Electronic Supplementary Information for Dalton Transactions

Coordination Polymers Containing Ferrocene Backbone. Synthesis, Structure and Electrochemistry

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Alternate procedure for the synthesis of **3-6**:

A mixture of **2** (0.050 g, 0.050 mmol), 4-methylpyridine (0.005 g) /4,4′-bipyridine (0.008 g) or 4,4′-trimethylenebipyridine (0.010 g) or 4,4′-vinylenebipyridine (0.009 g) were heated in toluene (20 mL) under reflux for 2h. The reaction mixture was cooled and the solvent removed in vacuo to afford a yellow solid. This was washed with hexane (10 mL), Et_2O (2 mL) dried and recrystallised to give pure samples of **3-6**.

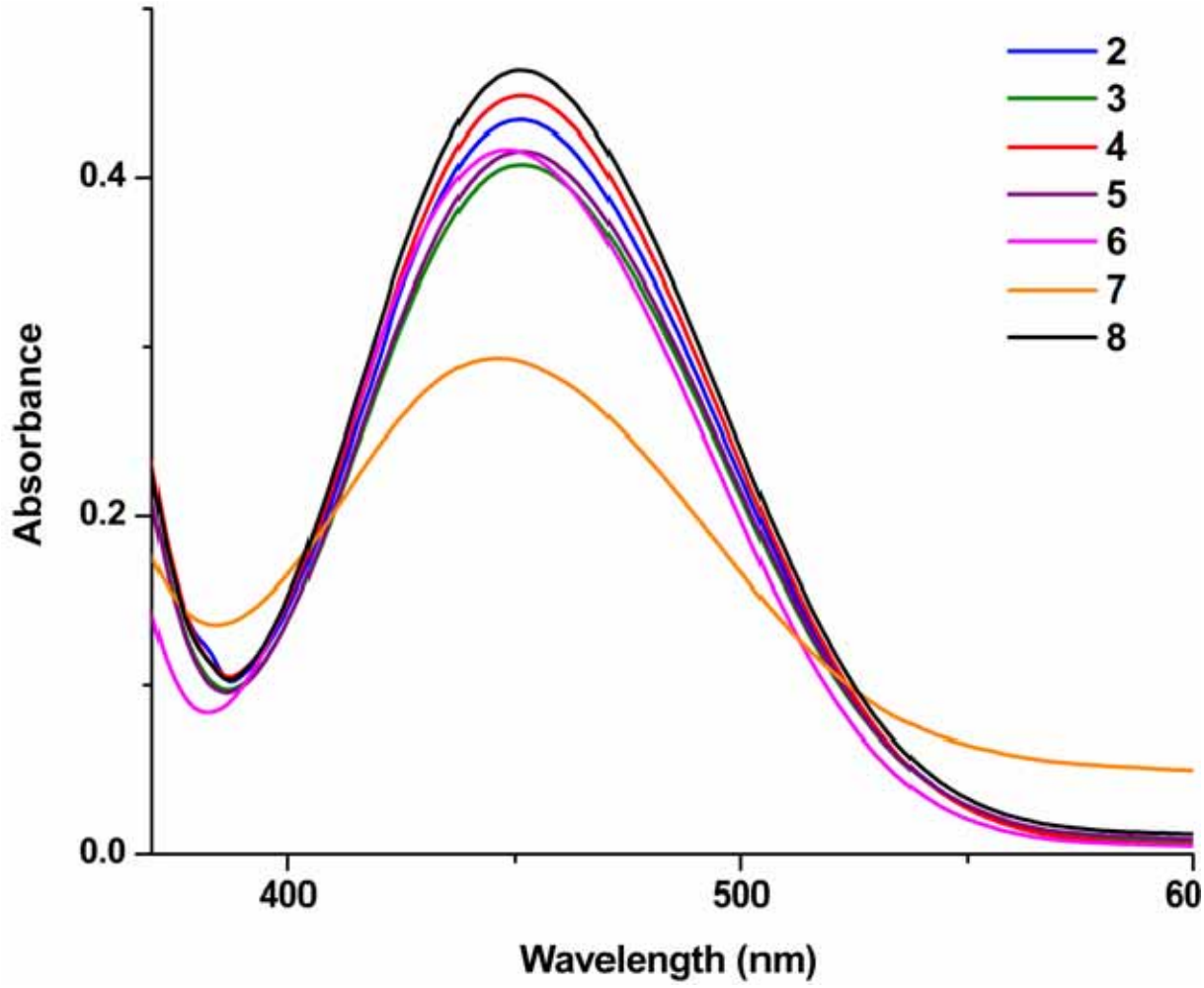

Figure S1. UV-visible spectra of **2-8**.

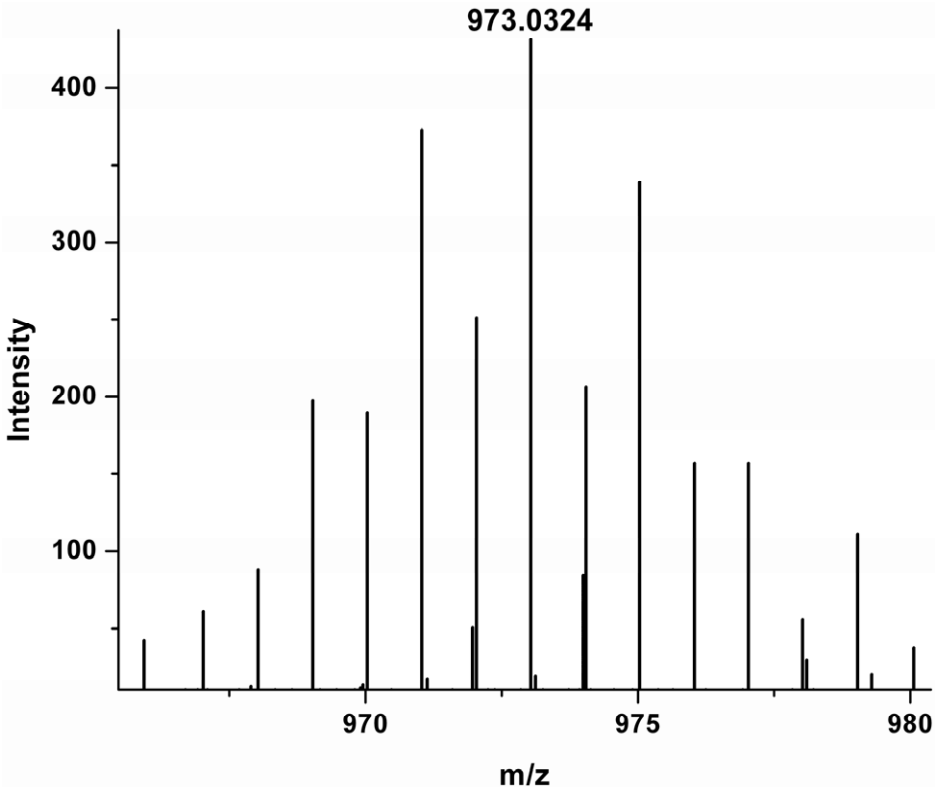

Figure S2. ESI-MS of **2**.

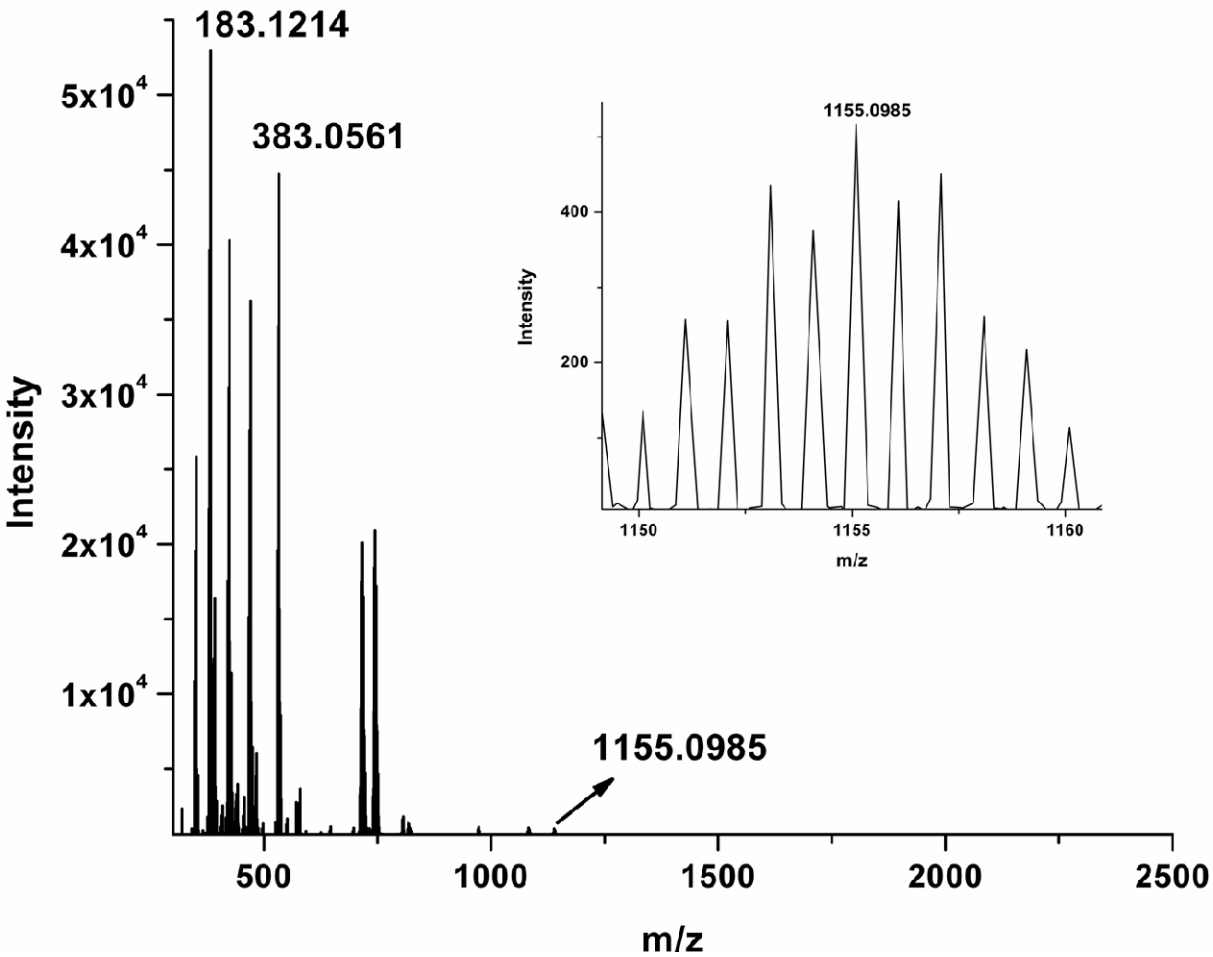

Figure S3. ESI-MS of **6**. Inset picture shows the isotopic pattern of $[(Ph_3Sn)_2LH(bpe)]^+$.

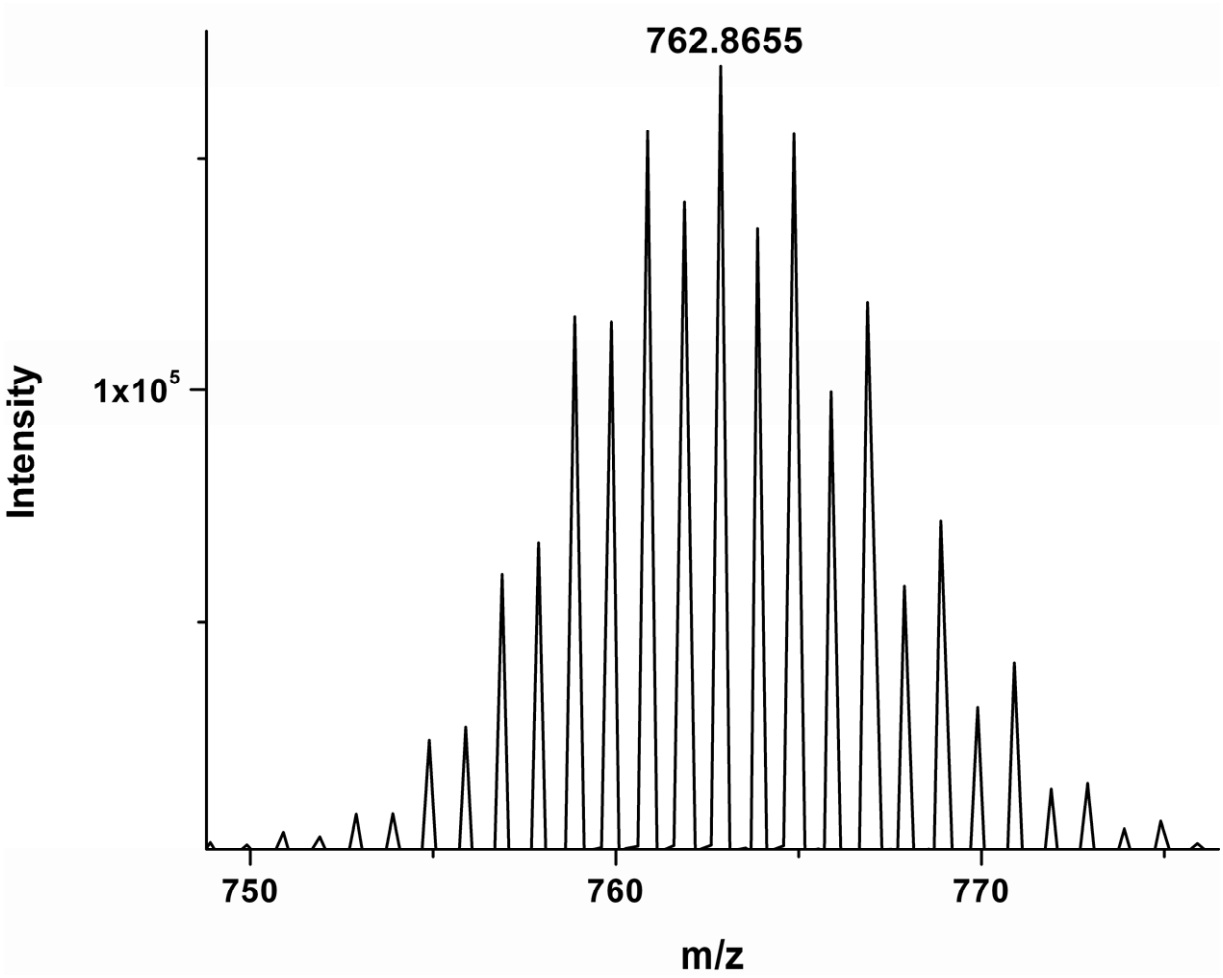

Figure S4. ESI-MS of **7**.

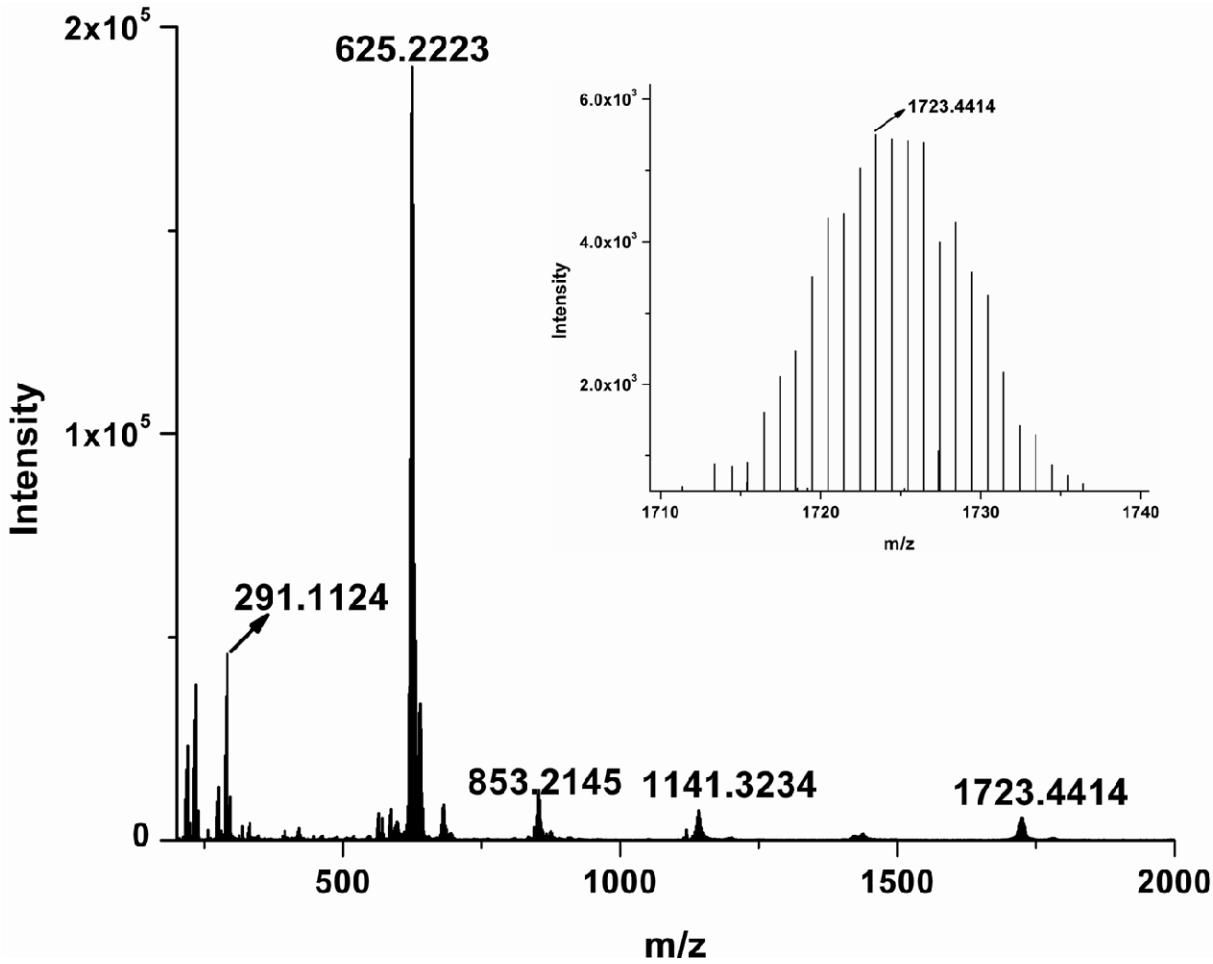

Figure S5. ESI-MS of **8**. Inset picture shows the isotopic pattern of $[(n\text{-}Bu_3Sn)_4(L)(LH)]^+$.

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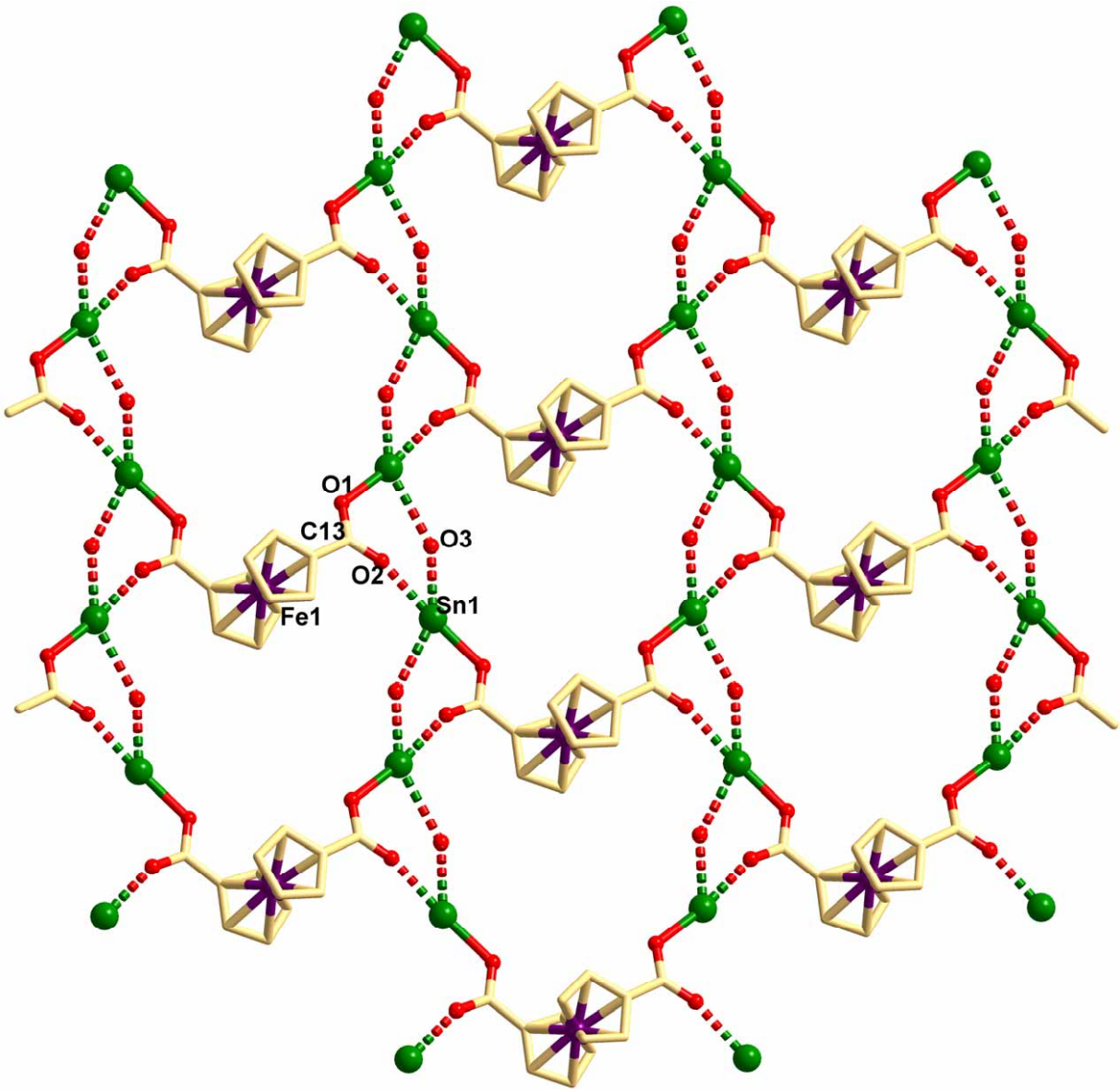

Figure S6. 2D polymeric structure of **8**. Hydrogen atoms have been omitted.

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Supramolecular structures of **2** and **5**

Compound **2** shows an interesting supramolecular assembly in the solid-state due to two different types of π-stacking interactions. A C-H… π interaction between the ferrocenyl C-H and the aromatic phenyl substituent on the tin (H22…π 2.5025(2) Å) leads to the formation of a 1D polymer. Further, two such 1D polymers are interconnected by C-H of the edge of aryl with face of other aryl groups leading to a 2D polymer (H42…π 3.4894 (42); H41…π 3.0791 (41); H38…π 2.8697 (41); H39…π 3.2544 (41) Å) (Figure S7). In compound **5** we have observed interaction between two 1D polymers through dichloromethane due to two different C-H…Cl interactions (H10…Cl2 2.8622(26) and H37…Cl1 2.8528(20) Å) between the chlorine atoms of dichloromethane and the C-H of the aryl group and a ferrocenyl group (Figure S8).

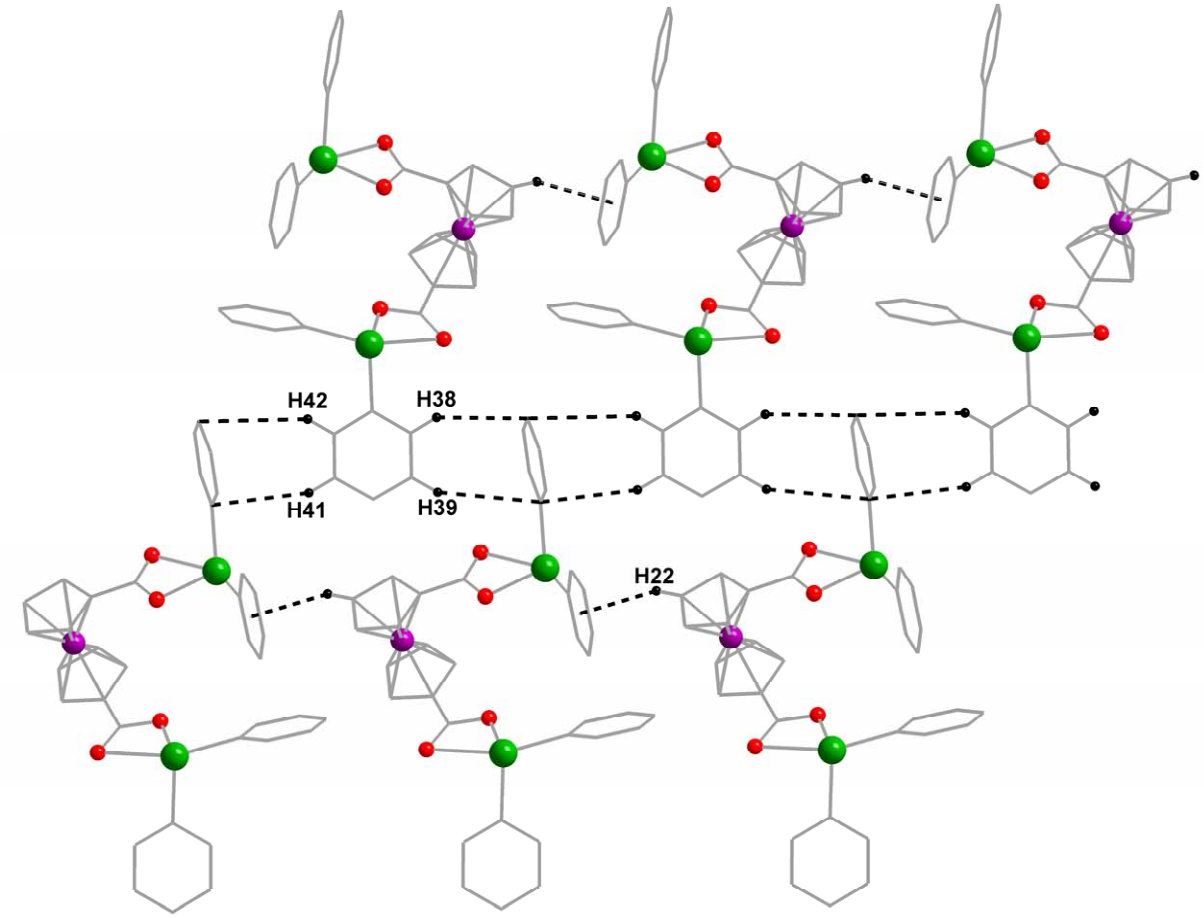
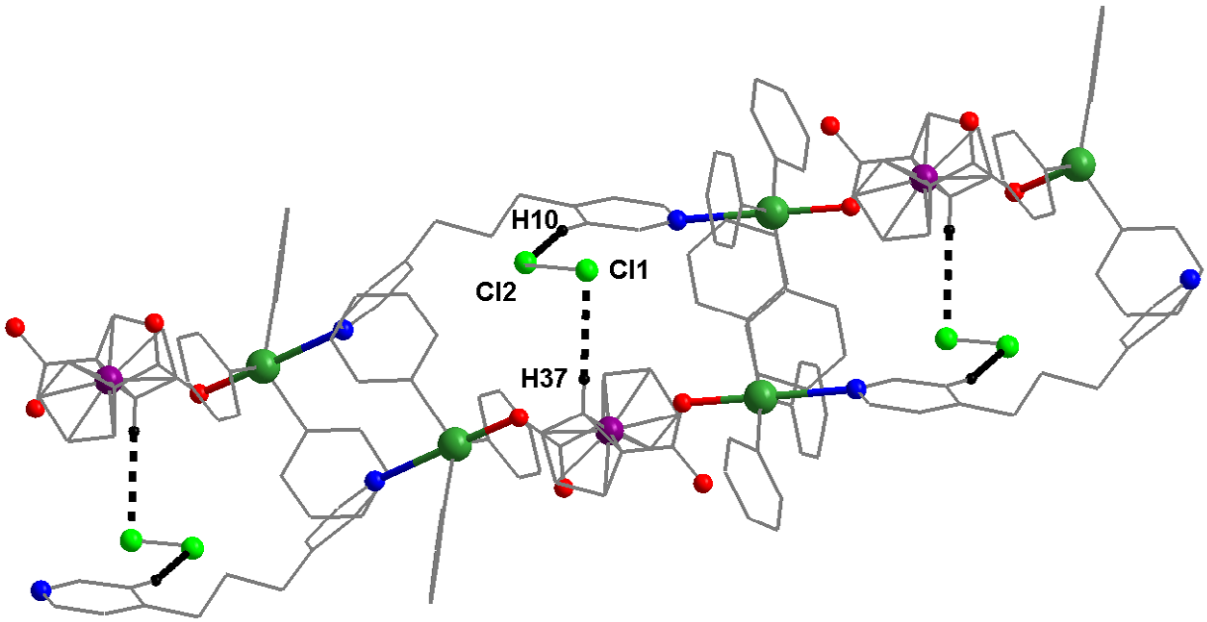


Figure S7. 2D polymeric structure of **2**. 2D polymers arises due to two different C-H…π interaction between molecules.



Figures S8. C-H…Cl interactions between two different 1D polymers of **5**. Except H10 and H37 remaining all the hydrogen atoms are removed for the clarity.

Table S1. Selected bond lengths (Å) and angles (°) for compounds **2-5**

		2	
Sn(1)-O(1)	2.093(3)	C(19)-O(1)	1.324(5)
Sn(2)-O(2)	2.061(3)	C(30)-O(2)	1.314(5)
Sn(1)-O(4)	2.552(3)	C(30)-O(3)	1.225(5)
Sn(2)-O(3)	2.794(3)	C(19)-O(4)	1.233(5)
O(1)-Sn(1)-O(4)	55.93(10)	O(1)-Sn(1)-C(7)	99.66(14)
O(1)-Sn(1)-C(13)	104.50(13)	C(13)-Sn(1)-C(7)	111.20(16)
O(1)-Sn(1)-C(1)	108.83(13)	C(1)-Sn(1)-C(7)	104.04(16)
C(13)-Sn(1)-C(1)	125.68(16)	C(13)-Sn(1)-O(4)	81.55(13)
C(1)-Sn(1)-O(4)	83.10(13)	O(2)-Sn(2)-C(31)	105.02(14)
C(7)-Sn(1)-O(4)	155.31(14)	O(2)-Sn(2)-C(43)	97.84 (14)
C(31)-Sn(2)-C(43)	113.83(17)	C(31)-Sn(2)-C(37)	116.97(17)
O(2)-Sn(2)-C(37)	113.53(14)	C(43)-Sn(2)-C(37)	108.08(16)
		3	
Sn(1)-O(2)	2.146(4)	O(1)-C(25)	1.210(7)
Sn(1)-N(1)	2.485(4)	O(2)-C(25)	1.301(6)
C(19)-Sn(1)-C(7)	126.4(2)	O(2)-Sn(1)-C(13)	89.54(17)
C(19)-Sn(1)-O(2)	96.28(17)	C(19)-Sn(1)-N(1)	84.40(17)
C(7)-Sn(1)-O(2)	97.86(16)	C(7)-Sn(1)-N(1)	83.97(16)
C(19)-Sn(1)-C(13)	118.04(19)	O(2)-Sn(1)-N(1)	177.07(14)
C(7)-Sn(1)-C(13)	113.52(19)	C(13)-Sn(1)-N(1)	87.64(17)
		4	
Sn(1)-O(1)	2.121(3)	Sn(2)-N(2)	2.628(4)
Sn(2)-O(3)	2.121(3)	C(1)-O(1)	1.314(6)
Sn(1)-N(1)	2.621(4)	C(1)-O(2)	1.220(6)
O(1)-Sn(1)-C(8)	98.82(16)	C(42)-Sn(2)-O(3)	102.01(15)
O(1)-Sn(1)-C(14)	94.44(15)	C(42)-Sn(2)-C(30)	130.11(18)
C(8)-Sn(1)-C(14)	130.65(19)	O(3)-Sn(2)-C(30)	92.86(15)
O(1)-Sn(1)-C(2)	90.93(16)	C(42)-Sn(2)-C(36)	113.34(18)
C(8)-Sn(1)-C(2)	112.99(18)	O(3)-Sn(2)-C(36)	90.87(16)
C(14)-Sn(1)-C(2)	114.08(18)	C(30)-Sn(2)-C(36)	113.74(19)
		5	
Sn(1)-O(1)	2.135(4)	C(32)-O(1)	1.295(7)
Sn(2)-O(3)	2.107(4)	C(32)-O(2)	1.237(7)

Sn(1)-N(2)	2.598(4)	C(43)-O(3)	1.313(7)
Sn(2)-N(1)	2.667(5)	C(43)-O(4)	1.216(7)
C(20)-Sn(1)-C(26)	129.5(2)	O(1)-Sn(1)-N(2)	179.26(14)
C(20)-Sn(1)-O(1)	95.17(18)	C(14)-Sn(1)-N(2)	89.95(18)
C(26)-Sn(1)-O(1)	97.37(17)	C(50)-Sn(2)-O(3)	97.19(17)
C(20)-Sn(1)-C(14)	115.4(2)	C(50)-Sn(2)-C(56)	126.9(2)
C(26)-Sn(1)-C(14)	113.5(2)	O(3)-Sn(2)-C(56)	96.47(19)
O(1)-Sn(1)-C(14)	89.56(18)	C(50)-Sn(2)-C(44)	116.5(2)
C(20)-Sn(1)-N(2)	84.54(18)	O(3)-Sn(2)-C(44)	89.89(19)
C(26)-Sn(1)-N(2)	83.33(17)	C(56)-Sn(2)-C(44)	114.6(2)

Table S2. Selected bond lengths (Å) and angles (°) for compounds **6-8**

		6	
Sn(1)-O(1)	2.127(3)	O(1)-C(6)	1.316(6)
Sn(1)-N(1)	2.579(4)	O(2)-C(6)	1.214(6)
C(13)-Sn(1)-O(1)	99.31(17)	C(7)-Sn(1)-C(19)	117.12(19)
C(13)-Sn(1)-C(7)	124.4(2)	C(13)-Sn(1)-N(1)	83.35(16)
O(1)-Sn(1)-C(7)	95.09(17)	O(1)-Sn(1)-N(1)	177.29(14)
C(13)-Sn(1)-C(19)	116.5(2)	C(7)-Sn(1)-N(1)	82.94(17)
O(1)-Sn(1)-C(19)	89.23(17)	C(19)-Sn(1)-N(1)	90.02(17)
C(7)-Sn(1)-C(19)	117.12(19)		
		7	
Sn(1)-O(1)	2.138(3)	C(4)-O(1)	1.278(5)
Sn(2)-O(2)	2.494(3)	C(4)-O(2)	1.229(5)
C(2)-Sn(1)-C(3)	123.4(2)	O(1)-Sn(1)-O(2)	173.55(12)
C(2)-Sn(1)-C(1)	119.7(3)	C(1)-Sn(1)-O(1)	89.08(18)
C(3)-Sn(1)-C(1)	115.4(3)	C(2)-Sn(1)-O(2)	83.37(16)
C(2)-Sn(1)-O(1)	95.81(17)	C(3)-Sn(1)-O(2)	88.47(17)
C(3)-Sn(1)-O(1)	97.28(18)		
		8	
Sn(1)-O(1)	2.156(3)	C(13)-O(1)	1.275(6)
Sn(1)-O(2)	2.444(4)	C(13)-O(2)	1.251(6)
Sn(1)-O(3)	2.507(8)		
C(5)-Sn(1)-C(1)	122.0(2)	C(5)-Sn(1)-O(2)	83.51(17)
C(5)-Sn(1)-C(9)	111.3(2)	C(1)-Sn(1)-O(2)	81.73(19)
C(1)-Sn(1)-C(9)	124.1(2)	C(9)-Sn(1)-O(2)	88.75(18)
C(5)-Sn(1)-O(1)	89.90(17)	O(1)-Sn(1)-O(2)	171.66(13)
C(1)-Sn(1)-O(1)	97.58(19)	C(5)-Sn(1)-O(3)	42.1(2)
C(9)-Sn(1)-O(1)	98.43(18)	C(1)-Sn(1)-O(3)	101.1(2)
C(9)-Sn(1)-O(3)	107.3(2)	O(2)-Sn(1)-O(3)	41.74(19)
O(1)-Sn(1)-O(3)	131.0(2)		