

Electronic supplementary information (ESI)

Monoorganooxotin Cage, Diorganotin Ladders, Diorganotin Double Chain and Triorganotin Single Chain Formed with Phosphonate and Arsonate Ligands

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Table S1. Selected bond lengths [Å] and angles [°] for compounds 1-5^a

Compound 1			
O(1)-Sn(1)	2.144(3)	O(5)-P(2)	1.525(3)
O(1)-Sn(2)	2.152(3)	O(5)-Sn(1)	2.076(3)
O(2)-Sn(3)	2.120(4)	O(6)-P(2)	1.529(4)
O(2)-Sn(2)	2.181(4)	O(6)-Sn(3)	2.082(3)
O(3)-Sn(3)	2.142(3)	O(7)-P(2)	1.515(3)
O(3)-Sn(1)	2.187(4)	O(8)-P(1)	1.531(3)
O(4)-Sn(2)	2.050(3)	O(9)-P(1)	1.531(4)
O(4)-Sn(1)	2.054(3)	O(10)-P(1)	1.526(3)
O(4)-Sn(3)	2.081(3)	O(10)-Sn(1)	2.075(3)
Sn(1)-O(1)-Sn(2)	101.87(12)	O(10)-Sn(1)-O(3)	167.00(12)
Sn(3)-O(2)-Sn(2)	100.66(13)	O(5)-Sn(1)-O(3)	84.50(13)
Sn(3)-O(3)-Sn(1)	100.06(14)	O(1)-Sn(1)-O(3)	92.99(13)
Sn(2)-O(4)-Sn(1)	108.72(13)	O(4)-Sn(2)-O(1)	74.48(11)
Sn(2)-O(4)-Sn(3)	106.55(13)	O(4)-Sn(2)-O(2)	74.68(12)
Sn(1)-O(4)-Sn(3)	106.72(13)	O(1)-Sn(2)-O(2)	92.71(14)
O(4)-Sn(1)-O(10)	93.24(13)	O(4)-Sn(3)-O(6)	86.61(12)
O(4)-Sn(1)-O(5)	87.64(11)	O(4)-Sn(3)-O(2)	75.41(12)
O(10)-Sn(1)-O(5)	89.36(12)	O(6)-Sn(3)-O(2)	161.99(14)
O(4)-Sn(1)-O(1)	74.59(11)	O(4)-Sn(3)-O(3)	75.55(13)
O(10)-Sn(1)-O(1)	89.34(13)	O(6)-Sn(3)-O(3)	90.16(13)
O(5)-Sn(1)-O(1)	162.08(12)	O(2)-Sn(3)-O(3)	86.43(14)
O(4)-Sn(1)-O(3)	75.11(13)		
Compound 2			
O(4)-Sn(1)	2.133(4)	Sn(1)-O(1)	2.023(4)
O(5)-Sn(2)	2.173(4)	Sn(3)-O(3)	2.152(4)
O(6)-Sn(3)	1.994(4)	O(2)-Sn(1)#1	2.148(5)
O(7)-Sn(2)	2.019(4)	O(9)-Sn(2)#2	2.165(5)
O(8)-Sn(3)	2.159(4)		
O(1)-Sn(1)-O(4)	86.02(17)	O(9)#2-Sn(2)-O(5)	175.75(17)
O(1)-Sn(1)-O(2)#1	84.85(16)	O(6)-Sn(3)-O(3)	84.54(17)
O(4)-Sn(1)-O(2)#1	170.61(18)	O(6)-Sn(3)-O(8)	87.63(18)
O(7)-Sn(2)-O(9)#2	88.68(18)	O(3)-Sn(3)-O(8)	172.16(17)
O(7)-Sn(2)-O(5)	88.05(17)		
Compound 3			

O(1)-As(1)	1.662(5)	O(2)-Sn(1)#1	2.020(6)
O(1)-Sn(1)	2.146(5)	O(3)-As(1)	1.662(6)
O(2)-As(1)	1.695(5)	O(3)-Sn(1)#2	2.177(5)
As(1)-O(1)-Sn(1)	132.3(3)	O(1)-As(1)-O(2)	111.0(3)
As(1)-O(2)-Sn(1)#1	135.4(3)	O(2)#1-Sn(1)-O(1)	87.6(2)
As(1)-O(3)-Sn(1)#2	134.5(3)	O(2)#1-Sn(1)-O(3)#3	83.8(2)
O(3)-As(1)-O(1)	111.5(3)	O(1)-Sn(1)-O(3)#3	168.0(2)
O(3)-As(1)-O(2)	108.0(3)		

Compound 4

As(1)-O(4)	1.654(3)	O(1)-Sn(1)	2.494(3)
As(1)-O(5)	1.664(3)	O(2)-Sn(1)#1	2.528(3)
As(1)-O(6)	1.706(3)	O(3)-S(1)	1.445(3)
O(1)-S(1)	1.459(3)	O(4)-Sn(1)#2	2.099(3)
O(2)-S(1)	1.443(4)	O(5)-Sn(1)	2.082(3)
O(5)-Sn(1)-O(4)#2	89.98(13)	O(4)#2-Sn(1)-O(1)	170.26(12)
O(5)-Sn(1)-C(1)	97.74(16)	C(1)-Sn(1)-O(1)	86.10(16)
O(4)#2-Sn(1)-C(1)	92.76(17)	C(5)-Sn(1)-O(1)	81.76(16)
O(5)-Sn(1)-C(5)	102.10(17)	O(5)-Sn(1)-O(2)#1	174.62(11)
O(4)#2-Sn(1)-C(5)	102.82(17)	O(4)#2-Sn(1)-O(2)#1	84.67(13)
C(1)-Sn(1)-C(5)	154.6(2)	C(1)-Sn(1)-O(2)#1	83.13(16)
O(5)-Sn(1)-O(1)	80.60(13)	C(5)-Sn(1)-O(2)#1	78.60(17)
O(1)-Sn(1)-O(2)#1	104.77(13)		

Compound 5

O(1)-As(1)	1.591(5)	O(4)-As(2)	1.665(6)
O(1)-Sn(2)	2.130(5)	O(4)-Sn(3)	1.992(6)
O(2)-As(1)	1.696(5)	O(5)-As(2)	1.587(5)
O(2)-Sn(4)	1.968(5)	O(5)-Sn(2)#1	2.154(5)
O(3)-As(1)	1.681(5)	O(6)-As(2)	1.663(5)
O(3)-Sn(1)	2.251(5)	O(6)-Sn(1)	2.251(5)
O(6)-Sn(1)-O(3)	175.9(2)	O(4)-Sn(3)-C(43)	114.7(2)
C(61)-Sn(2)-O(1)	86.9(2)	C(37)-Sn(3)-C(43)	111.5(3)
C(61)-Sn(2)-C(67)	126.3(2)	O(4)-Sn(3)-C(49)	100.7(3)
O(1)-Sn(2)-C(67)	95.4(2)	C(37)-Sn(3)-C(49)	116.4(2)
C(61)-Sn(2)-C(55)	116.9(2)	C(43)-Sn(3)-C(49)	109.7(2)
O(1)-Sn(2)-C(55)	88.75(19)	O(2)-Sn(4)-C(7)	102.0(3)
C(67)-Sn(2)-C(55)	116.9(2)	O(2)-Sn(4)-C(1)	103.7(3)
C(61)-Sn(2)-O(5)#2	91.8(2)	C(7)-Sn(4)-C(1)	121.0(3)
O(1)-Sn(2)-O(5)#2	176.9(2)	O(2)-Sn(4)-C(13)	95.2(3)

C(67)-Sn(2)-O(5)#2	83.0(3)	C(7)-Sn(4)-C(13)	111.8(3)
C(55)-Sn(2)-O(5)#2	94.3(2)	C(1)-Sn(4)-C(13)	117.5(3)
O(4)-Sn(3)-C(37)	103.4(3)		

^aSymmetry codes. For **1** #1 -x+1, -y+1, -z. For **2** #1 -x+2, -y+2, -z+1; #2 -x+1, -y+2, -z. For **3** #1 -x+1, y, -z+3/2; #2 x, -y+1, z+1/2; x, -y+1, z-1/2. For **4** #1 -x+1, -y+1, -z+2; -x+1, -y, -z+2. For **5** #1 x+1, y, z; #2 x-1, y, z.