Electronic Supplementary Material (ESI) for CrystEngComm

Metal-organic frameworks constructed with imidazole dicarboxylates bearing aromatic substituents at the 2-position

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Supporting Information

Table S1. Hydrogen bond distances (Å) and angles (deg) for 1-7.

D-H...A	d(H...A)	d(D...A)	∠(DHA)
1			
O(5)-H(5B)...N(2)#2	2.38(4)	2.941(7)	124(4)
O(5)-H(5B)...O(2)#1	2.31(5)	3.044(7)	145(7)
O(5)-H(5A)...O(1)#3	2.02	2.874(7)	179.5
2			
O(7)-H(7B)...O(1)#3	1.81(3)	2.648(2)	169(3)
O(8)-H(8A)...O(8)#4	2.40(2)	2.974(5)	127(2)
O(8)-H(8B)...O(7)#5	2.325(13)	3.117(3)	160(2)
O(6)-H(6B)...O(5)#6	1.944(10)	2.783(2)	171(2)
O(6)-H(6A)...O(1)#2	1.928(10)	2.770(2)	173.9(18)
N(2)-H(2)...O(8)#1	2.04	2.896(3)	174.8
O(5)-H(5)...O(3)#7	1.89	2.702(2)	169.8
3			
O(5)-H(5)...O(1)#1	2.19	2.910(2	146.3

O(5)-H(5)...O(2)#1	2.35	2.912(2	126.5
O(10)-H(10)...O(7)#3	1.81	2.626(8)	170.9
4			
O(2)-H(2)...O(3)	1.65	2.461(4)	171.7
O(5)-H(5)...O(11)	1.94	2.752(5)	170.1
O(8)-H(8A)...O(7)	1.64	2.462(4)	175.5
O(10)-H(10)...O(6)#2	2.07	2.884(4)	169.3
O(10)-H(10)...O(7)#2	2.61	3.171(4)	127.5
O(11)-H(11A)...O(7)#3	2.11	2.956(4)	179.3
O(11)-H(11B)...O(9)#4	2.44	2.977(4)	121.8
5			
O(5)-H(5A)...O(2)#1	2.21	3.060(4)	179.6
O(5)-H(5B)...N(1)#2	1.97	2.803(4)	167.0
N(2)-H(2)...O(5)#1	2.20(4)	2.987(4)	170.0(4)
7			
O(8)-H(8)...O(5)#4	2.02	2.836(7)	176.6
O(6)-H(1W)...O(4)#5	1.91(6)	2.796(4)	170(6)
O(6)-H(1W)...O(9)#5	2.47(6)	3.120(4)	130(5)
O(5)-H(3W)...O(7)#6	2.310(15)	3.146(8)	170(7)
O(5)-H(2W)...O(6)	2.40(4)	3.187(8)	155(8)
O(7)-H(5W)...O(1)#6	2.09(4)	2.817(4)	144(6)
O(7)-H(4W)...O(6)	2.39(11)	2.817(5)	111(9)

O(7)-H(4W)...O(9)#5	2.43(5)	3.213(5)	154(10)

Symmetry codes for **1** #1 –x+1,y+1/2,-z+1/2;#2 -x+1,-y-1/2,-z+1/2; #3 -x+1,-y,-z+1; For **2**: #1: x, -y+1/2, z+1/2. #2: x, -y+1/2, z-1/2. #3: x+1, y, z+1. #4: -x+2, -y+1, z. #5: x+1, y, z. #6: -x+2, -y+1, z. #7 -x+1, y+1/2, -z+1. For **3**: #1: 2-x, 1/2+y, 1/2-z. #3: x-1/2, -y+3/2, z. For **4**: #1: 2-x, 1/2+y, 1/2-z. #2: 2-x, -1/2+y, 1/2-z. #3: x-1, y, z. #4 -x+2,-y+1,-z+1 For **5:** #1: 1-x, -1/2+y, 1/2-z. #2: 1-x, -y, -z. For **7 :** #4 y+2/3,-x+y+1/3,-z+7/3. #5 x-y-1/3,x-2/3,-z+7/3. #6 -x+y+4/3,-x+2/3,z-1/3.

Table S2. NBO Charge Distributions of the Free Ligands H_3PhIDC, H_3HOPhIDC and H_3MPhDC.

H_3PhIDC		H_3HOPhIDC		H_3MePhIDC	
Atom Number	**NBO Charge**	**Atom Number**	**NBO Charge**	**Atom Number**	**NBO Charge**
O1	-0.66617	O1	-0.690	O1	-0.690
O6	-0.66085	O2	-0.545	O2	-0.684
O2	-0.69129	O3	-0.624	O3	-0626
O13	-0.65133	O4	-0.683	O4	-0.546
N7	-0.53170	N5	-0.508	N5	-0.508
N4	-0.49906	N6	-0.452	N6	-0.452
C10	0.80683	O7	-0.660	C7	0.103
C8	0.01558	C8	0.768	C8	-0.020
C9	0.05461	C9	0.760	C9	0.410
C12	0.77963	C10	-0.020	C10	0.768
C11	0.44052	C11	0.103	C11	0.760
C14	-0.43529	C12	0.409	C12	-0.125
C17	-0.56473	C13	-0.124	C13	-0.141
H15	0.22625	C14	-0.136	C14	-0.229
H16	0.23251	C15	-0.240	C15	0.343
H18	0.20938	C16	-0.165	C16	-0.163
H19	0.20176	C17	-0.276	C17	-0.286
H20	0.20415	C18	0.334	C18	-0.531
H21	0.54017	H19	0.496	H19	0.496
		H20	0.495	H20	0.495
		H21	0.240	H21	0.239
		H22	0.225	H22	0.225
		H23	0.470	H23	0.196
		H24	0.205	H24	0.171
		H25	0.193	H25	0.171
		H26	0.425	H26	0215
				H27	0.191
				H28	0.425

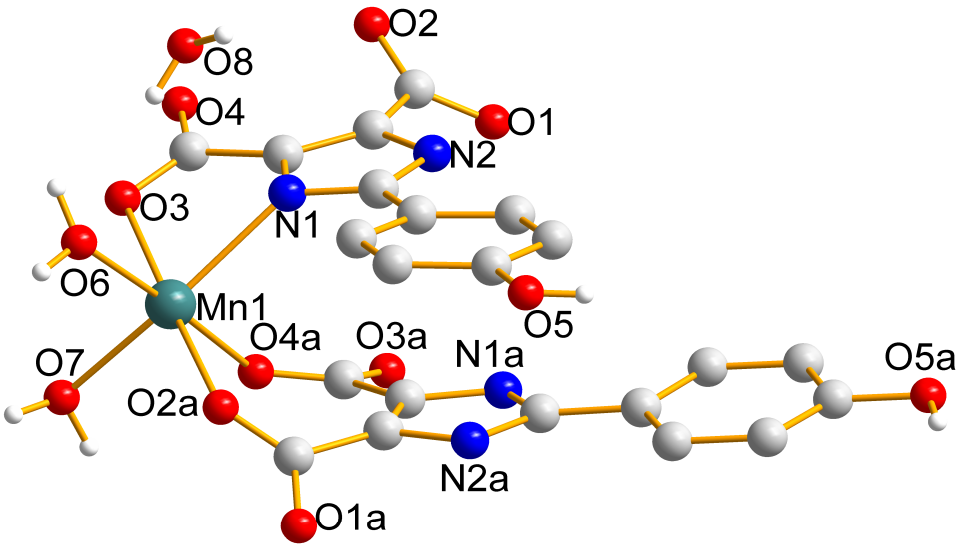

Figure S1. The segment of polymer **2**, showing the local coordination environment of Mn(II) ion (symmetry code: a: x, -y+1/2, z+1/2).

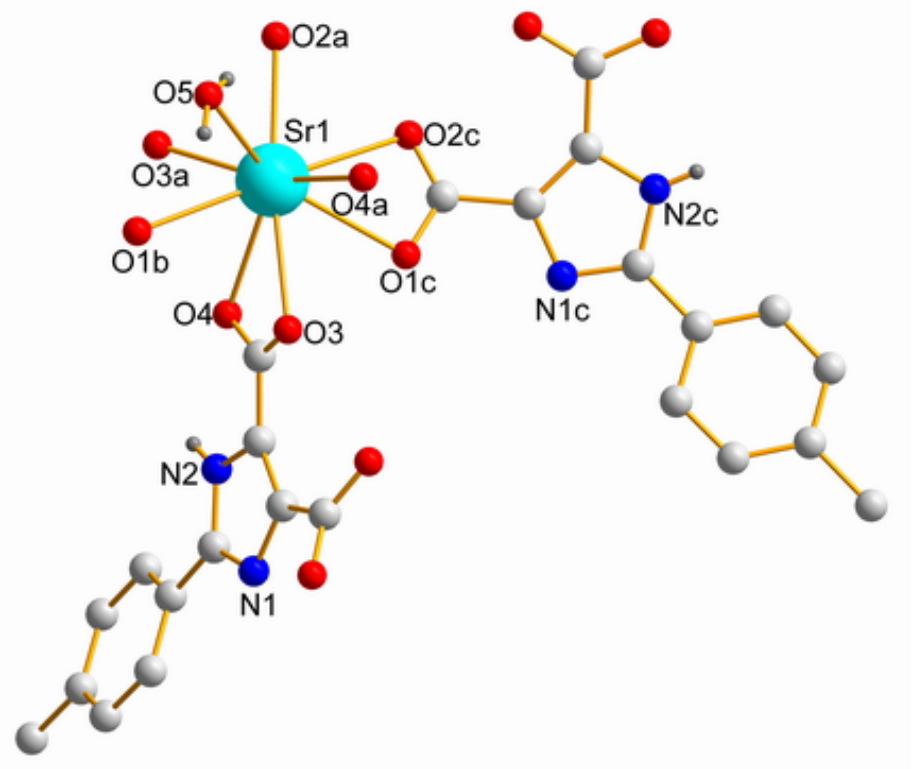

Figure S2. The coordination environment of the Sr(II) atom in **5** (symmetry code: a: 1-x, -1/2+y, 1/2-z; b: 1-x, -y, -z; c: x, -1/2-y, 1/2+z, partial $MePhHIDC^{2-}$ anions omitted for clarity).