.000000	0.000000
O	1.479000	-1.250000	-0.535000
Sn	0.000000	-2.420455	0.000000
O	-1.479000	-1.250000	0.535000
Si	-2.384100	0.000000	0.000000
O	-1.479000	1.250000	-0.535000
H	0.433400	3.292000	-1.394000
H	-0.433400	3.292000	1.394000
H	3.229000	-0.434100	1.143000
H	3.229000	0.434100	-1.143000
H	0.433400	-3.292000	1.394000
H	-0.433400	-3.292000	-1.394000
H	-3.229000	0.434100	1.143000
H	-3.229000	-0.434100	-1.143000

Table 6c: B3LYP/(v)TZb Calculated Structures for **6** and **7**

Cyclo-[$(H_2SiO)_2(H_2SnO)_2$] (**6**, planar, C_{2v})
E = -891.894733202

Si	0.000000	1.627500	2.474784
O	0.000000	0.000000	2.563495
Si	0.000000	-1.627500	2.474784
O	0.000000	-2.155757	0.941863
Sn	0.000000	-1.901507	-0.999450
O	0.000000	0.000000	-1.405351
Sn	0.000000	1.901507	-0.999450
O	0.000000	2.155757	0.941863
H	-1.220000	2.122000	3.157004
H	1.220000	2.122000	3.157004
H	-1.220000	-2.122000	3.157004
H	1.220000	-2.122000	3.157004
H	-1.457000	-2.566500	-1.577996
H	1.457000	-2.566500	-1.577996
H	-1.457000	2.566500	-1.577996
H	1.457000	2.566500	-1.577996

Cyclo-[$(H_2SiO)_2(H_2SnO)_2$] (**6**, puckered, C_1)
E = -891.896757823

Si	-1.551832	2.343723	0.452251
O	-0.174285	2.528687	-0.416861
Si	1.458915	2.395749	-0.494283
O	1.992036	1.021918	0.192202
Sn	1.849131	-0.939354	0.164092
O	0.059214	-1.410093	-0.460121
Sn	-1.820725	-0.974920	-0.157661
O	-1.863770	0.772612	0.748685
H	-1.415255	3.033966	1.757777
H	-2.640521	2.943947	-0.357725
H	2.069146	3.534288	0.232962
H	1.809666	2.434115	-1.936118
H	2.064798	-1.432448	1.780798
H	2.944855	-1.535591	-0.993950
H	-2.488188	-2.077381	0.954634
H	-2.569525	-0.844811	-1.682707

Cyclo-[$H_2Si(OSiH_2O)_2SnH_2$] (**7**, planar, C_{2v})
E = -1178.09784263

Sn	0.000000	0.000000	1.807023
O	0.000000	1.578697	0.658480
Si	0.000000	2.364482	-0.760976
O	0.000000	1.342280	-2.035266
Si	0.000000	0.000000	-2.955230
O	0.000000	-1.342280	-2.035266
Si	0.000000	-2.364482	-0.760976
O	0.000000	-1.578697	0.658480
H	-1.461856	0.000000	2.672649
H	1.461856	0.000000	2.672649
H	1.221578	3.199678	-0.852590
H	-1.221578	3.199678	-0.852590
H	1.223057	0.000000	-3.788478
H	-1.223057	0.000000	-3.788478
H	1.221578	-3.199678	-0.852590
H	-1.221578	-3.199678	-0.852590

Cyclo-[$H_2Si(OSiH_2O)_2SnH_2$] (**7**, puckered, C_1)
E = -1178.09893476

Sn	-1.776663	-0.007054	-0.042308
O	-0.614034	1.536781	-0.369528
Si	0.718352	2.304383	0.165464
O	2.040087	1.341639	0.126043
Si	2.920163	-0.015233	-0.068041
O	1.960652	-1.305185	-0.358066
Si	0.731484	-2.304703	0.061560
O	-0.594939	-1.472524	0.509757
H	-2.499658	-0.383016	-1.533428
H	-2.777043	0.317387	1.291254
H	0.531300	2.737360	1.573894
H	0.966292	3.462496	-0.722065
H	3.695354	-0.246025	1.173076
H	3.806966	0.152328	-1.239087
H	1.152749	-3.138097	1.211752
H	0.443054	-3.137672	-1.131387