Electronic Supplementary Material (ESI) for Dalton Transactions
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Supporting Information

Assembly of Hexa- and Trinuclear Monoorganostannoxanes: Hemi-Labile Nature of Intramolecular N→Sn Coordination in $RSnCl_3$ (R = 2-phenylazophenyl)

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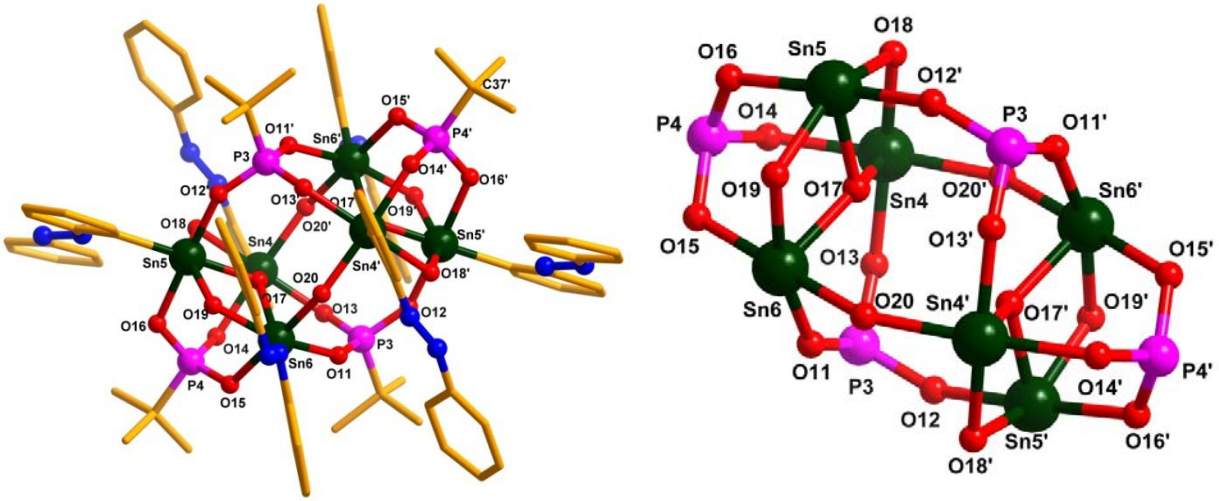

a) b)

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).

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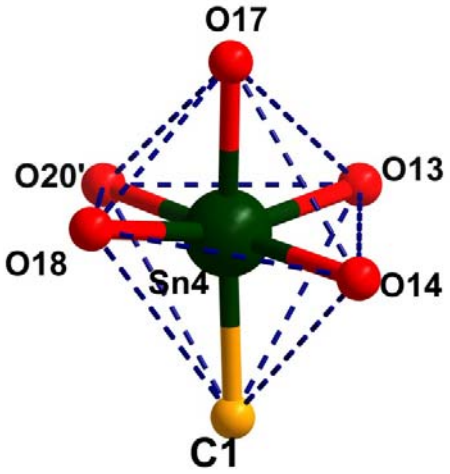

Figure S2 Coordination environment of Sn in **1**

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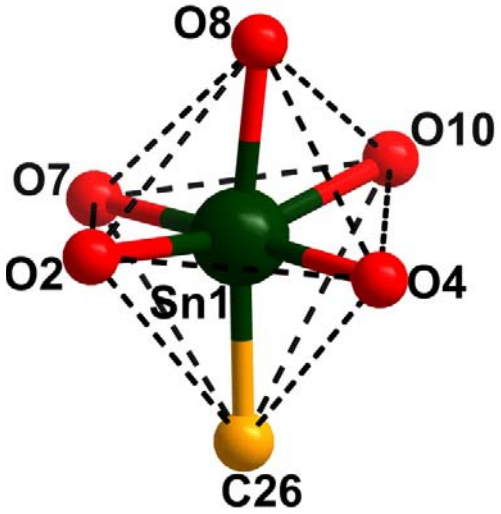
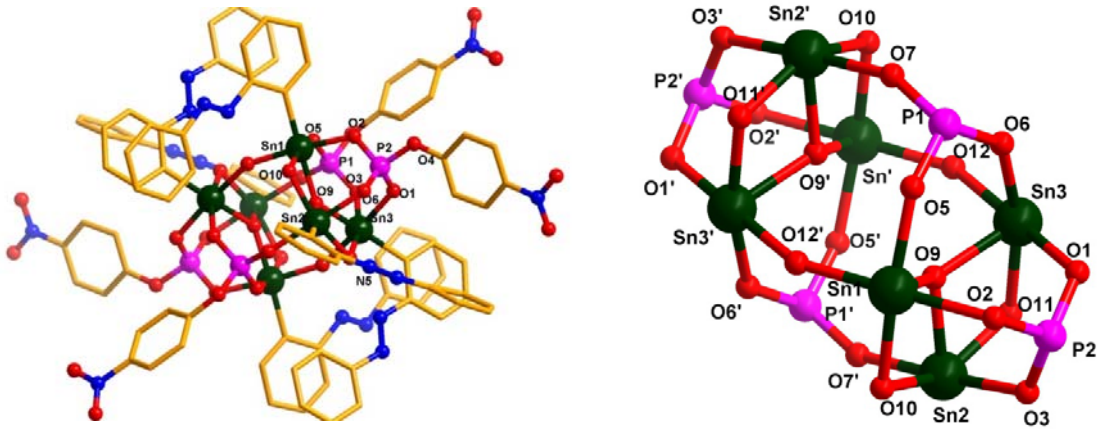


Figure S3 Coordination environment of Sn in **2**



a) b)

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(9) -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).

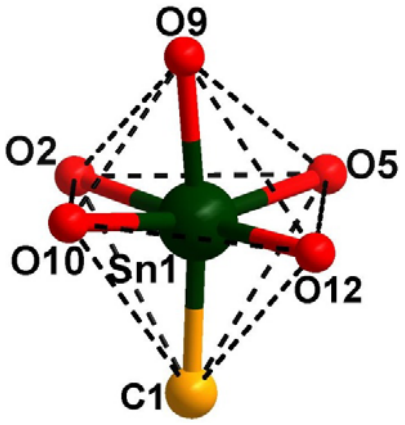


Figure S5 Coordination environment of Sn in **3**

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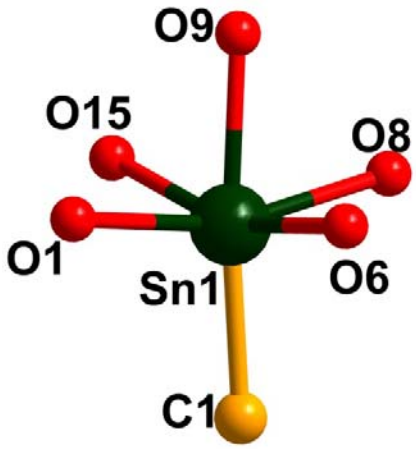

Figure S6 Coordination environment of Sn in **4**

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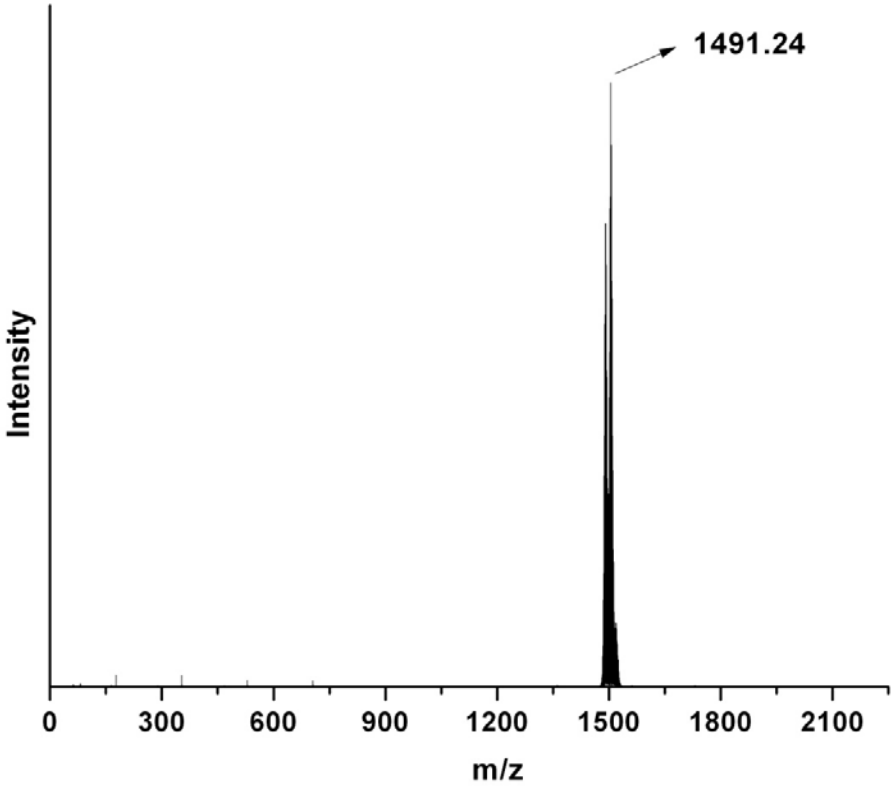
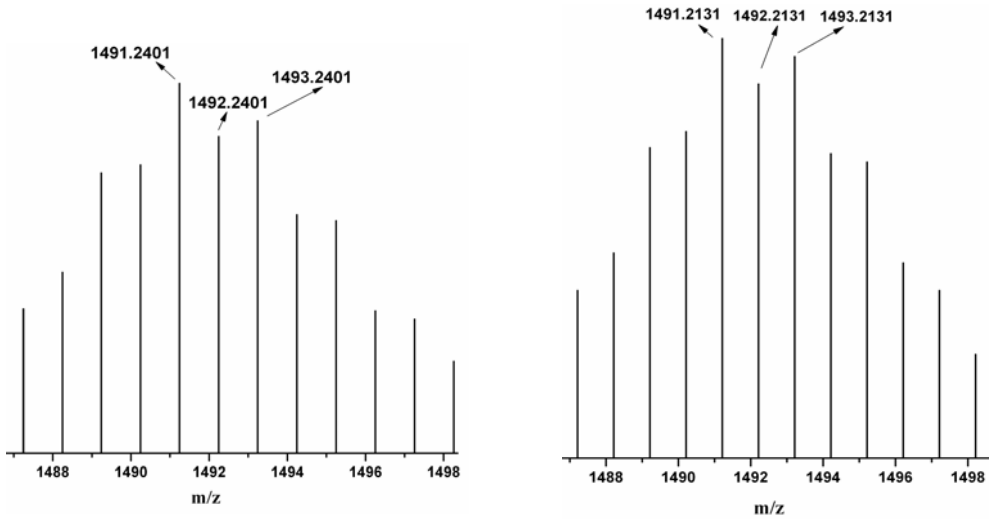


Figure S7 ESI MS of **4**



a) **b)**

Figure S8. ESI MS pattern of **4**. a) Experimental b) Simulated

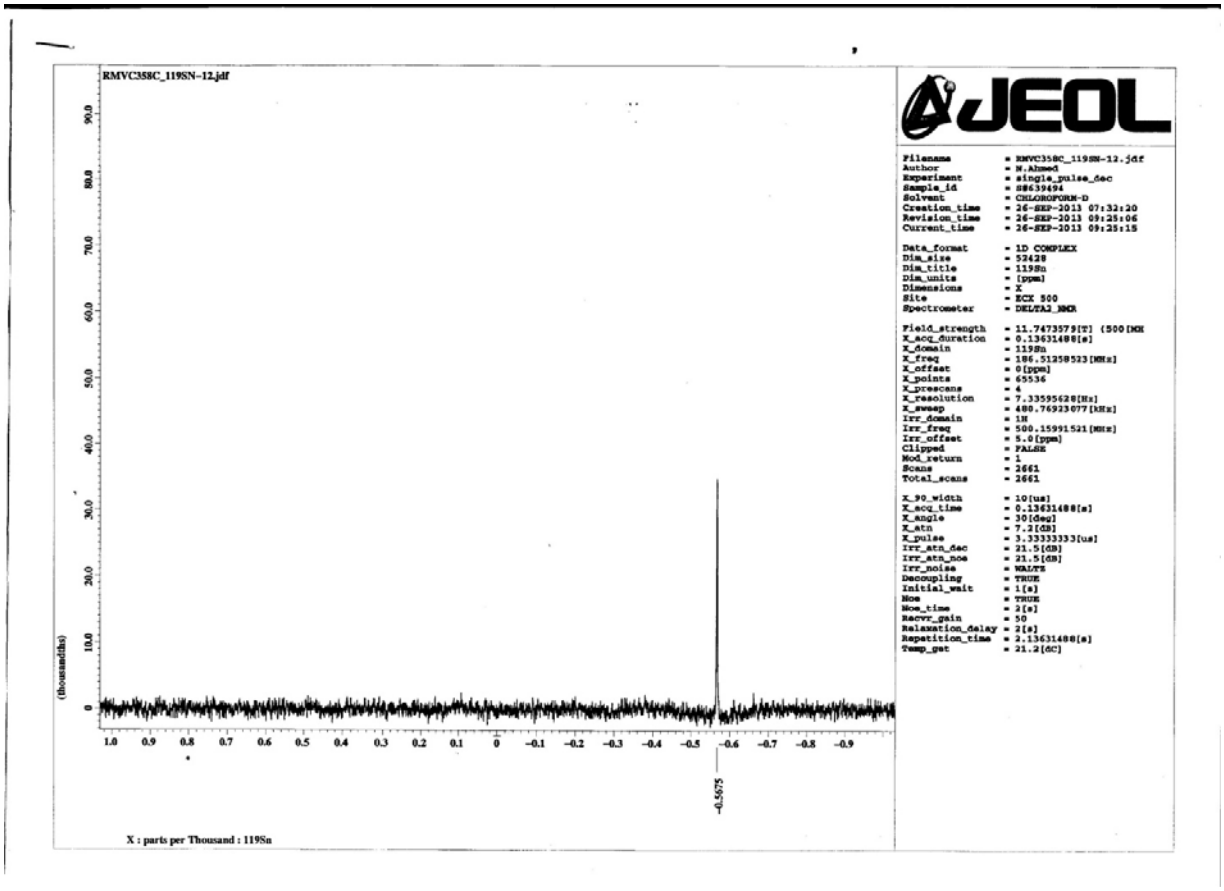


Figure S9. ^{119}Sn NMR spectrum of **4**

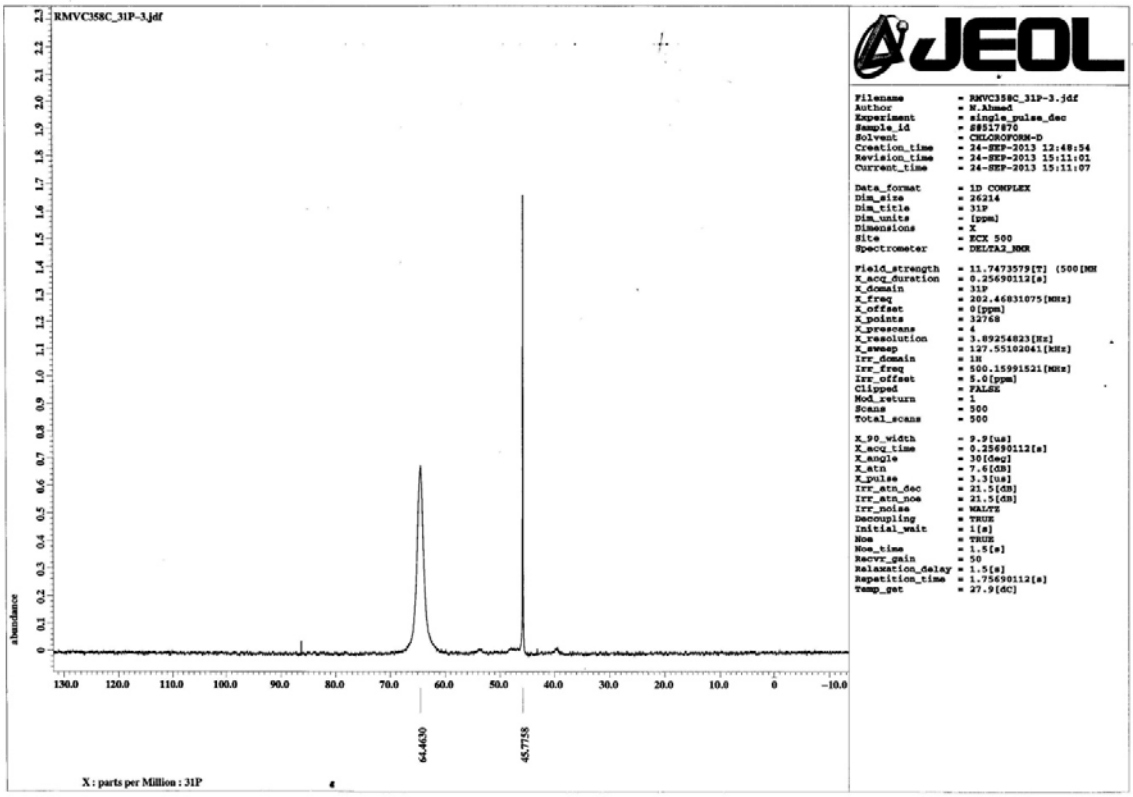
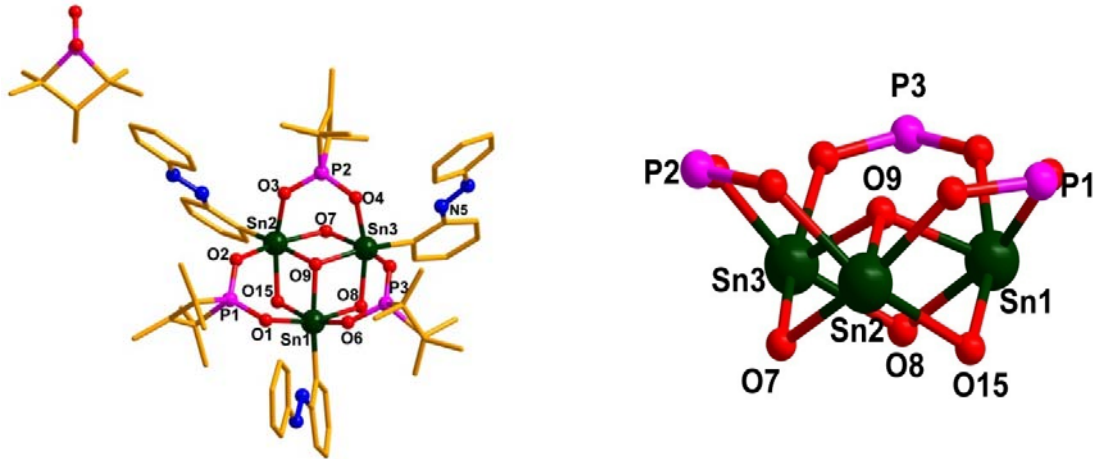


Figure S10. ^{31}P NMR spectrum of **4**



a) **b)**

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(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)

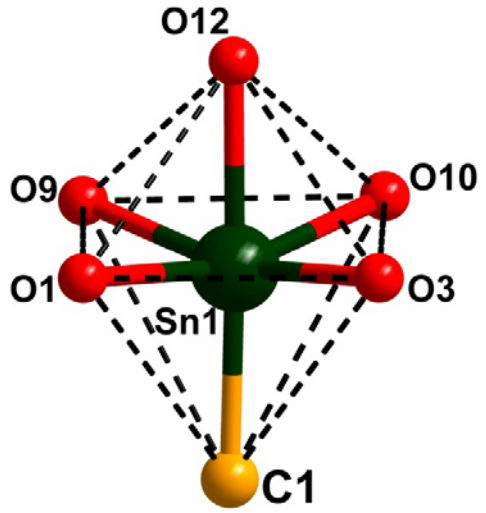


Figure S12 Coordination environment of Sn in **5**

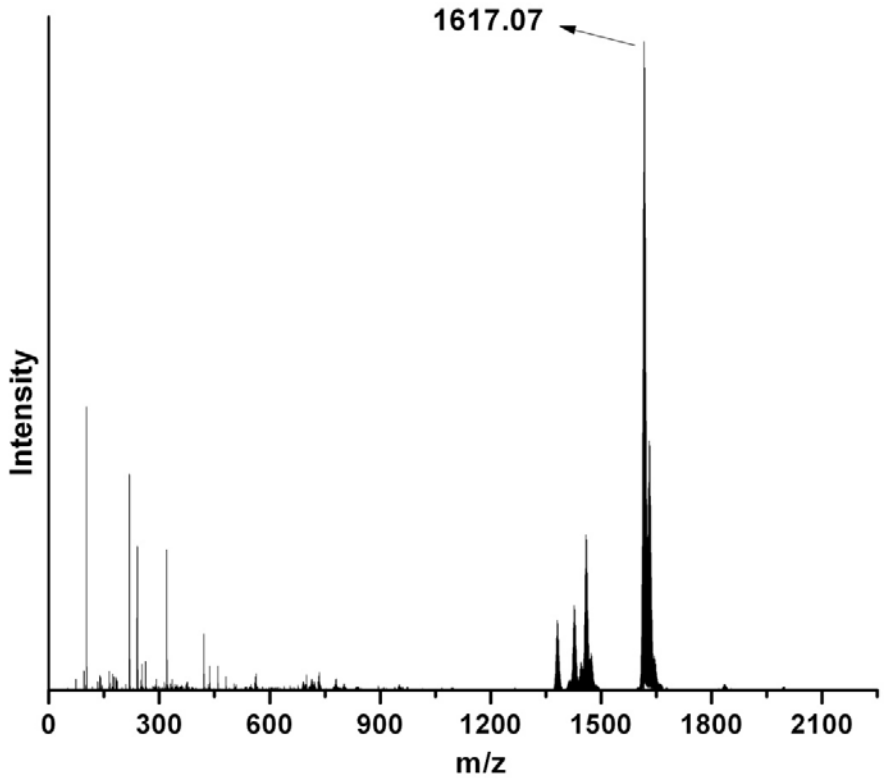


Figure S13 ESI MS of **5**

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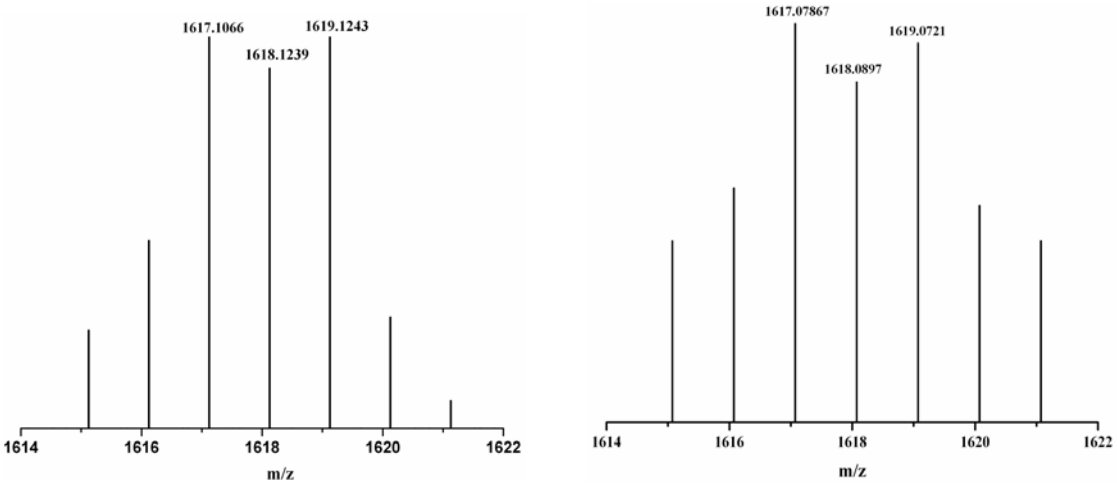

Figure S14.ESI MS pattern of **5**. a) Experimental b) Simulated

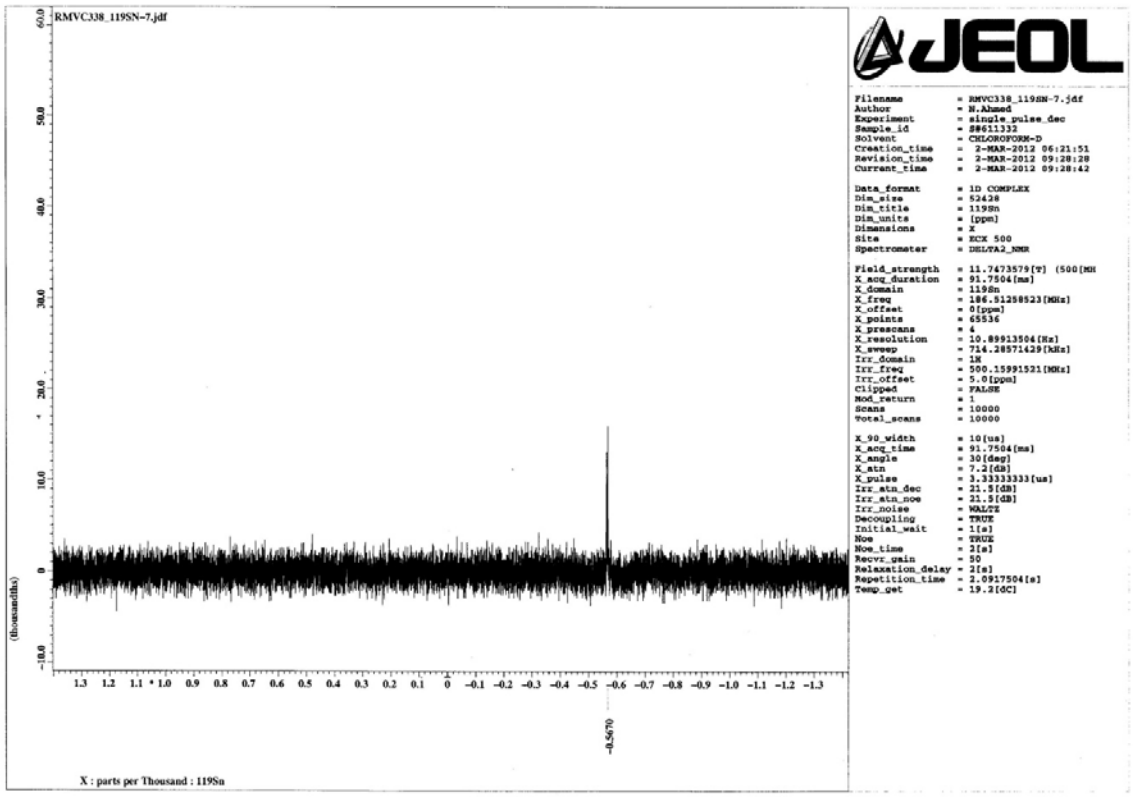

Figure S15. ^{119}Sn NMR spectrum of **5**

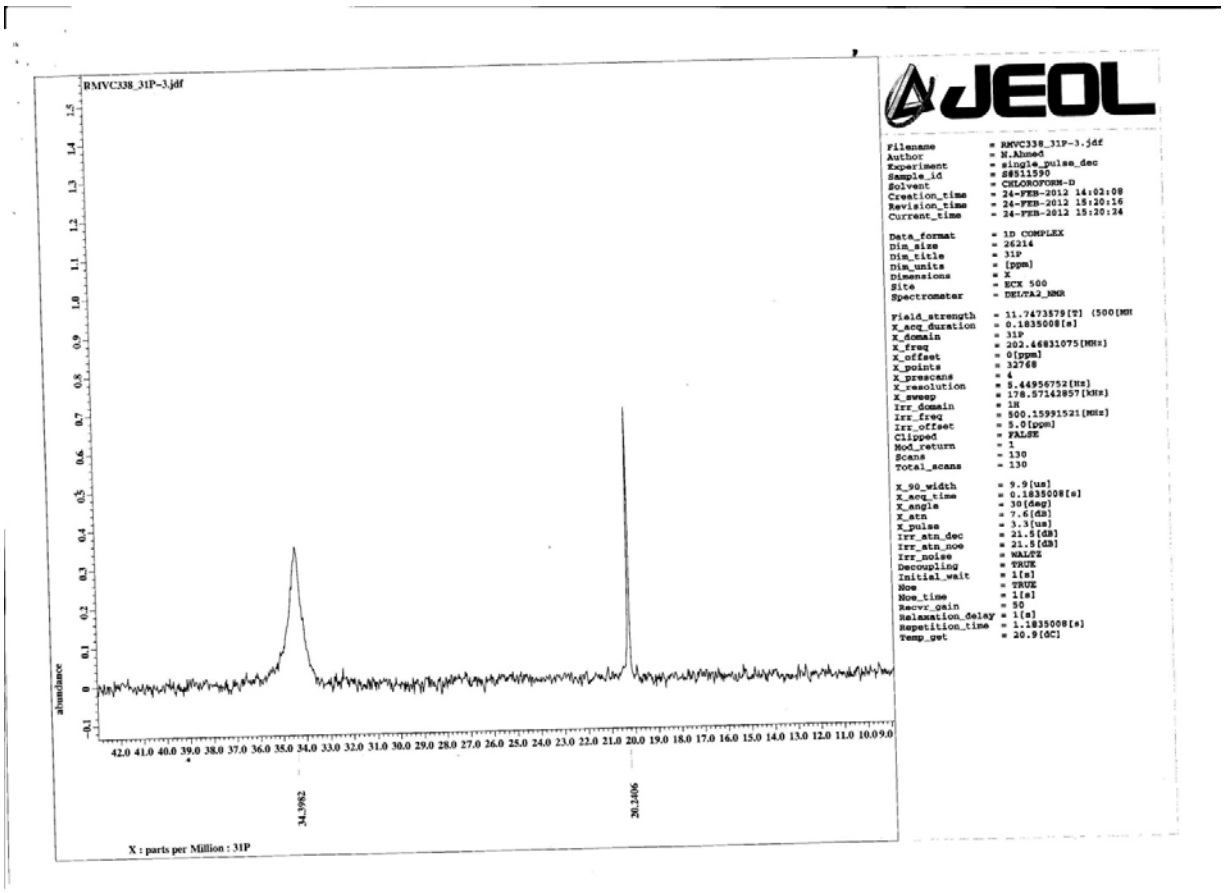

Figure S16. ^{31}P NMR spectrum of **5**