Electronic Supplementary Information (ESI) for CrystEngComm

Syntheses, structures and photoluminsent properties of a series of Ag(I) coordination architectures based on 2,4-diamino-6-methyl-1,3,5-triazine and dicarboxylates: from 0D discrete molecule to 3D network

Di Sun,‡ Yun-Hua Li,‡ Hong-Jun Hao, Fu-Jing Liu, Yang Zhao, Rong-Bin Huang* and Lan-Sun Zheng

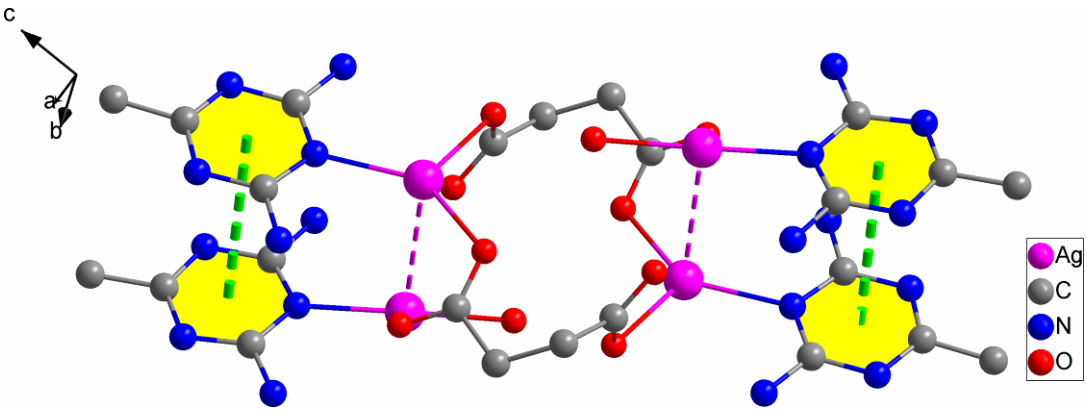
State Key Laboratory of Physical Chemistry of Solid Surface, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, 361005, China

‡*These authors contributed equally to this work.*

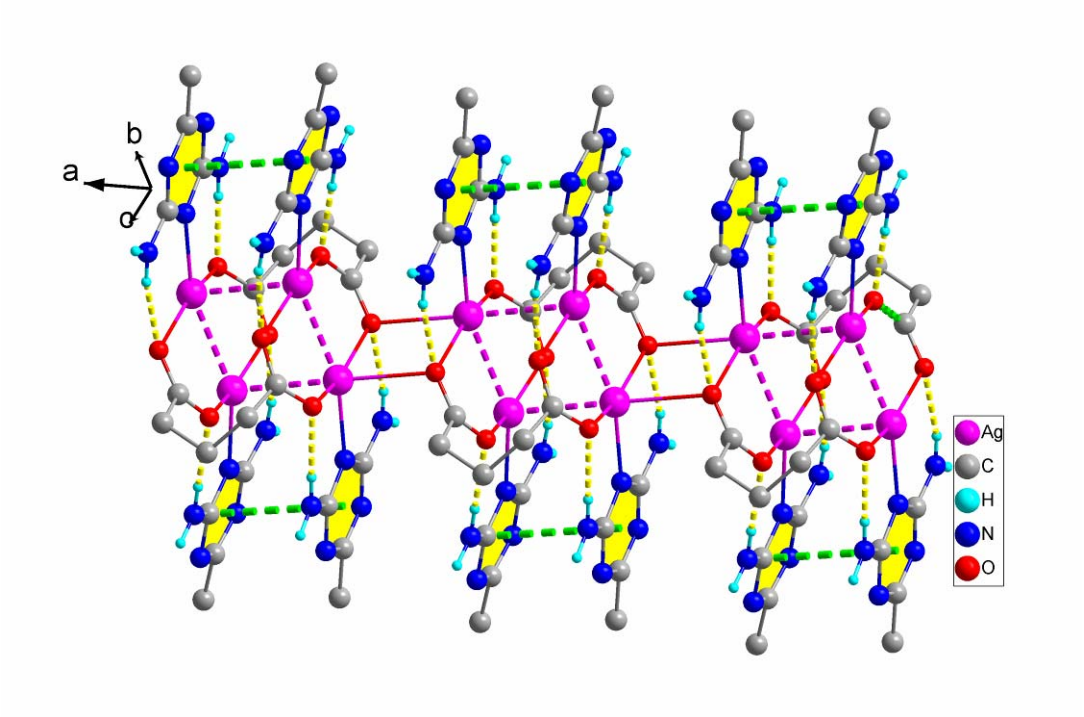
(1) Table S1 The hydrogen bond geometries for **1-5**.

Complex **1**				
D—H···A	D—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1	0.88	1.97	2.830(5)	165
N1—H1B···O2^{iv}	0.88	2.02	2.898(5)	174
N2—H2A···O1^{i}	0.88	2.25	3.093(5)	160
N2—H2B···O1W	0.88	1.97	2.806(5)	159
O1W—H1WA···O2^{v}	0.85	1.95	2.793(5)	174
O1W—H1WB···N5^{vi}	0.85	2.12	2.969(5)	174
Symmetry code: (i) −*x*+1/2, *y*, −*z*+1/2; (iv) *x*−1/2, −*y*+1, z−1/2; (v) *x*+1/2, −*y*+1, *z*−1/2; (vi) −*x*+1, −*y*+2, −z.				
Complex **2**				
N4—H4D···O1	0.88	2.26	3.134(12)	173
N4—H4E···N8^{iii}	0.88	2.22	3.099(12)	175
N5—H5A···N7^{iv}	0.88	2.06	2.935(12)	176
N5—H5B···O4^{i}	0.88	2.10	2.906(12)	153
N9—H9A···O2	0.88	2.10	2.891(12)	149
N9—H9B···N3^{iii}	0.88	2.01	2.881(12)	171
N10—H10C···O4^{i}	0.88	2.64	3.249(14)	127
N10—H10D···N2^{iv}	0.88	2.26	3.138(12)	174
O1W—H1WA···O2^{v}	0.85	2.11	2.957(13)	174
O1W—H1WB···O3	0.85	2.31	3.123(12)	161
Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) −*x*, −*y*, −*z*; (v) −*x*, −*y*+1, −*z*+1.				
Complex **3**				
N4—H4D···O3^{i}	0.88	2.05	2.927(6)	173
N4—H4E···N7^{iii}	0.88	2.20	3.080(6)	177
N5—H5A···N8^{iv}	0.88	2.19	3.062(6)	173
N5—H5B···O2	0.88	2.10	2.968(6)	169
N9—H9A···N3^{iv}	0.88	2.17	3.046(6)	173
N9—H9B···O4	0.88	2.08	2.948(6)	169
N10—H10A···N2^{iii}	0.88	2.20	3.075(6)	178
N10—H10B···O1^{i}	0.88	2.03	2.907(5)	174
Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*, −*z*+2; (iv) −*x*+1, −*y*+1, −*z*+2.				
Complex **4**				
N3—H3A···O2	0.88	2.03	2.910(4)	176
N3—H3B···N7^{iii}	0.88	2.07	2.949(4)	176
N6—H6A···O1^{i}	0.88	2.02	2.890(4)	172
N6—H6B···N2^{iv}	0.88	2.28	3.047(4)	146
Symmetry codes: (i) −*x*+2, *y*, −*z*+3/2; (iii) *x*−1/2, *y*+1/2, *z*; (iv) *x*+1/2, *y*−1/2, *z*.				
Complex **5**				
N3—H3D···N2^{ii}	0.88	2.24	3.101(6)	164.8
N3—H3E···O2^{i}	0.88	2.12	2.888(6)	145.8
N5—H5B···O2	0.88	2.15	2.969(6)	155.1
N5—H5A···O1^{iii}	0.88	2.01	2.838(6)	157.0
Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+3, −*y*+1, −*z*+2; (iii) *x*, −*y*+3/2, *z*−1/2.				

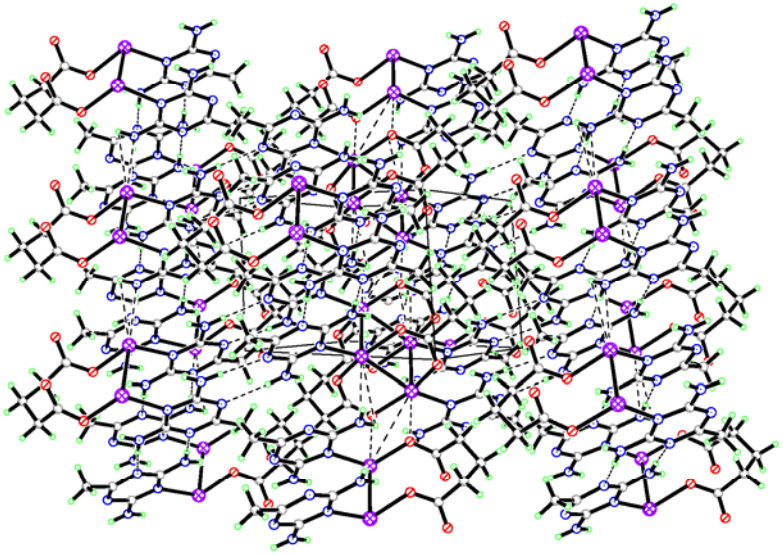
(2) Figure S1 Intramolecular face-to-face π···π interaction in **2**



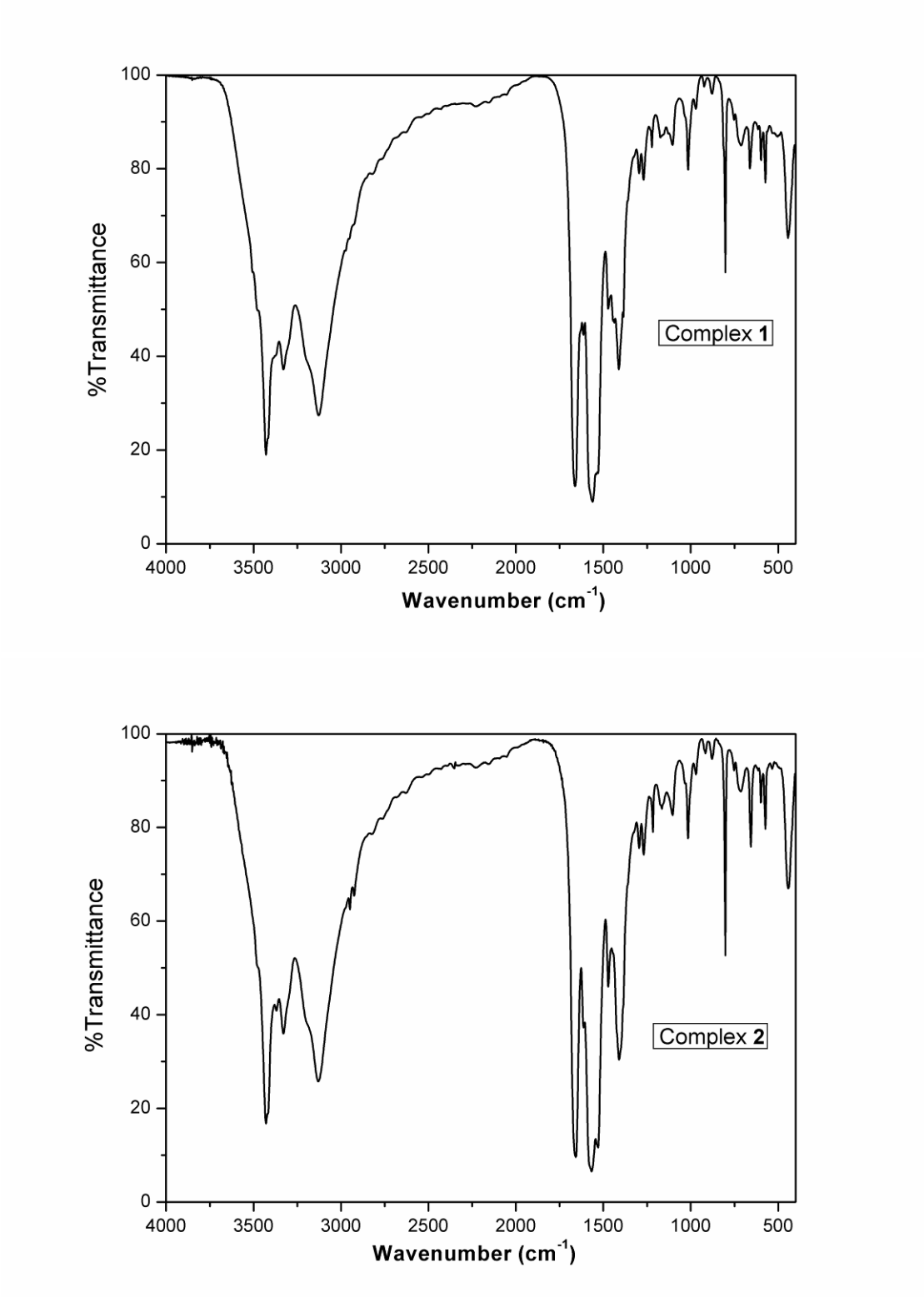
(3) Figure S2 Intrachain face-to-face π···π interaction and intrachain N-H···O_{glu} hydrogen bonds in **3**

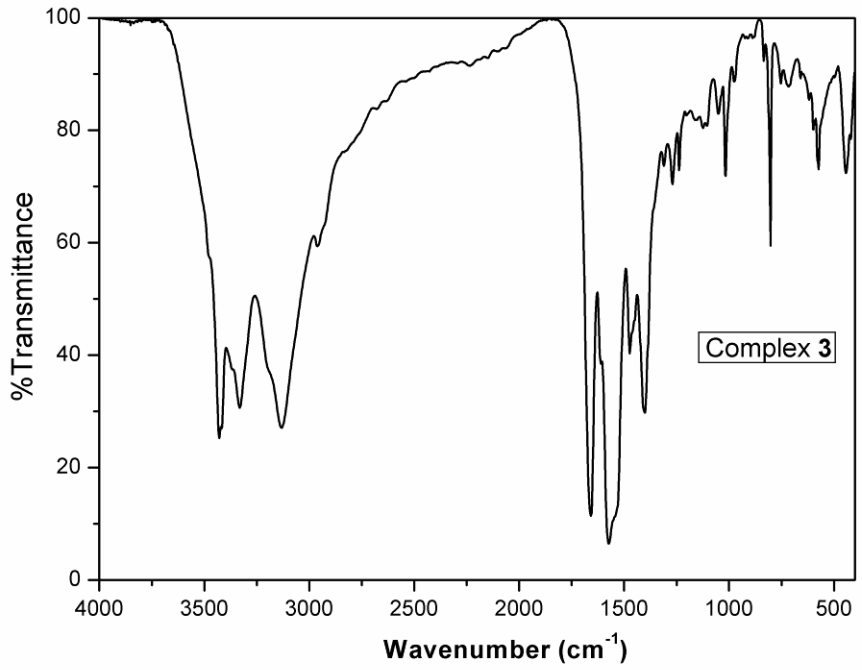


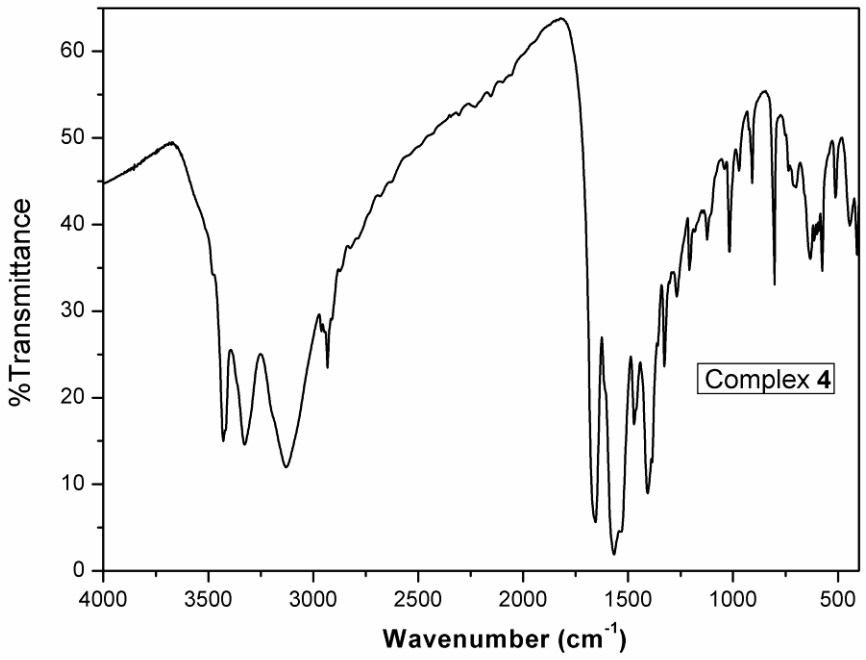
(4) Figure S3 The 3D supramolecular framework in **3**

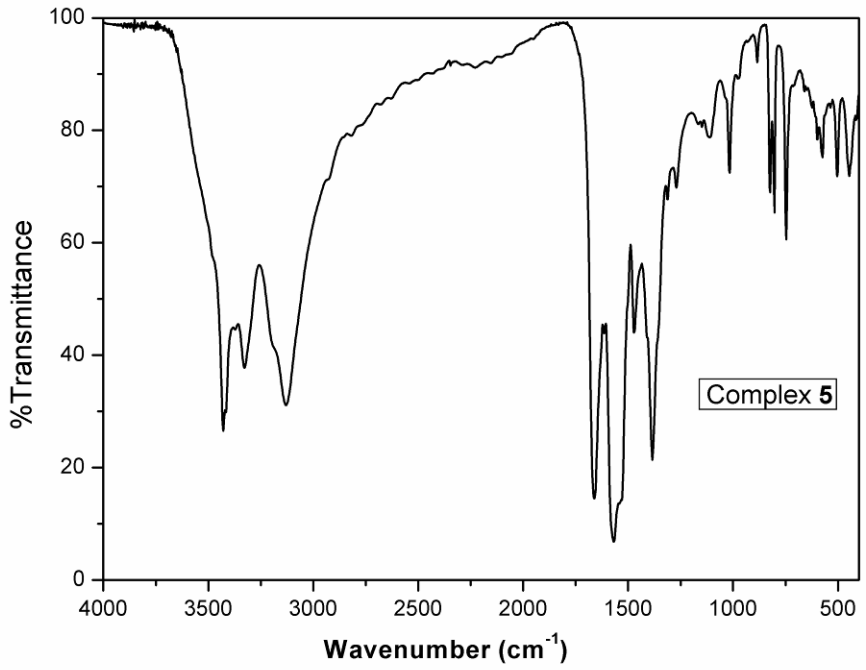


(5) Fig. S4 IR of complex 1-5

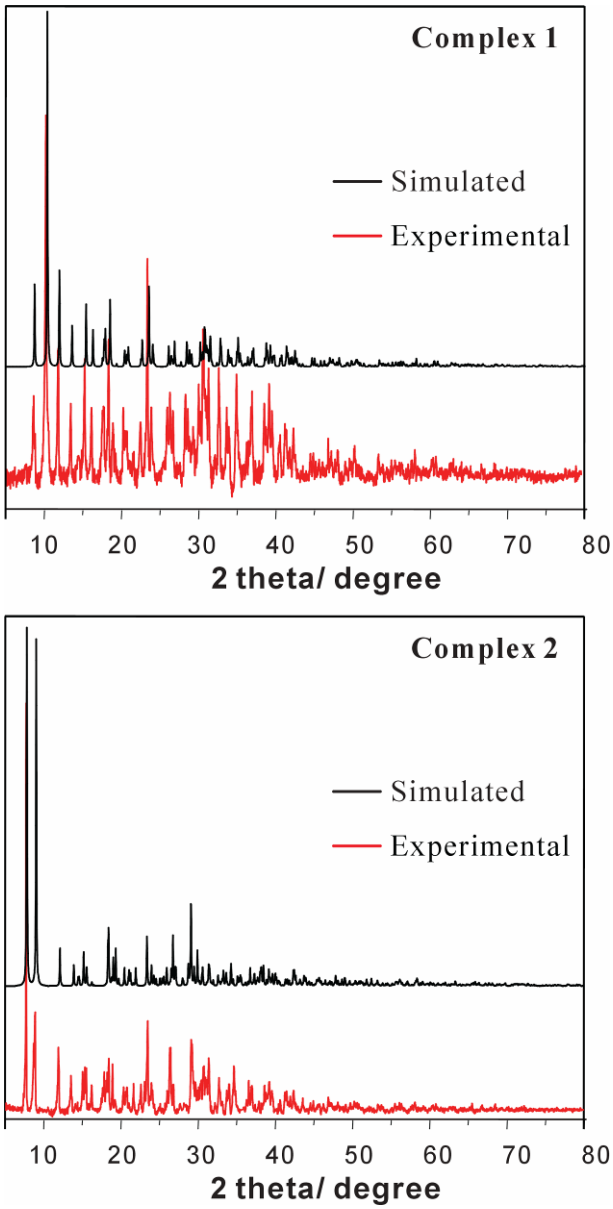


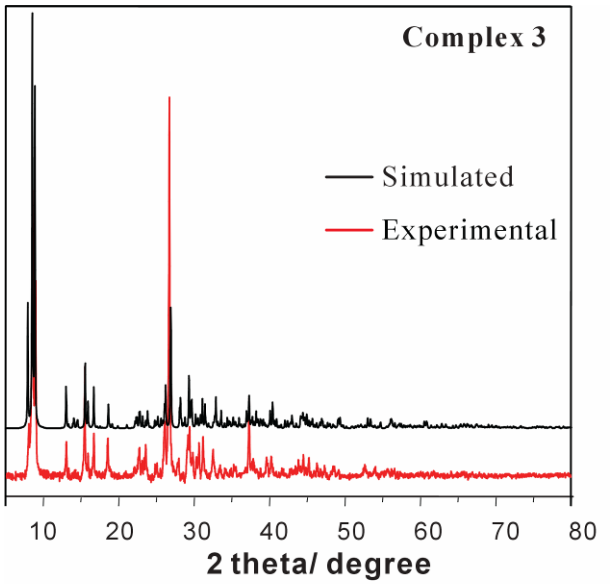


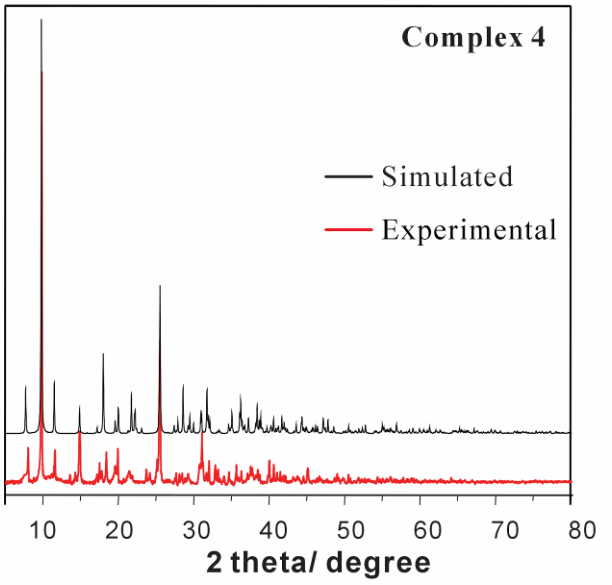


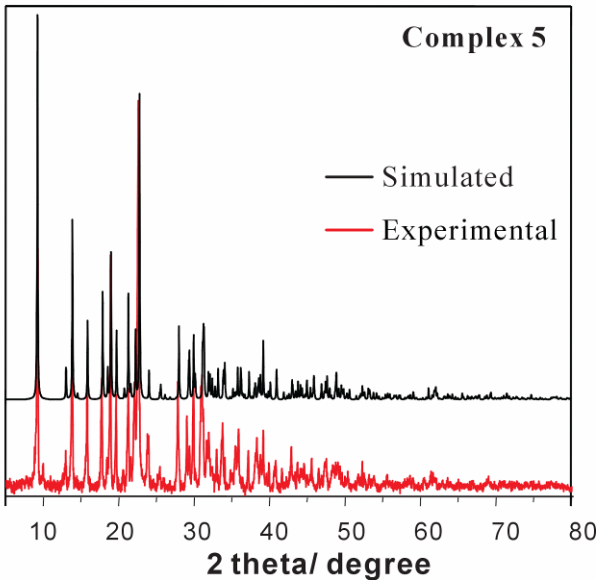


(6) Fig. S5 The powder XRD patterns and the simulated one from the single-crystal diffraction data for complex 1-5




Complex 3
Simulated
Experimental
10
20
30
40
50
60
70
80
2 theta/ degree


Complex 4
Simulated
Experimental
10
20
30
40
50
60
70
80
2 theta/ degree


Complex 5
Simulated
Experimental
10
20
30
40
50
60
70
80
2 theta/ degree

(7) Fig. S6 The photoluminescence spectrum of 2,4-diamino-6-methyl-1,3,5-triazine (dmt).