Syntheses, crystal structures, and properties of complexes constructed with polybenzoate and 2,2′-bibenzimidazole

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Table 1: Selected Hydrogen-Bonding Geometry (Å, °) of Complexes **1**-**6**.

D-H···A	D-H	H···A	D···A	D-H···A
Complex **1**[a]				
N(3)-H(3b)···O(2)#1	0.86	2.11	2.784(6)	134.6
N(4)-H(4b)···O(4)#2	0.86	2.03	2.793(6)	147.5
Complex **2**[b]				
N(3)-H(3b)···O(2)#1	0.86	2.09	2.769(5)	135.2
N(4)-H(4b)···O(4)#2	0.86	2.02	2.789(5)	148.2
. Complex **3**[c]				
N(5)-H(5a)···O(3)#1	0.86	1.85(5)	2.695(5)	170(5)
N(6-H(6a)···O(4)#1	0.89(5)	1.85(5)	2.725(5)	167(5)
N(7)-H(7a)···O(1w)#2	0.83(5)	2.06(6)	2.848(6)	158(5)
N(8)-H(8a)···O(2)#3	0.79(6)	2.07(6)	2.776(6)	149(6)
O(1w)-H(1b)··O(3)#4	0.82(9)	2.17(9)	2.973(6)	168(8)
O(1w)-H(1c)··O(4)#5	0.89(8)	2.00(8)	2.870(6)	169(7)
Complex **4**[d]				
N(3)-H(3b) ···O(6w)#1	0.86	2.10	2.869(14)	148.1
N(4)-H(4b) ···O(6w)#1	0.86	1.98	2.785(13)	154.6
N(7)-H(7a) ···O(9)#2	0.86	1.93	2.755(12)	159.4
N(8)-H(8b) ···O(10)#2	0.86	1.81	2.666(12)	172.8
N(12)-H(12a) ···O(11)#1	0.86	2.01	2.785(13)	148.9
N(14)-H(14a) ···O(3)#3	0.86	2.03	2.778(12)	145.3
N(19)-H(19a)···O(3w)#4	0.86	2.06	2.84(2)	149.4
N(20)-H(20b) ···O(3w)#4	0.86	2.07	2.861(19)	151.5
Complex **5**[e]				
N(3)-H(3b)...O(3)#1	0.86	2.09	2.881(3)	152.4
N(4)-H(4b...O(4)#1	0.86	1.75	2.604(3)	173.3

N(7)-H(7a)...O(2)#2	0.86	1.95	2.753(3)	154.0
N(8)-H(8a)...O(2)#2	0.86	1.99	2.764(3)	150.0
Complex **6**[f]				
N(3)-H(3b) ···O(4)#1	0.86	2.02	2.857(8)	162.9
N(4)-H(4b) ···O(3)#1	0.86	1.78	2.632(8)	168.9
N(7)-H(7a) ···O(2)#1	0.86	1.80	2.648(7)	170.4
N(8)-H(8b) ···O(1)#1	0.86	1.88	2.737(7)	173.5
N(12)-H(12a) ···O(4)#2	0.86	2.13	2.913(9)	151.4

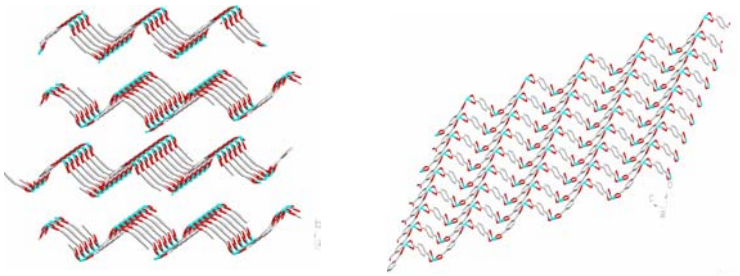
a, b:: #1 -x, y+1/2, -z+1/2 #2 -x, -y+1, -z+1

c: #1 x-1, -y+3/2, z-1/2 #2-x+1, y+1/2, -z+3/2 #3 -x+1, -y+2, -z+1 #4 x, -y+3/2, z+1/2 #5 x, y, z

d: #1 x, -y+1, z+1/2 #2 x+1, -y+1, z+1/2 #3 x-1/2, -y+3/2, z+1/2 #4 x, y, z

e: #1 -x+1,-y+1,-z+1 #2 -x+2,-y+2,-z+2

f: #1 x, y, z #2 x-1/2, -y+3/2, z-1/2



(a) (b)

Fig 1. (a).The arrangement of the undulating sheets in **1**. (b). Perspective view of the 2D sheet. (H_2bibzim ligands omitted for clarity)

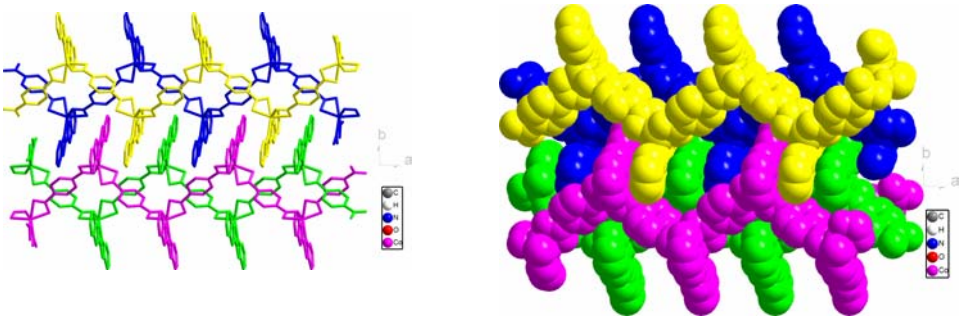


Fig 2. Molecular zipper formed by four chains in complexes **1** and **2**.

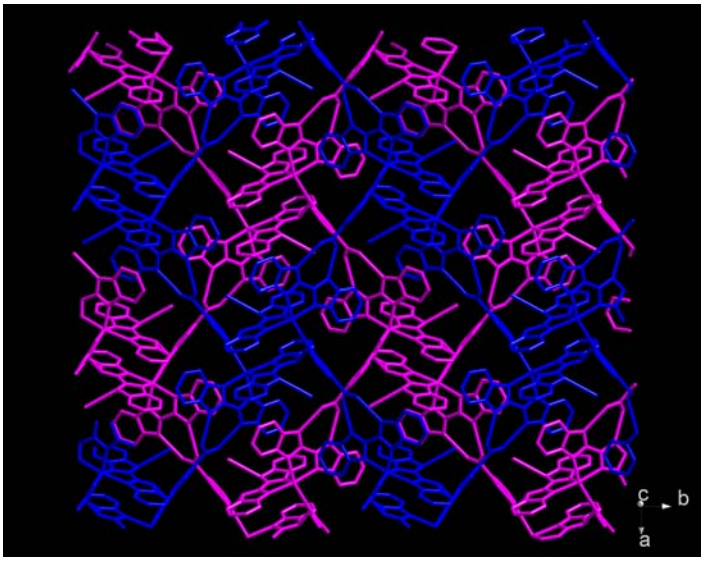


Fig 3. The hydrogen-bonding interactions connect the 2D sheets into 3D framework in **3**, and the H_2bibzim ligands of adjacent sheets halt the holes.

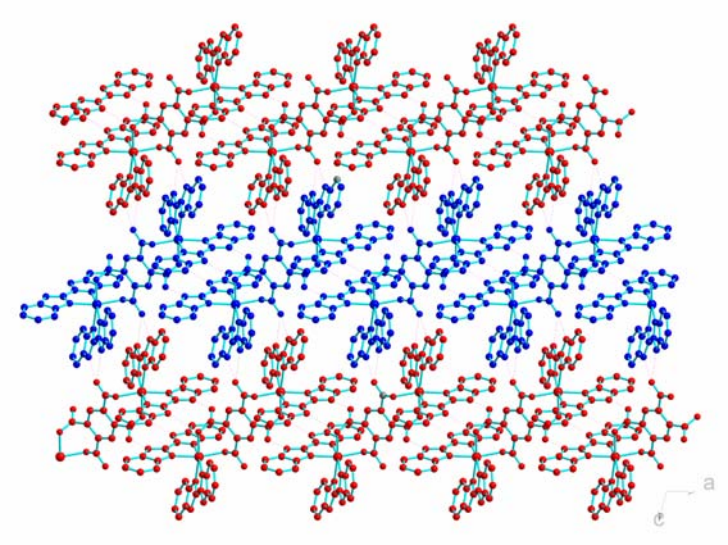


Fig 4. Hydrogen-bonding interactions connect the dinuclear unit into one-dimensional chain and further into two-dimensional sheet in complex **5**.

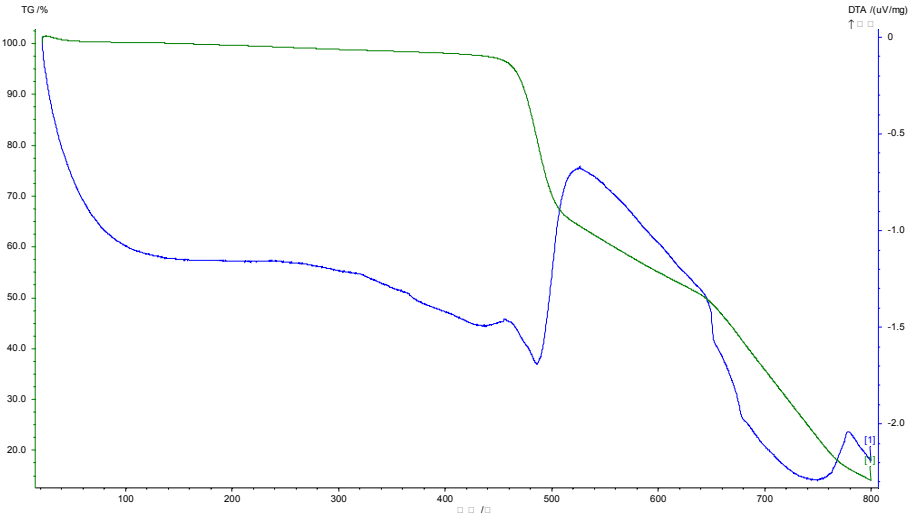


Fig 5. TGA and DSC traces of complex **1**.

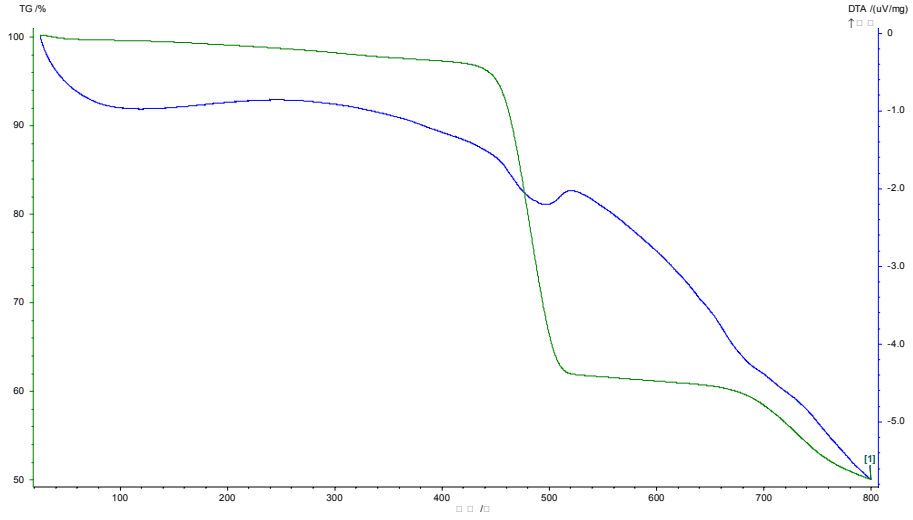


Fig 6. TGA and DSC traces of complex **2**.

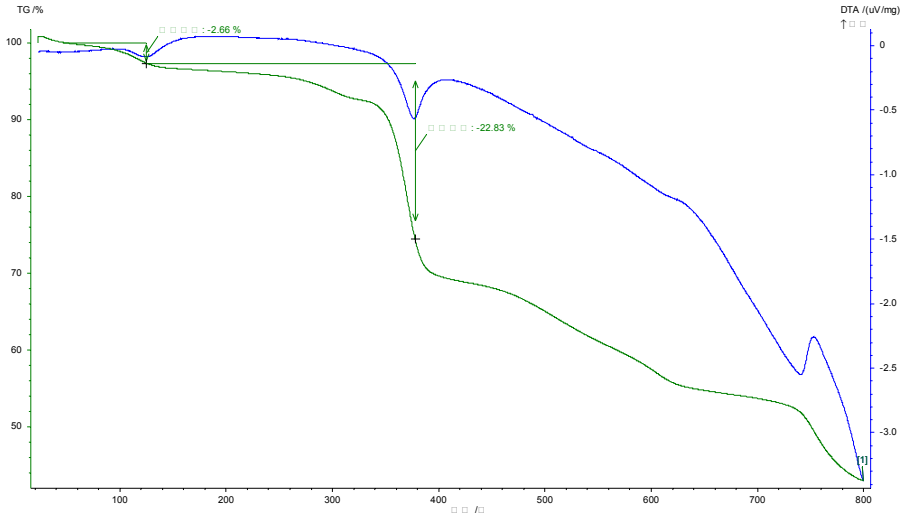


Fig 7. TGA and DSC traces of complex **3**.

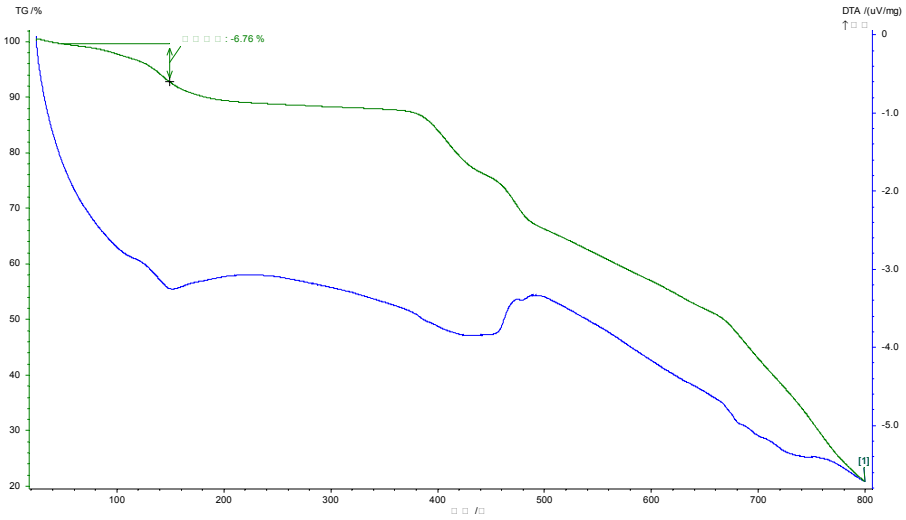


Fig 8. TGA and DSC traces of complex **4**.

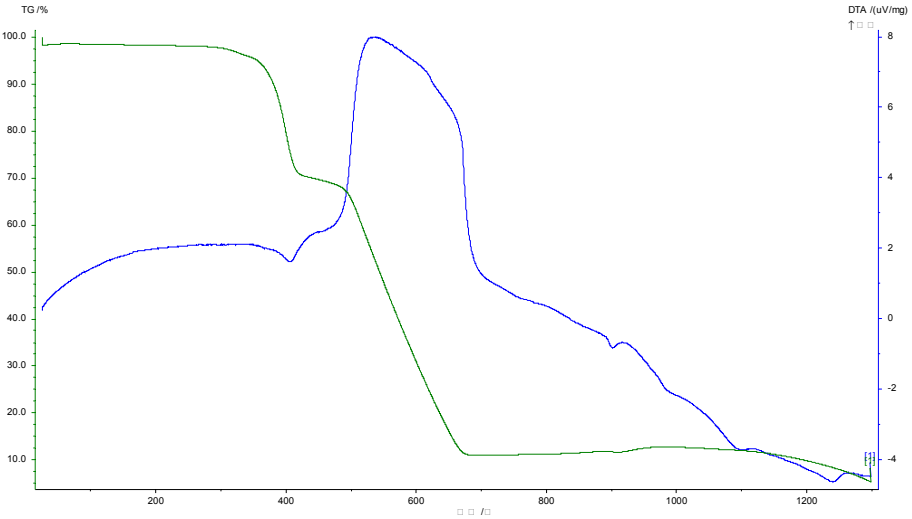


Fig 9. TGA and DSC traces of complex **5** (air atmosphere).

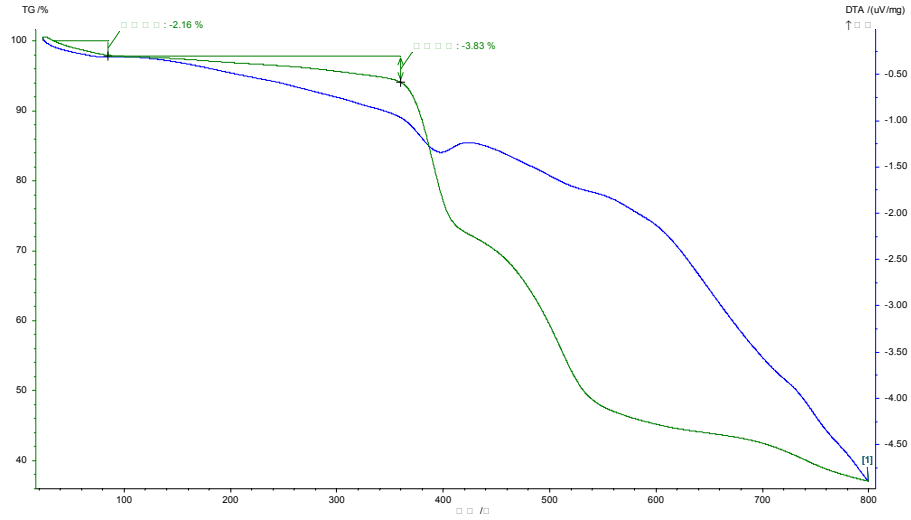


Fig 10. TGA and DSC traces of complex **6**.

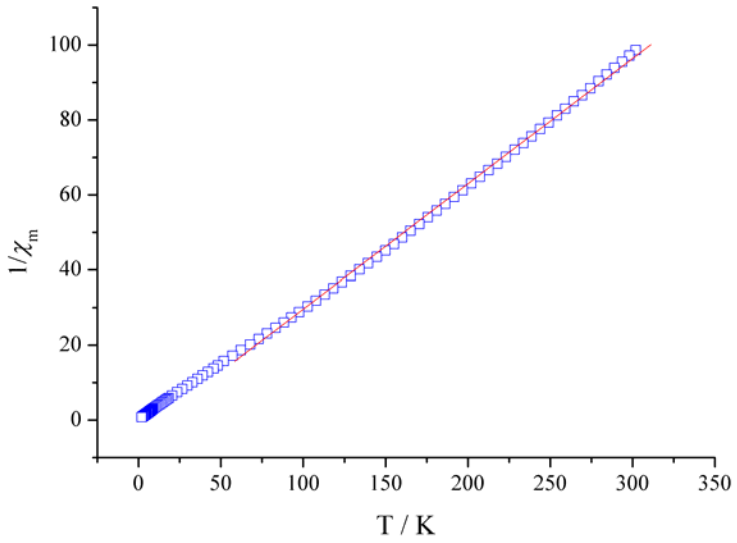


Fig 11. The inverse susceptibility with linear regression based upon the Curis-Weiss law for complex **1.**

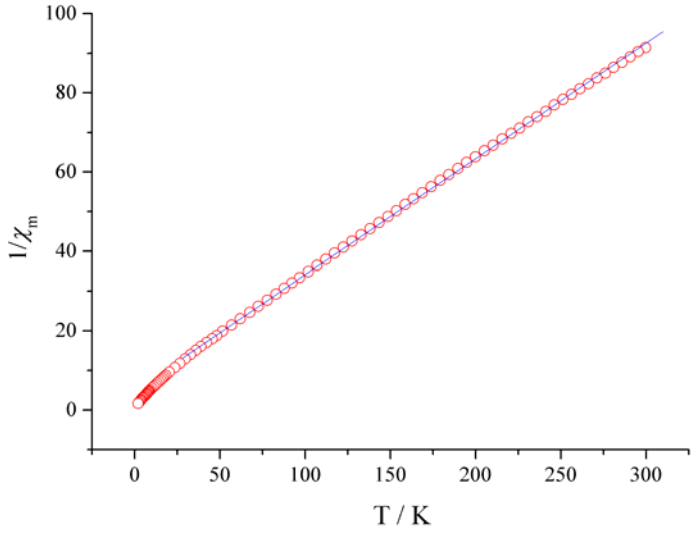
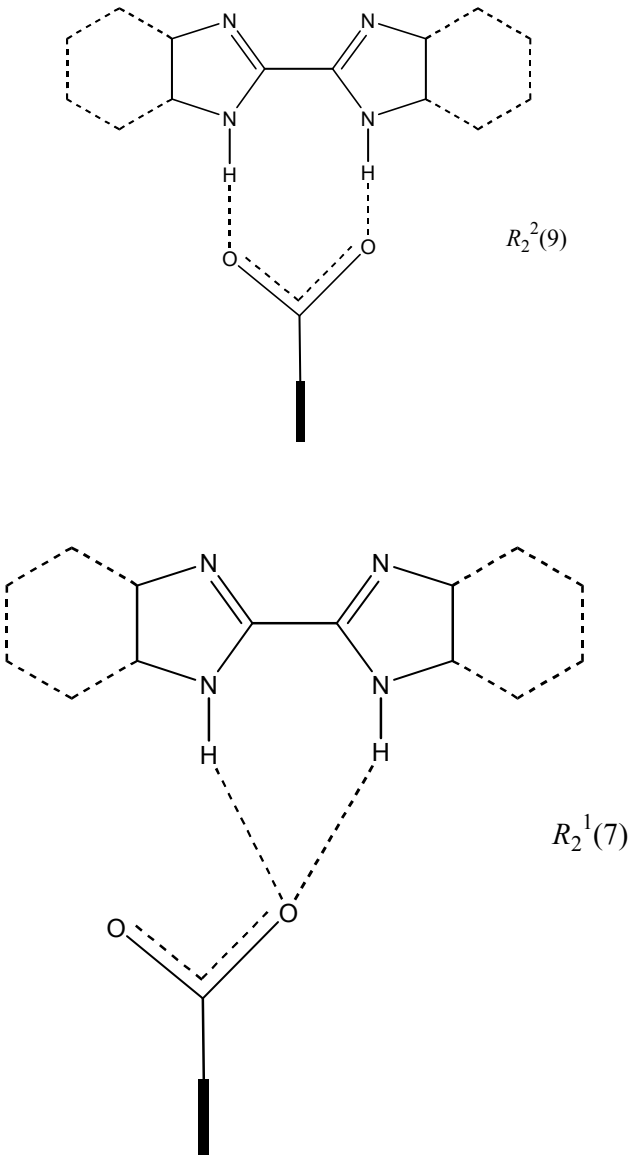


Fig 12. The inverse susceptibility with linear regression based upon the Curis-Weiss law for complex **4.**



Scheme 1. Presentation of heteromeric Hydrogen-bonded synthon $R_2^2(9)$ and $R_2^1(7)$ formed by H_2bibzim (or H_2biim) and uncoordinated carboxylate.