Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Bismuth-Ferrocene Carboxylates: Synthesis and Structure

Vadapalli Chandrasekhar,* and Ramesh K. Metre

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur – 208016, India.

[*] Prof. V. Chandrasekhar
Department of Chemistry
Indian Institute of Technology, Kanpur
Kanpur – 208016, India
Fax: (+91)-512-2597436
E-mail: vc@iitk.ac.in

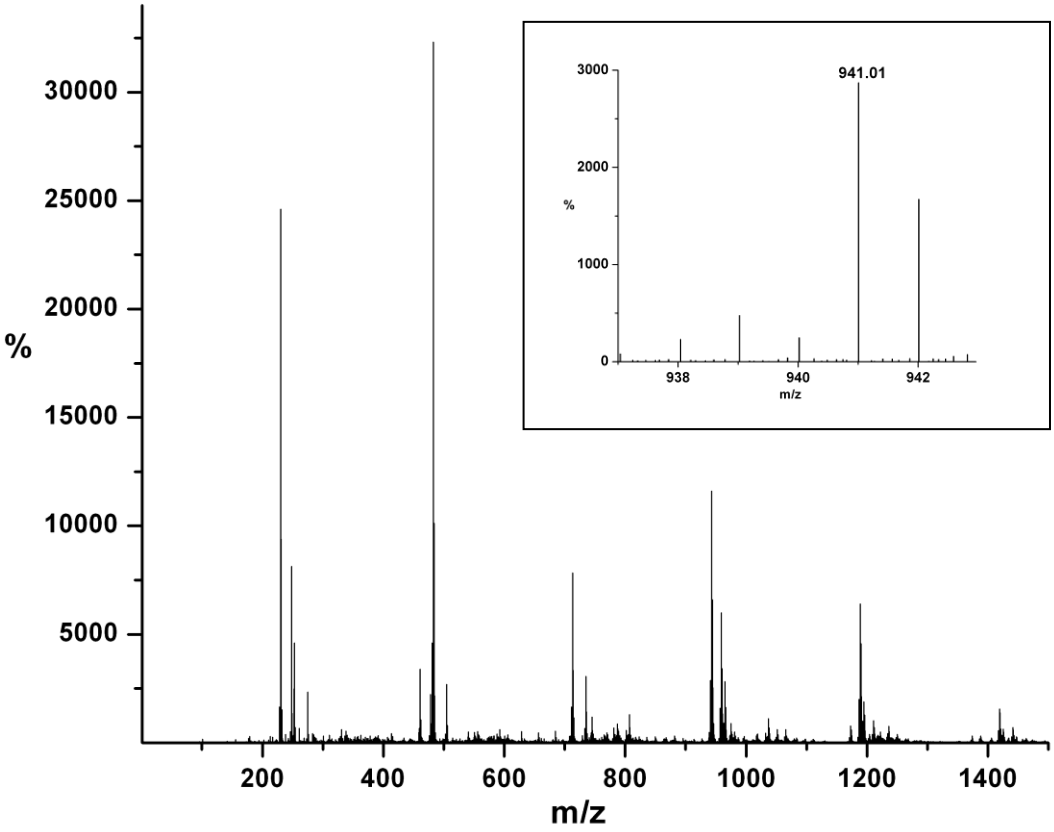


Figure S1 ESI-MS of **2**

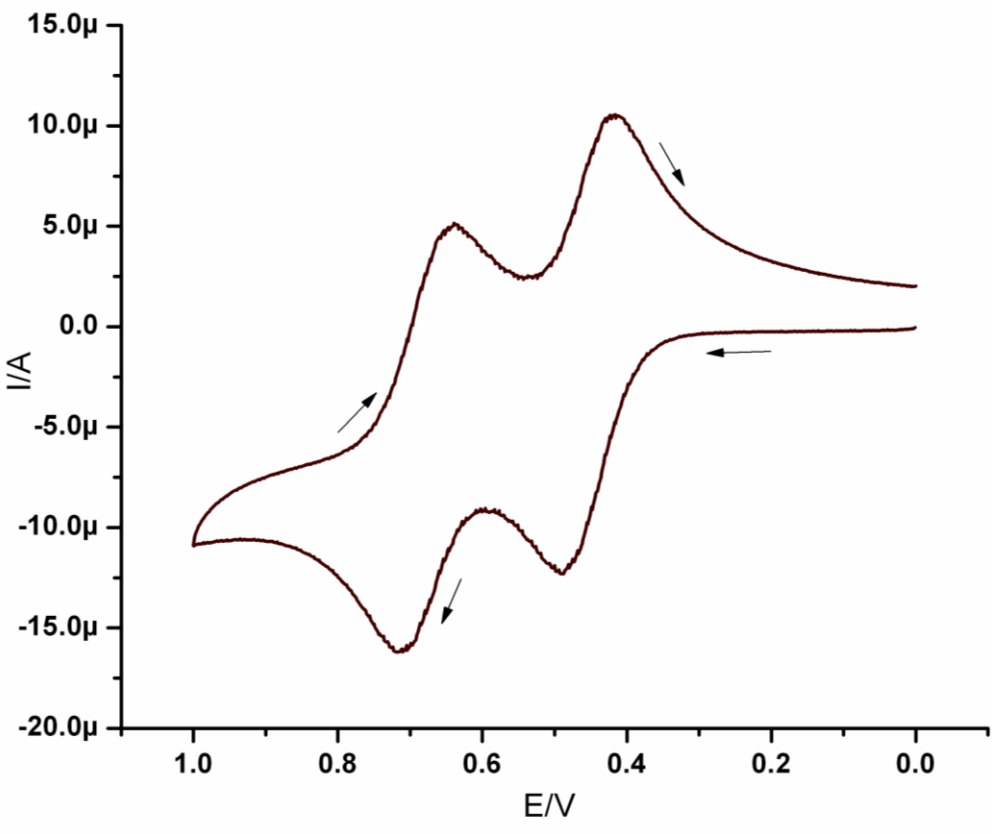


Figure S2. cyclic voltammogram of **2** (3.33×10^{-4} M) in presence of ferrocene (10^{-3} M) [vs Ag/AgCl; scan rate: 250 (mV/s)]

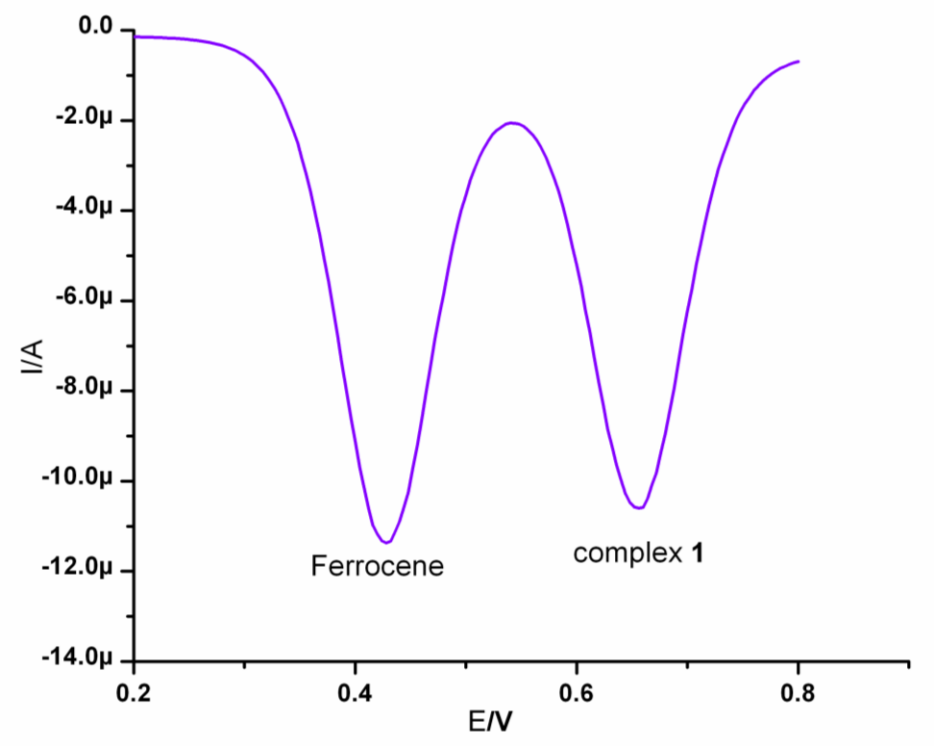
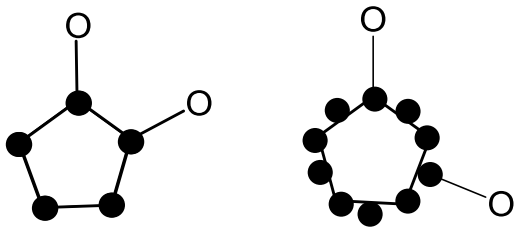


Figure S3. Differential pulse voltammogram of **2** (Ip = 1.13 x 10^{-5} A) and ferrocene (Ip =1.06 x 10^{-5} A).



Synclinal (eclipsed) Anticlinal (staggered)

Chart 2. **Conformations of the ferrocenedicarboxylate ligand in 1**[a]

[a] Synclinal (eclipsed) conformation corresponds to the situation where the two cyclopentadienyl groups are perfectly eclipsed while the 1,1′ substituents on these rings are not. In anticlinal (staggered) conformation the two cyclopentadienyl rings as well as two substituents on the 1,1′ positions are staggered.

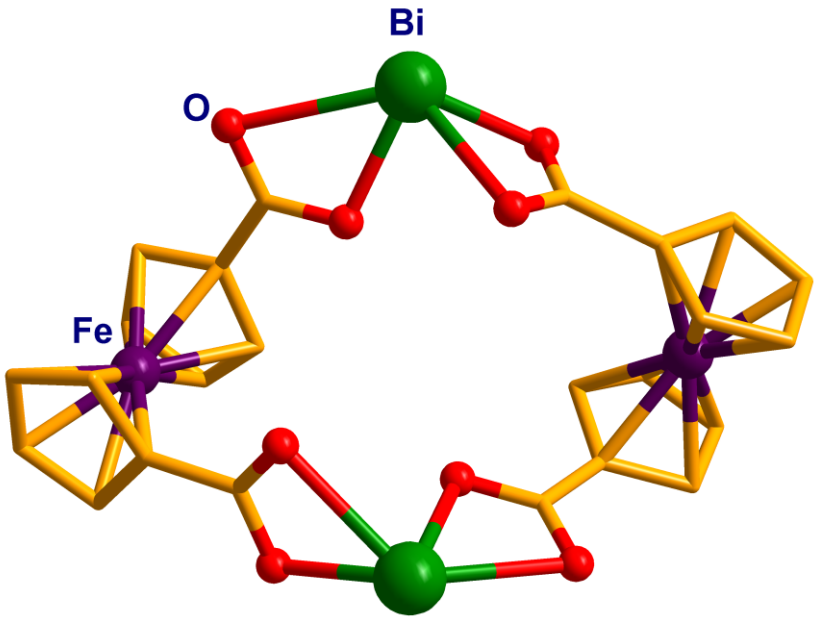


Figure S4 Heterobimetallic tetranuclear (Bi_2Fe_2) 16 membered macrocycle **1**

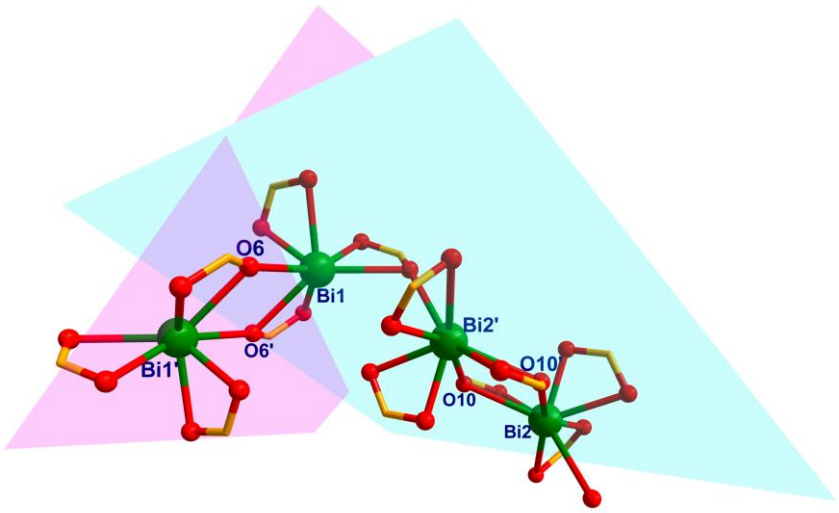


Figure S5. Figure showing planes passing through motif **A** and motif **B** in **1** with dihedral angle of 63.85(3)°. (ferrocenedicarboxylate units and hydrogen atoms have been omitted for the sake of clarity)

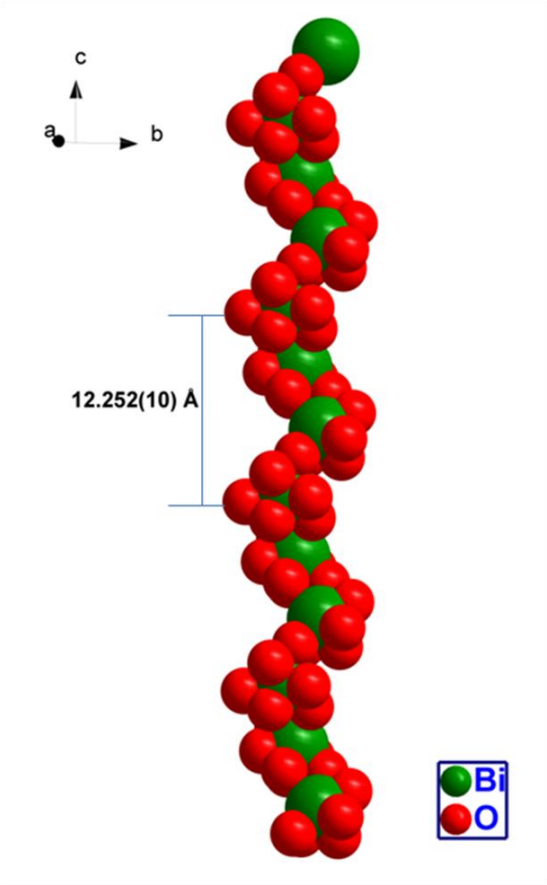


Figure S6 . 1D helical chain of **2**. Only Bi and O atoms are shown while other atoms have been omitted for sake of clarity.

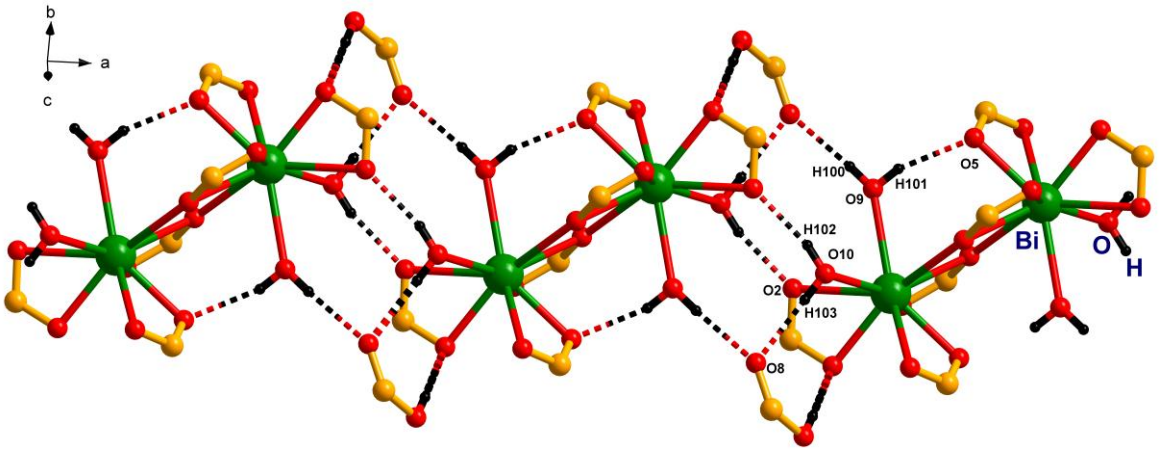


Figure S7. View showing intermolecular O-$H_{(water)}$…$O_{(ferrocene)}$ and O-$H_{(ferrocene)}$--- $O_{(ferrocene)}$ interactions of compound **3.** Ferrocene units of all ferrocene carboxylate ligands have been omitted for the sake clarity.The metric parameters involved are: O9-H101, 0.816 (4), H101-O5, 2.054 (3) Å and O10-H103-O8, 164.54 (38)°. O9-H100, 0.813 (4), H100-O8, 2.069 (4) Å and O9-H100-O8, 174.13 (41)°. O10-H102, 0.826 (4), H102-O2, 1.962 (4) Å and O10-H102-O2, 167.56 (43)° .O7-H7, 0.839 (1), H7-O1, 1.869 (3) Å and O7-H7-O1, 174.43 (41)°

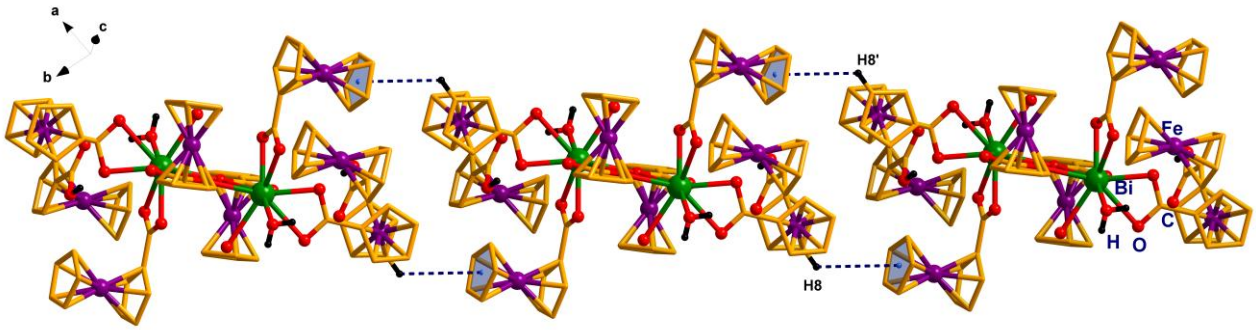


Figure S8. Intermolecular C-H…π in the 1D-network of **3**. Metric parameters: C8-H8…π, 3.5088(1) Å, C8-H8…π, 119.068(34)°

Table 1. Selected bond distance (Å) and bond angle (°) data for **1** and **2**

Compound **1**				Compound **2**			
Bond distances(Å)		Bond angles(°)		Bond distances(Å)		Bond angles(°)	
Bi(1)-O(2)	2.212(12)	O(11)-Bi(1)-O(6)	129.2(4)	Bi(1)-O(6)	2.192(6)	O(2)-Bi(1)-O(4)	78.1(2)
Bi(1)-O(5)	2.556(11))	O(6)-Bi(1)-O(11)#1	75.4(4)	Bi(1)-O(2)	2.236(6)	O(6)-Bi(1)-O(1)	77.2(2)
Bi(1)-O(11)	2.287(9)	O(6)-Bi(1)-O(1)	127.9(4)	Bi(1)-O(4)	2.271(6)	O(4)-Bi(1)-O(1)	131.9(2)
Bi(1)-O(1)	2.493(13)	O(11)#1-Bi(1)-O(5)	129.3(4)	Bi(1)-O(1)	2.449(6)	O(2)-Bi(1)-O(5)	127.5(2)
Bi(1)-O(6)	2.271(10)	O(1)-Bi(1)-O(5)	129.0(4)	Bi(1)-O(5)	2.597(7)	O(1)-Bi(1)-O(5)	124.2(2)
Bi(1)-O(12)	2.607(11)	O(2)-Bi(1)-O(12)#1	134.9(3)	Bi(1)-O(3)	2.674(6)	O(6)-Bi(1)-O(3)	132.2(2)
Bi(2)-O(7)	2.190(11)	O(11)#1-Bi(1)-O(12)#1	52.1(3)	Bi(1)-O(3) #1	2.702(6)	O(2)-Bi(1)-O(3)	72.3(2)
Bi(2)-O(4)	2.503(11)	O(7)-Bi(2)-O(3)	87.3(4)			O(1)-Bi(1)-O(3)	114.1(2)
Bi(2)-O(9)	2.258(11)	O(7)-Bi(2)-O(9)	79.3(4)			O(5)-Bi(1)-O(3)	118.5(2)
Bi(2)-O(3)	2.207(11)	O(4)-Bi(2)-O(10)	130.9(4)			O(6)-Bi(1)-O(3)#1	78.1(2)
Bi(2)-O(10)	2.628(11)	O(7)-Bi(2)-O(12)#3	88.0(4)			O(2)-Bi(1)-O(3)#1	121.0(2)
Bi(2)-O(12) #3	2.658(10)	O(9)-Bi(2)-O(12)#3	147.4(4)			O(4)-Bi(1)-O(3)#1	150.8(2)
						O(1)-Bi(1)-O(3)#1	66.78(19)
						O(5)-Bi(1)-O(3)#1	76.91(19)
						O(3)-Bi(1)-O(3)#1	149.73(19)

For compound 1: Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z+1 #3 -x,-y+1,-z+1

For compound 2: Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1

Table 2. Important bond distance (Å) and bond angle (°) data for **3**

Compound **3**			
Bond distances(Å)		Bond angles(°)	
Bi(1)-O(3)	2.306(3)	O(4)-Bi(1)-O(4)#1	69.26(11)
Bi(1)-O(5)	2.324(3)	O(9)-Bi(1)-O(4)#1	74.63(10)
Bi(1)-O(1)	2.335(3)	O(10)-Bi(1)-O(4)#1	84.53(11)
Bi(1)-O(6)	2.574(3)	O(3)-Bi(1)-O(5)	77.95(11)
Bi(1)-O(2)	2.592(3)	O(3)-Bi(1)-O(6)	123.67(11)
Bi(1)-O(4)	2.637(3)	O(5)-Bi(1)-O(2)	134.22(11)
Bi(1)-O(9)	2.657(4)	O(6)-Bi(1)-O(2)	116.02(10)
Bi(1)-O(10)	2.659(4)	O(1)-Bi(1)-O(4)	128.51(10)
Bi(1)-O(4)#1	2.665(3)	O(6)-Bi(1)-O(4)	120.32(10)
		O(2)-Bi(1)-O(4)	118.37(10)
		O(5)-Bi(1)-O(9)	141.33(11)
		O(1)-Bi(1)-O(9)	127.49(11)
		O(6)-Bi(1)-O(9)	147.44(11)
		O(3)-Bi(1)-O(10)	148.33(11)
		O(5)-Bi(1)-O(10)	126.73(11)
		O(4)-Bi(1)-O(10)	146.46(10)
		O(3)-Bi(1)-O(4)#1	121.72(10)
		O(5)-Bi(1)-O(4)#1	82.40(11)
		O(1)-Bi(1)-O(4)#1	152.95(10)
		O(6)-Bi(1)-O(4)#1	81.64(10)
		O(2)-Bi(1)-O(4)#1	143.32(10)

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