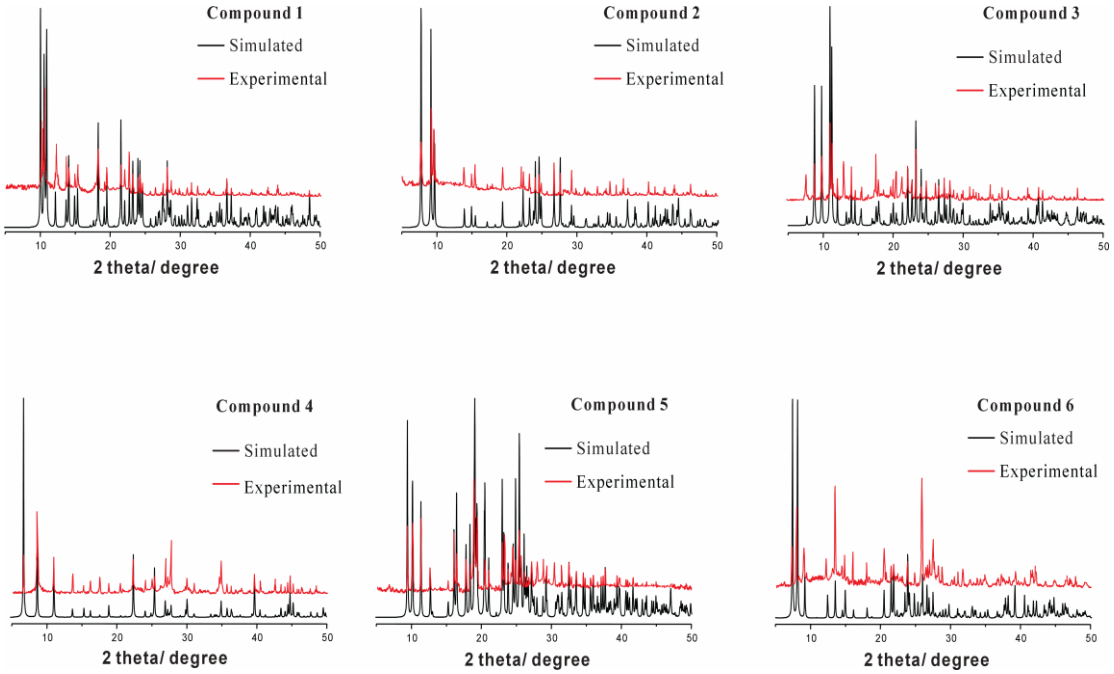
Electronic Supplementary Information (ESI) for *CrystEngComm*

Reactant Ratio-Modulated Six New Copper(I)-Iodide Coordination Complexes Based on Diverse [Cu_mI_m] Aggregates and Biimidazole Linkers: Syntheses, Structures and Temperature-Dependent Luminescence Properties

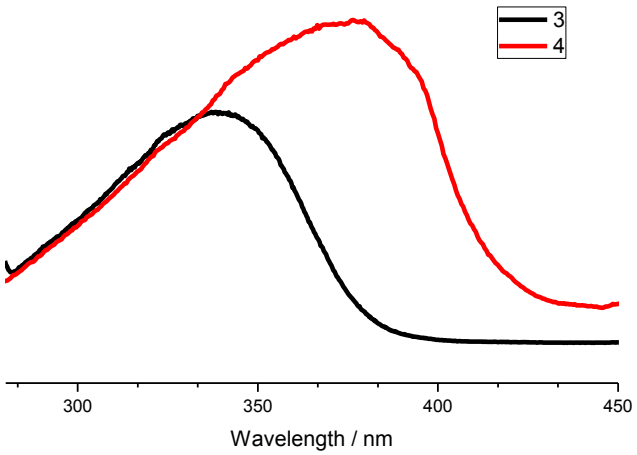
Shuai Yuan, Hua Wang, Deng-Xu Wang, Hai-Feng Lu, Sheng-Yu Feng, Di Sun,*

Key Lab of Colloid and Interface Chemistry, Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, P. R. China. E-mail: dsun@sdu.edu.cn. Fax: +86-531-88364218.

1. Figure S1. The XRD patterns of 1 - 6.



2. Figure S2. Excitation spectra for 3 and 4 at 298 K.



3. Table S1. Crystal Data Collection and Structure Refinement for 3 at four different temperatures.

Temperature/K	**100(2)**	**160(2)**	**220(2)**	**298(2)**
Empirical formula	$C_{18}H_{27}Cu_3I_3N_6$	$C_{18}H_{27}Cu_3I_3N_6$	$C_{18}H_{27}Cu_3I_3N_6$	$C_{18}H_{27}Cu_3I_3N_6$
Formula weight	898.78	898.78	898.78	898.78
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1	P-1
a/Å	10.2669(12)	10.2961(9)	10.352(2)	10.3645(8)
b/Å	10.7531(14)	10.7386(10)	10.760(2)	10.7637(9)
c/Å	11.8781(15)	11.9132(10)	11.977(2)	12.0346(10)
α/°	106.838(2)	106.7680(10)	106.782(3)	106.9346(12)
β/°	90.109(2)	90.2070(10)	90.335(3)	90.3554(13)
γ/°	101.790(2)	101.7260(10)	101.715(3)	101.8012(11)
Volume/Å^3	1226.0(3)	1232.14(19)	1247.7(4)	1254.11(18)
Z	2	2	2	2
ρ_{calc} g/cm^3	2.435	2.423	2.392	2.380
m/mm^{-1}	6.374	6.342	6.263	6.231
F(000)	846.0	846.0	846.0	846.0
Crystal size/mm^3	0.15 × 0.10 × 0.10	0.15 × 0.10 × 0.10	0.15 × 0.10 × 0.10	0.15 × 0.10 × 0.10
2Θ range for data collection	3.6 to 50°	3.58 to 50°	3.56 to 49.98°	3.54 to 50°
Reflections collected	6135	6113	6102	6288
Independent reflections	4276[R(int) = 0.0169]	4280[R(int) = 0.0146]	4295[R(int) = 0.0173]	4372[R(int) = 0.0179]
Data/restraints/parameters	4276/0/271	4280/0/271	4295/0/271	4372/0/271
Goodness-of-fit on F^2	1.154	1.072	1.095	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0252, wR_2 = 0.0688	R_1 = 0.0249, wR_2 = 0.0598	R_1 = 0.0313, wR_2 = 0.0780	R_1 = 0.0304, wR_2 = 0.0667
Final R indexes [all data]	R_1 = 0.0293, wR_2 = 0.0804	R_1 = 0.0279, wR_2 = 0.0632	R_1 = 0.0398, wR_2 = 0.0892	R_1 = 0.0399, wR_2 = 0.0716
Largest diff. peak/hole / e Å^{-3}	0.86/-0.89	1.09/-0.70	0.96/-0.71	0.72/-0.68

4. Figure S3. The disordered dimb ligand in compound 4.