Electronic supplementary information (ESI)

Construction of coordination frameworks based on 4-imidazolyl tecton 1,4-di(1H-imidazol-4-yl)benzene and varied carboxylic acids

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Table S1 Selected bond lengths [Å] and bond angles [º] for complexes **1** - **9**.

1			
Mn(1)-O(1)	2.1592(15)	Mn(1)-N(2)	2.2405(19)
Mn(1)-O(2)#2	2.2565(16)		
O(1)-Mn(1)-O(1)#1	146.69(8)	O(1)-Mn(1)-N(2)	103.62(7)
O(1)#1-Mn(1)-N(2)	97.55(6)	N(2)-Mn(1)-N(2)#1	100.43(10)
O(1)-Mn(1)-O(2)#2	75.13(5)	O(1)#1-Mn(1)-O(2)#2	80.65(6)
N(2)-Mn(1)-O(2)#2	87.07(7)	N(2)#1-Mn(1)-O(2)#2	170.67(6)
O(2)#2-Mn(1)-O(2)#3	86.03(9)		
2			
Zn(1)-O(4)#1	1.9564(18)	Zn(1)-O(1)	1.9743(17)

Zn(1)-N(1)	2.008(2)	Zn(1)-N(3)#2	2.033(2)
O(4)#1-Zn(1)-O(1)	113.06(8)	O(4)#1-Zn(1)-N(1)	115.73(8)
O(1)-Zn(1)-N(1)	93.84(8)	O(4)#1-Zn(1)-N(3)#2	106.51(8)
O(1)-Zn(1)-N(3)#2	103.22(9)	N(1)-Zn(1)-N(3)#2	123.04(8)

3

Zn(1)-O(1)	1.960(5)	Zn(1)-O(5)	1.968(6)
Zn(1)-N(112)	2.018(6)	Zn(1)-N(212)	1.997(8)
Zn(2)-O(3)	1.961(5)	Zn(2)-O(9)#1	1.993(8)
Zn(2)-N(242)	2.010(6)	Zn(2)-N(312)	1.979(6)
Zn(3)-O(7)#2	1.994(8)	Zn(3)-O(13)	2.099(5)
Zn(3)-N(142)#3	2.002(7)	Zn(3)-N(342)	1.975(6)
Zn(4)-O(11)	1.963(6)	Zn(4)-O(15)	2.120(8)
Zn(4)-N(412)	2.005(6)	Zn(4)-N(442)	2.020(9)
O(1)-Zn(1)-O(5)	105.2(2)	O(1)-Zn(1)-N(112)	104.0(2)
O(1)-Zn(1)-N(212)	127.1(2)	O(5)-Zn(1)-N(112)	107.1(2)
O(5)-Zn(1)-N(212)	104.2(2)	N(112)-Zn(1)-N(212)	107.9(3)
O(3)-Zn(2)-O(9)#1	104.9(3)	O(3)-Zn(2)-N(242)	102.8(2)
O(3)-Zn(2)-N(312)	127.1(2)	O(9)#1-Zn(2)-N(242)	105.8(2)
O(9)#1-Zn(2)-N(312)	105.9(3)	N(242)-Zn(2)-N(312)	108.7(2)
O(7)#2-Zn(3)-O(13)	94.4(2)	O(7)#2-Zn(3)-N(142)#3	103.9(3)
O(7)#2-Zn(3)-N(342)	98.9(3)	O(13)-Zn(3)-N(142)#3	113.4(2)
O(13)-Zn(3)-N(342)	120.7(2)	N(142)#3-Zn(3)-N(342)	118.7(2)
O(11)-Zn(4)-O(15)	136.6(3)	O(11)-Zn(4)-N(412)	102.9(2)
O(11)-Zn(4)-N(442)	100.7(3)	O(15)-Zn(4)-N(412)	104.7(3)
O(15)-Zn(4)-N(442)	92.8(4)	N(412)-Zn(4)-N(442)	121.3(3)

4

Co(1)-O(1)	2.0374(19)	Co(1)-N(2)	2.092(2)
Co(1)-O(4)#2	2.2171(19)	Co(2)-O(2)	1.978(2)
Co(2)-O(5)#4	2.027(2)	Co(2)-N(4)#5	2.044(2)
Co(2)-O(4)#3	2.0886(18)	Co(2)-O(3)#3	2.2499(19)
O(1)#1-Co(1)-O(1)	180.000(1)	O(1)#1-Co(1)-N(2)	89.22(9)
O(1)-Co(1)-N(2)	90.78(9)	N(2)-Co(1)-N(2)#1	180.000(1)
O(1)#1-Co(1)-O(4)#2	88.83(8)	O(1)-Co(1)-O(4)#2	91.17(8)

N(2)-Co(1)-O(4)#2	87.66(8)	N(2)#1-Co(1)-O(4)#2	92.34(8)
O(1)#1-Co(1)-O(4)#3	91.17(8)	O(1)-Co(1)-O(4)#3	88.83(8)
N(2)-Co(1)-O(4)#3	92.34(8)	N(2)#1-Co(1)-O(4)#3	87.66(8)
O(4)#2-Co(1)-O(4)#3	180.000(1)	O(2)-Co(2)-O(5)#4	96.89(9)
O(2)-Co(2)-N(4)#5	103.93(10)	O(5)#4-Co(2)-N(4)#5	99.85(9)
O(2)-Co(2)-O(4)#3	100.89(8)	O(5)#4-Co(2)-O(4)#3	149.60(8)
N(4)#5-Co(2)-O(4)#3	99.52(9)	O(2)-Co(2)-O(3)#3	157.23(9)
O(5)#4-Co(2)-O(3)#3	96.58(8)	N(4)#5-Co(2)-O(3)#3	91.71(9)
O(4)#3-Co(2)-O(3)#3	59.63(7)		

5

Co(1)-O(1)	1.9714(19)	Co(1)-O(3)#1	1.9858(16)
Co(1)-N(12)	2.016(2)	Co(1)-N(42)	2.007(2)
O(1)-Co(1)-O(3)#1	100.50(6)	O(1)-Co(1)-N(12)	113.53(10)
O(1)-Co(1)-N(42)	117.79(9)	O(3)#1-Co(1)-N(12)	114.30(9)
O(3)#1-Co(1)-N(42)	101.08(9)	N(12)-Co(1)-N(42)	108.88(9)

6

Ni(1)-O(1)	2.1121(15)	Ni(1)-O(2)	2.1221(15)
Ni(1)-O(7)#1	2.1348(13)	Ni(1)-O(8)#1	2.0958(14)
Ni(1)-N(112)	2.0178(16)	Ni(1)-N(442)	2.0402(16)
Ni(2)-O(3)#2	2.1709(13)	Ni(2)-O(4)#2	2.0851(14)
Ni(2)-O(5)	2.0715(15)	Ni(2)-O(6)	2.1695(15)
Ni(2)-N(142)	2.0286(16)	Ni(2)-N(212)#3	2.0471(17)
Ni(3)-O(9)	2.1158(15)	Ni(3)-O(10)	2.1237(15)
Ni(3)-O(13)	2.0713(14)	Ni(3)-O(14)	2.1741(13)
Ni(3)-N(242)	2.0384(16)	Ni(3)-N(312)	2.0189(18)
Ni(4)-O(11)	2.1364(13)	Ni(4)-O(12)	2.1160(14)
Ni(4)-O(15)	2.1656(15)	Ni(4)-O(16)	2.0713(15)
Ni(4)-N(342)#1	2.0325(18)	Ni(4)-N(412)	2.0476(17)
O(1)-Ni(1)-O(2)	62.18(5)	O(1)-Ni(1)-O(7)#1	94.75(5)
O(1)-Ni(1)-O(8)#1	151.33(5)	O(1)-Ni(1)-N(112)	101.65(6)
O(1)-Ni(1)-N(442)	100.29(6)	O(2)-Ni(1)-O(7)#1	89.46(5)
O(2)-Ni(1)-O(8)#1	98.83(5)	O(2)-Ni(1)-N(112)	163.31(6)
O(2)-Ni(1)-N(442)	92.93(6)	O(7)#1-Ni(1)-O(8)#1	62.02(5)

O(7)#1-Ni(1)-N(112)	87.78(5)	O(7)#1-Ni(1)-N(442)	164.07(6)
O(8)#1-Ni(1)-N(112)	94.39(6)	O(8)#1-Ni(1)-N(442)	102.05(6)
N(112)-Ni(1)-N(442)	94.24(6)	O(3)#2-Ni(2)-O(4)#2	61.38(5)
O(3)#2-Ni(2)-O(5)	95.32(5)	O(3)#2-Ni(2)-O(6)	88.41(5)
O(3)#2-Ni(2)-N(142)	88.08(6)	O(3)#2-Ni(2)-N(212)#3	162.59(6)
O(4)#2-Ni(2)-O(5)	151.38(5)	O(4)#2-Ni(2)-O(6)	98.61(5)
O(4)#2-Ni(2)-N(142)	94.40(6)	O(4)#2-Ni(2)-N(212)#3	101.28(6)
O(5)-Ni(2)-O(6)	62.07(5)	O(5)-Ni(2)-N(142)	101.60(6)
O(5)-Ni(2)-N(212)#3	100.70(6)	O(6)-Ni(2)-N(142)	162.86(6)
O(6)-Ni(2)-N(212)#3	93.07(6)	N(142)-Ni(2)-N(212)#3	95.28(6)
O(9)-Ni(3)-O(10)	62.10(5)	O(9)-Ni(3)-O(13)	151.43(5)
O(9)-Ni(3)-O(14)	95.53(5)	O(9)-Ni(3)-N(242)	101.80(6)
O(9)-Ni(3)-N(312)	101.92(6)	O(10)-Ni(3)-O(13)	98.66(5)
O(10)-Ni(3)-O(14)	89.63(5)	O(10)-Ni(3)-N(242)	92.78(6)
O(10)-Ni(3)-N(312)	163.68(6)	O(13)-Ni(3)-O(14)	61.57(5)
O(13)-Ni(3)-N(242)	99.95(6)	O(13)-Ni(3)-N(312)	94.78(6)
O(14)-Ni(3)-N(242)	161.51(6)	O(14)-Ni(3)-N(312)	88.66(6)
N(242)-Ni(3)-N(312)	93.98(6)	O(11)-Ni(4)-O(12)	61.60(5)
O(11)-Ni(4)-O(15)	88.91(5)	O(11)-Ni(4)-O(16)	95.19(5)
O(11)-Ni(4)-N(342)#1	87.43(6)	O(11)-Ni(4)-N(412)	165.24(6)
O(12)-Ni(4)-O(15)	98.77(5)	O(12)-Ni(4)-O(16)	151.40(5)
O(12)-Ni(4)-N(342)#1	94.02(6)	O(12)-Ni(4)-N(412)	103.71(6)
O(15)-Ni(4)-O(16)	62.06(5)	O(15)-Ni(4)-N(342)#1	163.06(6)
O(15)-Ni(4)-N(412)	92.23(6)	O(16)-Ni(4)-N(342)#1	101.81(6)
O(16)-Ni(4)-N(412)	98.35(6)	N(342)#1-Ni(4)-N(412)	95.50(7)

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Co(1)-O(1)	1.9868(17)	Co(1)-O(3)#1	1.9851(11)
Co(1)-N(112)	2.0398(14)	Co(1)-N(142)#2	2.0414(19)
O(1)-Co(1)-O(3)#1	132.77(7)	O(1)-Co(1)-N(112)	97.41(6)
O(1)-Co(1)-N(142)#2	120.23(6)	O(3)#1-Co(1)-N(112)	106.53(5)
O(3)#1-Co(1)-N(142)#2	93.91(6)	N(112)-Co(1)-N(142)#2	102.34(7)

8

Co(1)-O(1)	1.9910(14)	Co(1)-O(3)	1.9931(13)

Co(1)-N(112)	2.0432(15)	Co(1)-N(142)	2.0058(19)
O(1)-Co(1)-O(3)	107.06(5)	O(1)-Co(1)-N(112)	98.51(6)
O(1)-Co(1)-N(142)	106.45(6)	O(3)-Co(1)-N(112)	99.42(6)
O(3)-Co(1)-N(142)	126.90(6)	N(112)-Co(1)-N(142)	114.84(6)
9			
Co(1)-O(1)	1.980(6)	Co(1)-O(3)#1	1.931(6)
Co(1)-N(12)	2.006(6)	Co(1)-N(42)#2	2.036(5)
O(1)-Co(1)-O(3)#1	107.6(2)	O(1)-Co(1)-N(12)	114.1(2)
O(1)-Co(1)-N(42)#2	96.3(2)	O(3)#1-Co(1)-N(12)	122.8(2)
O(3)#1-Co(1)-N(42)#2	99.6(2)	N(12)-Co(1)-N(42)#2	112.3(2)

Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -x+1,y,-z+1/2, #2 -x+1,-y+1,-z, #3 x,-y+1,z+1/2. For **2**: #1 -x+1,y-1/2,-z+3/2, #2 -x,-y,-z+1. For **3**: #1 -x+1,-y+1,-z+1, #2 -x+1,-y,-z, #3 x+1,y-2,z. For **4**: #1 -x+3,-y+2,-z+1, #2 -x+4,-y+3,-z+1, #3 x-1,y-1,z, #4 x-1,y,z, #5 -x+3,-y+1,-z. For **5**: #1 -x+1,-y,-z+1. For **6**: #1 x-1,y,z, #2 x+1,y,z, #3 x,y,z-1. For **7**: #1 x,-y+1/2+1,z+1/2-1, #2 -x+2,y+1/2,-z+1/2. For **9**: #1 -x+1,-y+1,-z, #2 x-1,y,z-1.

Table S2 Hydrogen bonding data for complexes **1 – 9**.

D-H···A	d(D···A) (Å)	∠D-H···A (°)
	Compound **1**	
N1-H1A···O2#1	2.823(2)	163
	Compound **2**	
N2-H2A···O2#1	2.788(3)	164
N4-H4···O3#2	2.792(3)	135
C8-H8···O3#3	3.178(3)	126
C12-H12···O2#4	3.257(3)	158
C21-H21···O3#5	3.454(4)	155
	Compound **3**	
N111-H37···O4#1	2.860(11)	165
N141-H40···O16#2	2.811(12)	159
N211-H47···O10	2.656(10)	161
N241-H50···O13#3	2.914(10)	151
N311-H57···O12#4	2.727(11)	148
N341-H60···O6#5	2.676(11)	157
N411-H67···O2#6	2.885(10)	164
N441-H70···O8	2.740(10)	152
C25-H7···O14#7	3.147(12)	123
C102-H33···O4#1	3.324(10)	162
C105-H35···O16#2	3.312(13)	141
C142-H41···O8#8	3.172(12)	139
C402-H63···O2#6	3.328(11)	161
C412-H68···O12	3.187(11)	131
	Compound **4**	
N1-H1A···O3#1	2.812(3)	155
N3-H3B···O1W#2	2.827(4)	167
C21-H21B···O1#3	3.162(4)	146
	Compound **5**	
N11-H5···O4#1	2.864(4)	171
N41-H8···O5#2	2.765(4)	162
O5-H12···O4#1	2.861(3)	155(4)

O5-H13···O3#3	2.920(3)	159(4)
C5-H3···O2#4	3.308(4)	152
C13-H7···O4#5	3.171(4)	129
	Compound **6**	
N111-H45···O13#1	2.747(2)	175
N141-H40···O12#1	2.793(2)	173
N211-H55···O17#1	2.656(10)	176
N241-H58···O1#2	2.874(2)	136
N311-H65···O4#3	2.723(2)	174
N341-H68···O8#4	2.813(2)	175
N411-H75···O18	3.149(4)	173
N411-H78···O9#5	2.848(2)	139
O17-H81···O19	2.859(4)	165(3)
O17-H82···O16#6	2.711(2)	149(4)
O18-H83···O23	2.860(5)	168(3)
O18-H84···O5#7	2.705(3)	145(4)
O19-H85···O20	2.868(4)	174(3)
O19-H86···O11#6	2.769(2)	141(3)
O20-H87···O9#6	2.810(3)	165(3)
O20-H88···O24	2.806(4)	163(3)
O22-H91···O1#1	2.802(3)	167(3)
O24-H95···O14#6	2.774(3)	154(3)
O24-H96···O17	3.082(4)	160(3)
C102-H41···O13#1	3.374(2)	164
C103-H42···O12#1	3.326(2)	166
C105-H43···O24	3.409(3)	163
C106-H44···O19	3.302(3)	163
C206-H54···O17#1	3.427(3)	148
C305-H63···O8#4	3.360(3)	165
C306-H64···O4#3	3.339(3)	164
C406-H74···O18	3.377(4)	146
	Compound **7**	
N111-H15···O2#1	2.752(2)	169

N141-H18···O4#2	2.711(2)	169
C6-H9···O3	3.086(2)	116
	Compound **8**	
N111-H15···O6	2.750(3)	160
N141-H18···O4#1	2.750(2)	145
O5-H21···O1	2.904(3)	167(4)
O5-H22···O4#2	3.041(4)	173(3)
O6-H23···O2#3	2.782(3)	175(2)
O6-H24···O2#4	2.884(3)	167(4)
C143-H20···O5#5	3.206(4)	146
	Compound **9**	
N11-H5···O4#1	2.784(9)	175
N41-H8···O6#1	2.898(9)	170
O5-H20···O2#2	2.630(8)	165(10)
C3-H2···O6#1	3.325(10)	171
C13-H7···O1#3	3.203(10)	138
C43-H10···O1#4	3.383(10)	151

Symmetry transformations used to generate equivalent atoms: For **1**: #1 1/2+x,3/2-y,1/2+z. For **2**: #1 1-x,1/2+y,3/2-z; #2 -2+x,1/2-y,-1/2+z; #3 1-x,-1/2+y,3/2-z ; #4 -x,-y,1-z ; #5 2-x,-y,2-z. For **3**: #1 -x,1-y,1-z; #2 1-x,2-y,-z; #3 -1+x,y,1+z; #4 x,-1+y,1+z; #5 x,-1+y,z; #6 1+x,y,-1+z; #7 1-x,-y,1-z; #8 -x,2-y,-z. For **4**: #1 x,-1+y,z; #2 -1+x,y,z; #3 4-x,3-y,1-z. For **5**: #1 x,1+y,z; #2 1-x,1-y,2-z; #3 1-x,1-y,1-z; #4 2-x,1-y,2-z; #5 1-x,-y,1-z. For **6**: #1 1-x,1-y,1-z ; #2 1-x,-1/2+y,3/2-z; #3 1+x,1/2-y,1/2+z; #4 x,1/2-y,1/2+z; #5 1-x,1/2+y,3/2-z; #6 x,1/2-y,-1/2+z; #7 1-x,-1/2+y,1/2-z. For **7**: #1 1+x,3/2-y,1/2+z; #2 2-x,-1/2+y,3/2-z. For **8**: #1 2-x,1-y,1-z; #2 -1+x,y,z; #3 x,-1+y,z; #4 2-x,1-y,-z; #5 1-x,1-y,1-z. For **9**: #1 1+x,-1+y,z; #2 1-x,1-y,1-z; #3 1-x,-y,-z; #4 2-x,-y,1-z.

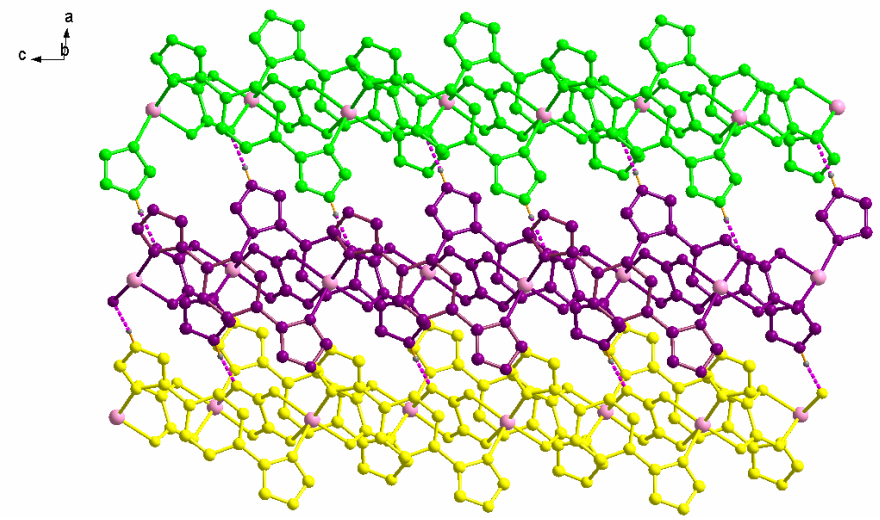


Fig. S1. 2D network of **1** linked by hydrogen bonds indicated by dashed line.

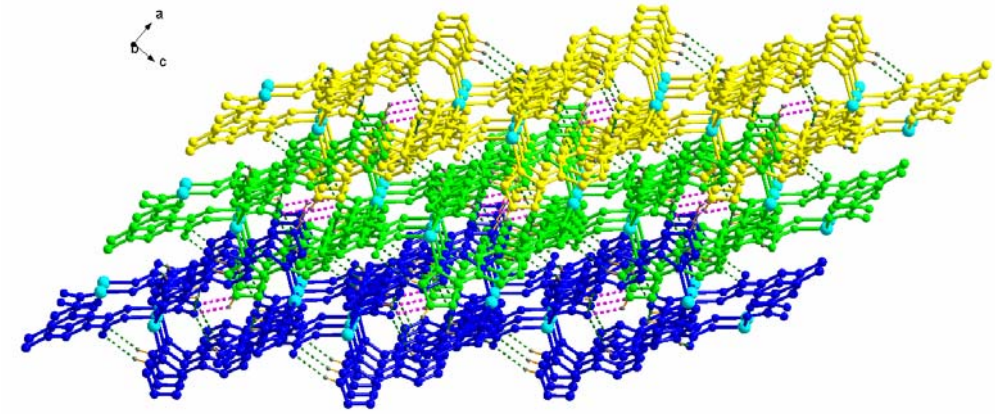


Fig. S2. The 3D structure of **2** linked by hydrogen bonds indicated by dashed lines.

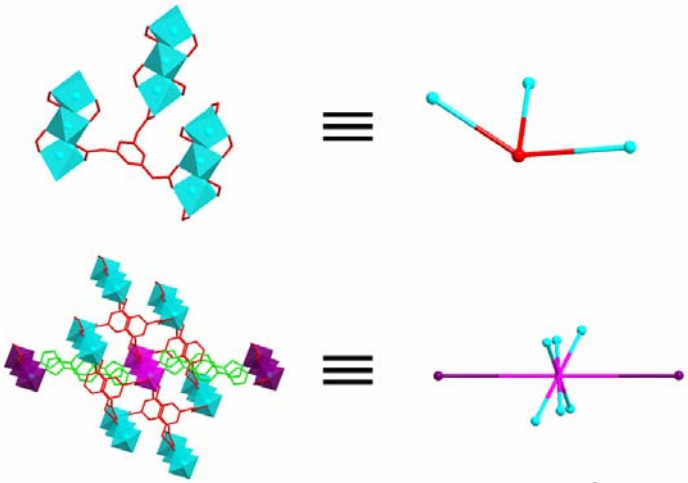


Fig. S3. Polyhedral representations of the 3-connected BTA^{3-} ligand and 8-connected trinuclear SBU of **4**.

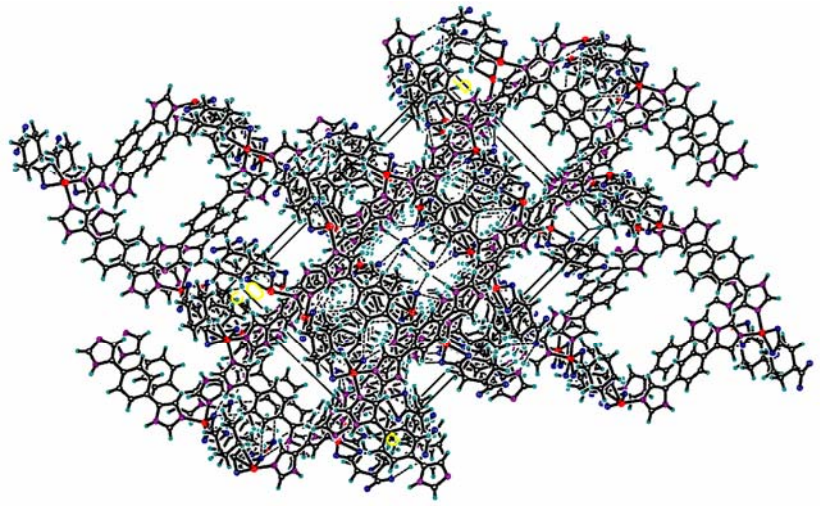


Fig. S4 The 3D structure of **6** linked by hydrogen bonds indicated by dashed lines.

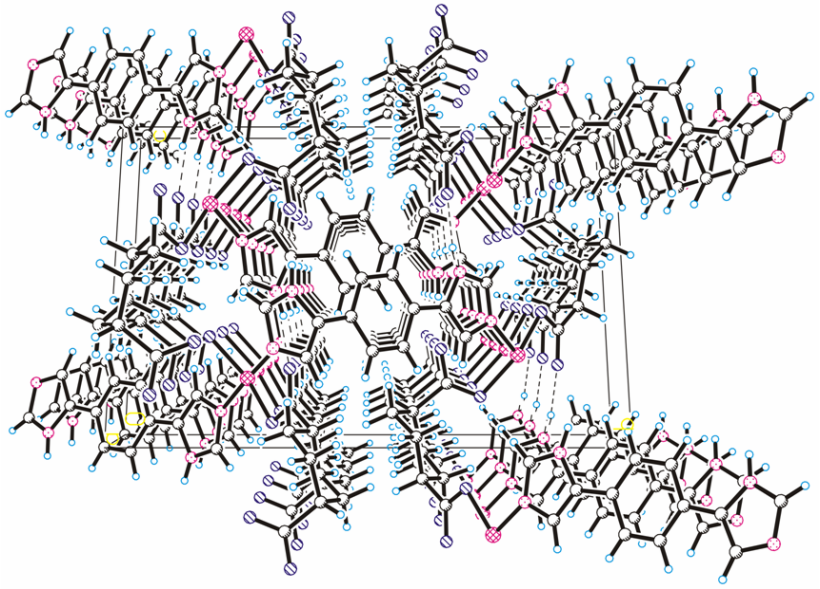


Fig. S5 The 3D structure of **7** linked by hydrogen bonds indicated by dashed lines.

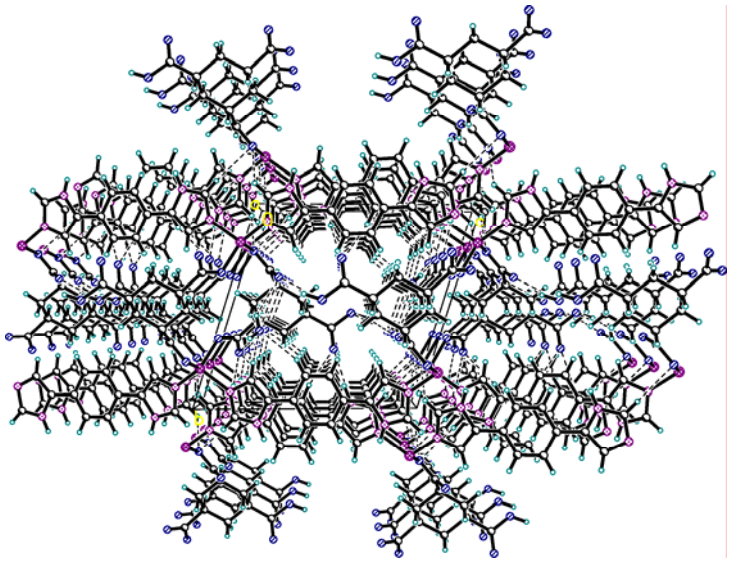


Fig. S6 The 3D structure of **9** linked by hydrogen bonds indicated by dashed lines.

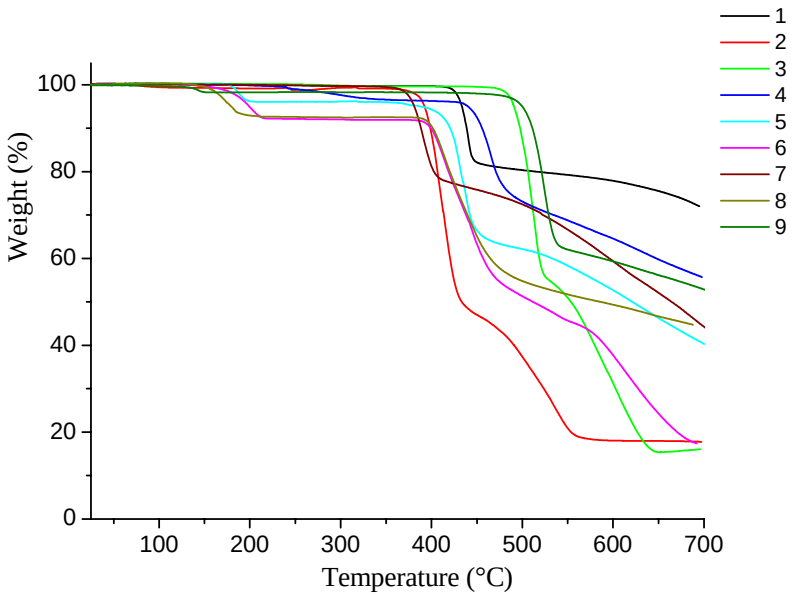
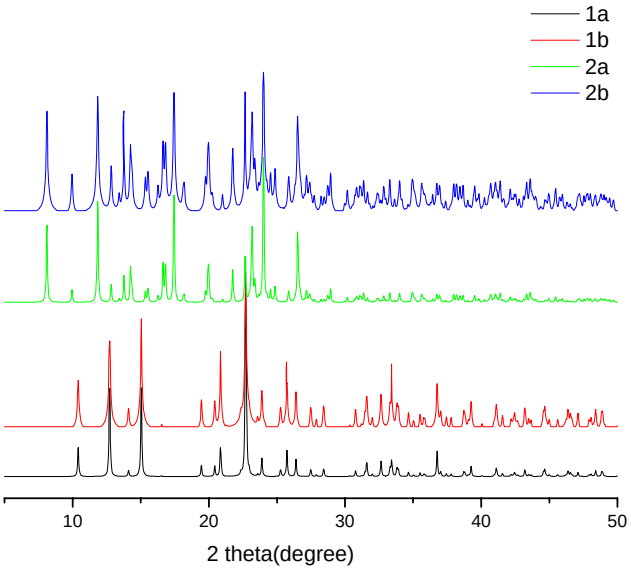
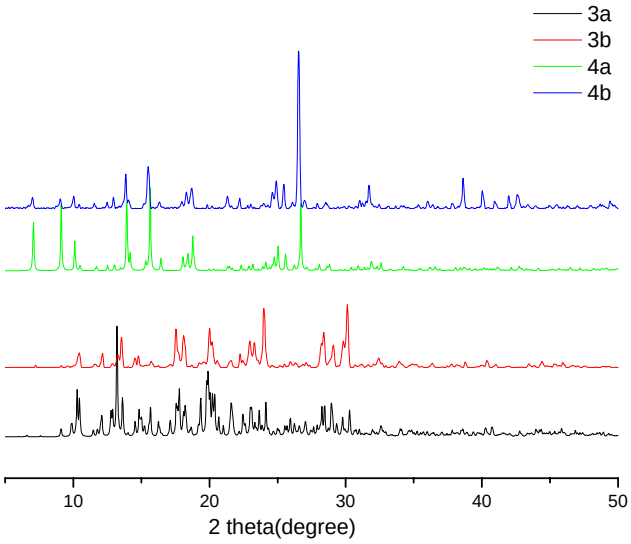
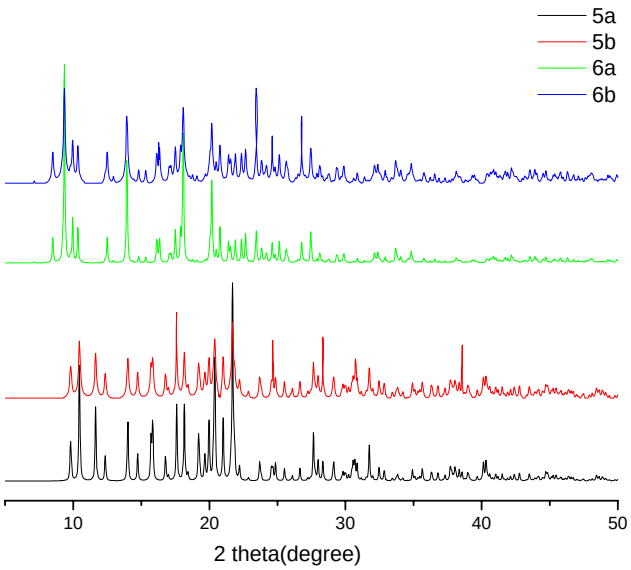


Fig. S7 The TG curves of **1 - 9**.







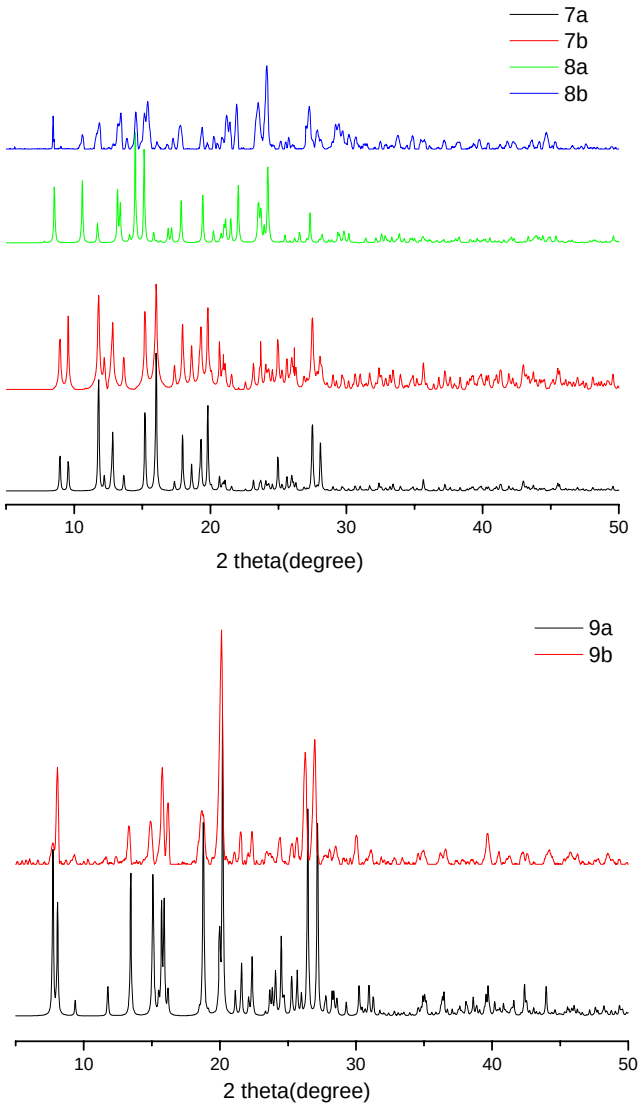


Fig. S8 PXRD patterns of **1 - 9:** a - simulated; b - as-synthesized**.**