Supporting Information

Assembly of Hexa- and Trinuclear Monoorganostannoxanes: Hemi-Labile Nature of Intramolecular N→Sn Coordination in RSnCl₃ (R = 2-phenylazophenyl)

Ramesh K. Metre,a Chandrajeet Mohapatra,a Dipankar Sahooa and Vadapalli Chandrasekhar*a,b

a Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India.

b Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, 21, Brundavan Colony, Narsingi, Hyderabad-500075, India.
Figure S1  a) Molecular structure of 1. Hydrogen atoms have been omitted for the sake of clarity.

b) Core structure of 1. Some atoms (Carbon, Nitrogen, Hydrogen) have been omitted for the sake of clarity. Bond distance (Å) and bond angle (°) parameters; Sn(4)-O(17) 2.070(5), Sn(4)-O(20)' 2.084(6), Sn(4)-O(18) 2.128(6), Sn(4)-C(1) 2.154(9), Sn(5)-O(12)' 2.063(6), Sn(5)-O(18) 2.110(6), Sn(5)-O(19) 2.115(6), Sn(6)-O(20) 2.088(5), Sn(6)-O(15) 2.096(5), Sn(6)-O(19) 2.127(6); Sn(6)-O(17)-Sn(4) 133.3(3), Sn(6)-O(17)-Sn(5) 105.2(3), Sn(4)-O(17)-Sn(5) 105.7(2), Sn(5)-O(18)-Sn(4) 102.4(2), Sn(5)-O(19)-Sn(6) 101.1(2), Sn(4)'-O(20)-Sn(6) 147.3(3), Sn(4)-O(18)-Sn(5) 102.421(2), Sn(4)'-O(20)-Sn(6) 147.3(3).
**Figure S2** Coordination environment of Sn in 1
**Figure S3** Coordination environment of Sn in 2
**Figure S4.** a) Molecular structure of 3. Hydrogen atoms have been omitted for the sake of clarity. b) Core structure of 3. Some atoms (Carbon, Nitrogen, Hydrogen) have been omitted for the sake of clarity. Bond distance (Å) and bond angle (°) parameters; Sn(1) -O(12) 2.059(7), Sn(1) -O(9) 2.052(7), Sn(1) -O(10) 2.113(9), Sn(2) -O(11) 2.072(7), Sn(2) -O(9) 2.064(7), Sn(2) -O(10) 2.094(7), Sn(3) -O(11) 2.095(7), Sn(3) -O(9) 2.078(7); Sn(1) -O(9) -Sn(2) 105.8(3), Sn(1) -O(9) -Sn(3) 133.6(3), Sn(2) -O(11) -Sn(3) 105.8(3), Sn(1) -O(12) -Sn(3) 152.2(4), Sn(2) -O(11) -Sn(3) 104.9(3), Sn(2) -O(10) -Sn(1) 102.6(3).
**Figure S5** Coordination environment of Sn in 3
Figure S6 Coordination environment of Sn in 4
Figure S7 ESI MS of 4
Figure S8. ESI MS pattern of 4. a) Experimental b) Simulated
**Figure S9.** $^{119}$Sn NMR spectrum of 4
Figure S10. $^{31}$P NMR spectrum of 4
Figure S11. a) Molecular structure of 5. Hydrogen atoms have been omitted for the sake of clarity. b) Core structure of 5. Some atoms (Carbon, Nitrogen, Hydrogen) have been omitted for the sake of clarity. Bond distance (Å) and bond angle (°) parameters; Sn(1)-O(9) 2.083(5), Sn(1)-O(1) 2.088(5), Sn(1)-O(6) 2.092(5), Sn(1)-O(8) 2.118(6), Sn(2)-O(9) 2.066(5), Sn(2)-O(7) 2.093(5), Sn(3)-O(9) 2.068(5), Sn(3)-O(5) 2.091(5); O(9)-Sn(1)-O(1) 86.63(19), O(9)-Sn(2)-O(3) 86.31(19), O(9)-Sn(1)-O(6) 84.03(18), O(1)-Sn(1)-O(6) 91.20(19), O(9)-Sn(2)-O(3) 83.98(18), O(7)-Sn(2)-O(2) 162.50(19), O(2)-Sn(2)-O(3) 89.88(18), O(5)-Sn(3)-O(4) 86.91(19), O(9)-Sn(3)-O(5) 85.71(18), O(9)-Sn(3)-O(7) 76.20(19)
Figure S12 Coordination environment of Sn in 5
Figure S13 ESI MS of 5
Figure S14. ESI MS pattern of 5. a) Experimental b) Simulated
Figure S15. $^{119}$Sn NMR spectrum of 5
Figure S16. $^{31}$P NMR spectrum of 5