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Solvent modulated assembly of two Zn Metal-Organic Frameworks: syntheses, luminescent, and gas adsorption properties

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Table S1. Selected bond length (Å) and angles (°) for complex **1**.

complex 1			
Zn1—O2	2.1185 (13)	Zn1—O4	2.3708 (15)
Zn1—N4	2.2099 (16)	Zn1—N6	2.1851 (15)
Zn1—N9	2.0941 (14)	Zn1—N10	2.0855 (13)
O2—Zn1—O4	58.36 (5)	O2—Zn1—N4	150.85 (5)
O2—Zn1—N6	88.02 (5)	N4—Zn1—O4	97.48 (5)
N6—Zn1—O4	88.59 (5)	N6—Zn1—N4	74.31 (6)
N9—Zn1—O2	100.40 (5)	N9—Zn1—O4	88.24 (5)
N9—Zn1—N4	94.32 (6)	N9—Zn1—N6	89.16(11)
N16—Zn1—N7 ii	103.24(9)	N27—Zn3—N12	167.68 (6)
N10—Zn1—O2	97.53 (5)	N10—Zn1—O4	155.72 (5)
N10—Zn1—N4	106.42 (6)	N10—Zn1—N6	93.70 (5)
N10—Zn1—N9	94.08 (5)		
Symmetry codes: (i) −x+1/2, y−1/2, z; (ii) −x+1/2, y+1/2, z; (iii) x−1/2, y, −z+1/2; (iv) x+1/2, y, −z+1/2			

Table S2. Selected bond length (Å) and angles (°) for complex **2**.

complex **2**			
Zn1—O1	1.910 (2)	Zn3—N12	2.026(2)
Zn1—N3 ^{i}	1.969(2)	Zn3—O1W	2.087(3)
Zn1—N7 ^{ii}	2.018(2)	Zn3—N23	2.078(2)
Zn1—N16	1.988(2)	Zn3—N27	2.189(3)
Zn3—O4^{3}	1.959(2)		
N3 ^{i}—Zn1—O1	115.11(9)	O1W—Zn3—N12	98.12(10)
N7 ^{ii} —Zn1—O1	97.05(8)	N23—Zn3—O4 ^{iii}	152.85(10)
N7 ^{ii}—Zn1—N3 ^{i}	115.26(8)	N23—Zn3—N12	103.18(10)
N16—Zn1—O1	117.59(9)	N23—Zn3—O1W	91.78(10)
N16—Zn1—N3 ^{i}	107.87(9)	N27—Zn3—O4 ^{iii}	89.16(11)
N16—Zn1—N7 ^{ii}	103.24(9)	N27—Zn3—N12	101.85(10)
N12—Zn3—O4 ^{iii}	102.01(9)	N27—Zn3—O1W	158.46(10)
O1W—Zn3—O4 ^{iii}	94.53(11)	N27—Zn3—N23	75.94(11)
Symmetry codes: (i) -1/2+X,+Y,1/2-Z; (ii)1/2-X,1/2+Y,+Z; (iii)-X,-Y,-Z.			

Table S3. The photophysical data for complex **1**, **2** and **2a**.

Complex	τ, ns, (Weight)	χ^2	Φ(%)
1	τ_1 = 1.29(70.12%); τ_2 = 4.78(26.37%);τ_3 = 23.45(3.50%)	1.218	2.72
2	τ_1 = 0.60(61.88%); τ_2 = 2.66(27.71%);τ_3 = 27.01(10.41%)	1.380	2.85
2a	τ_1 = 0.83(73.13%); τ_2 = 3.03(20.53%);τ_3 = 20.79(6.35%)	1.287	4.35

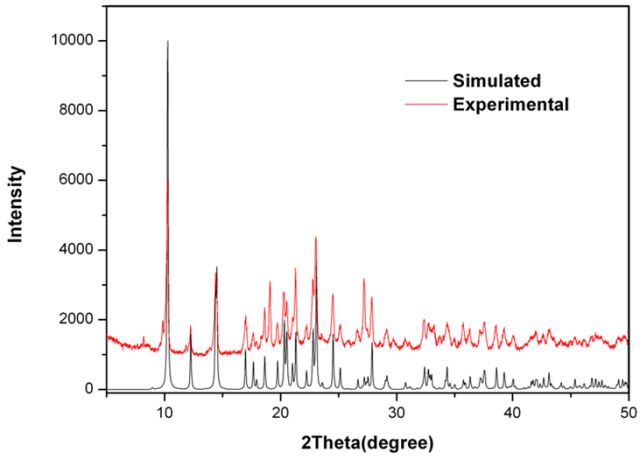

Figure S1. The simulated and experimental **PXRD** of complex **1**.

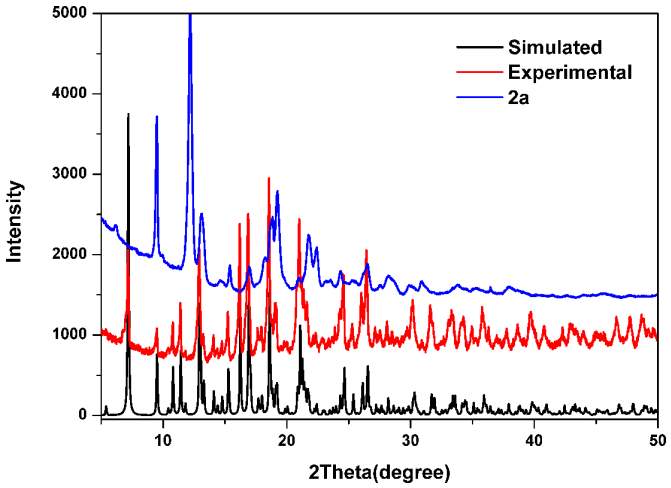

Figure S2. The simulated and experimental **PXRD** of complex **2** and experimental **PXRD** of complex **2a**.

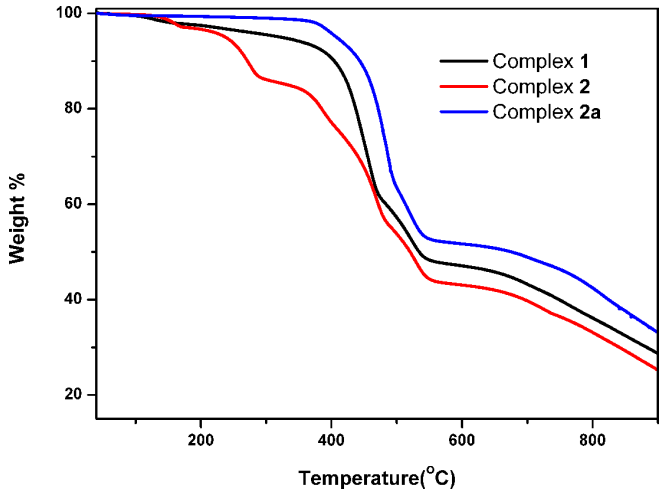

Figure S3. The TGA curves of complexes **1**, **2** and **2a.**

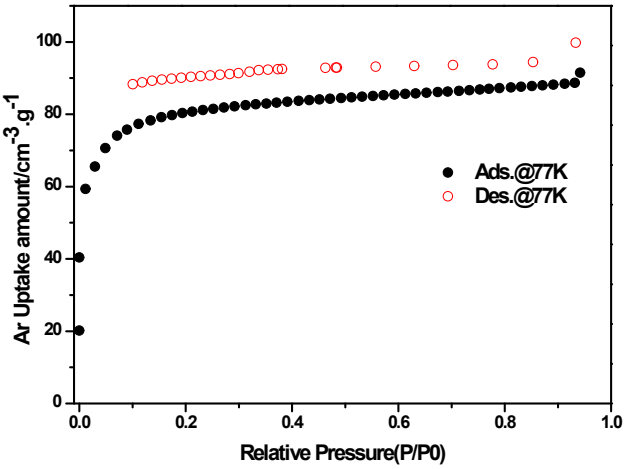

Figure S4. The Ar sorption isotherms at 77K for **2a**.

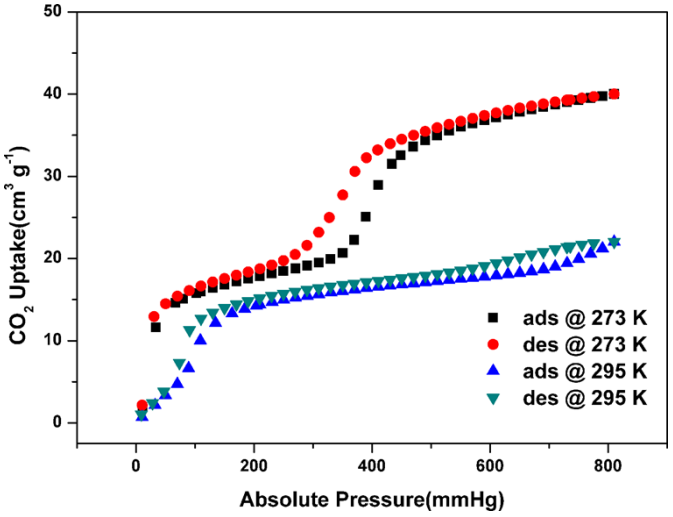

Figure S5. The CO_2 sorption isotherms at 273 and 295K for **2a**.

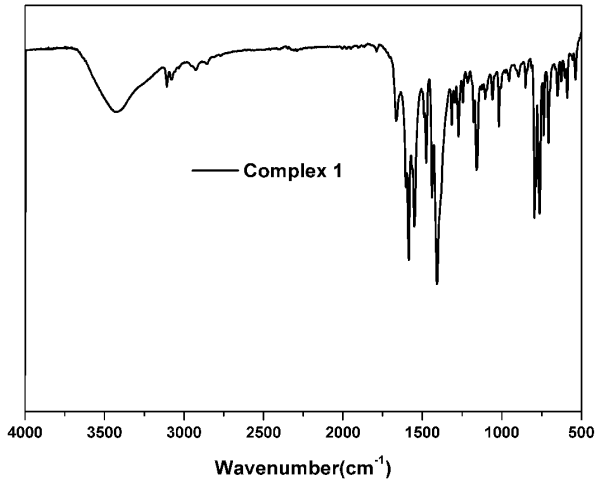

Figure S6. The IR spectrum of complex **1**.

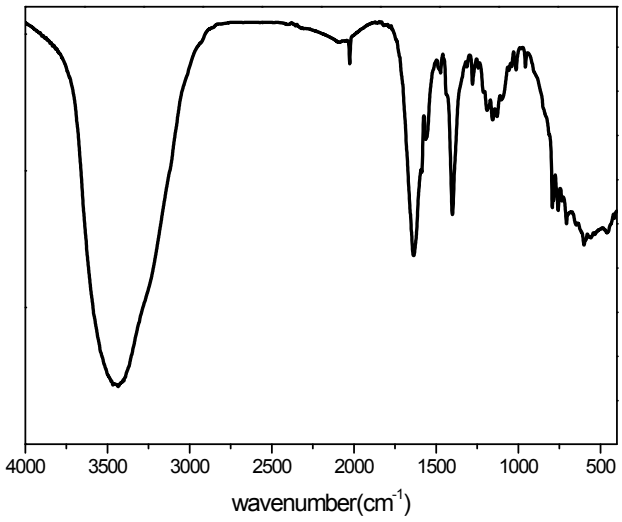

Figure S7. The IR spectrum of complex **2**.

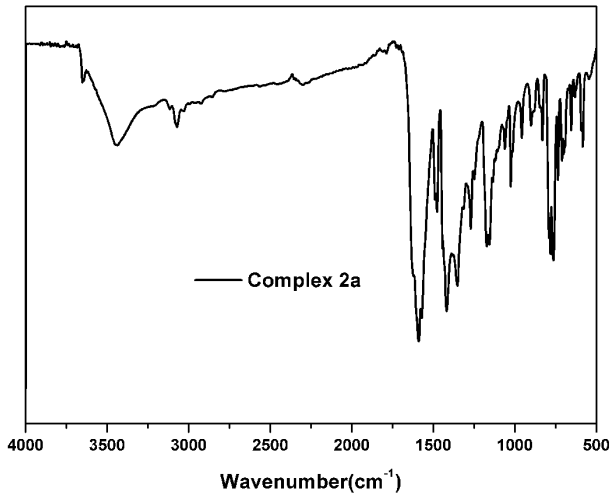

Figure S8. The IR spectrum of complex **2a**.

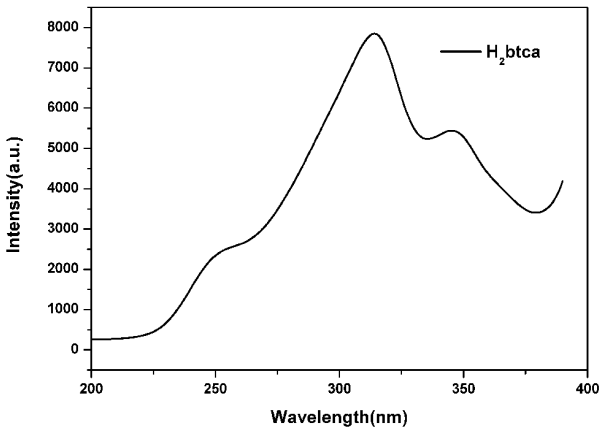

Figure S9. The photoluminescence excitation spectrum of H_2btca at 298 K

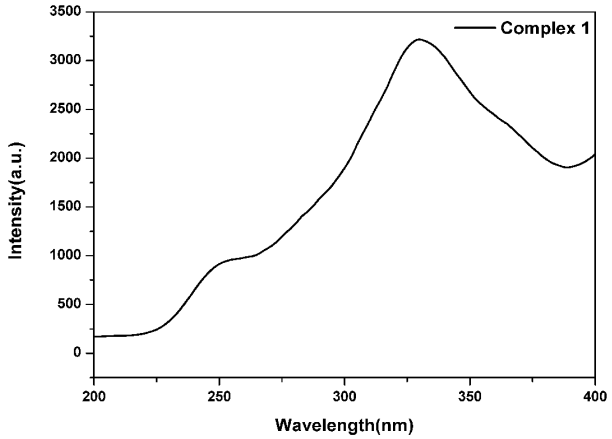

Figure S10. The photoluminescence excitation spectrum of complex **1** at 298 K

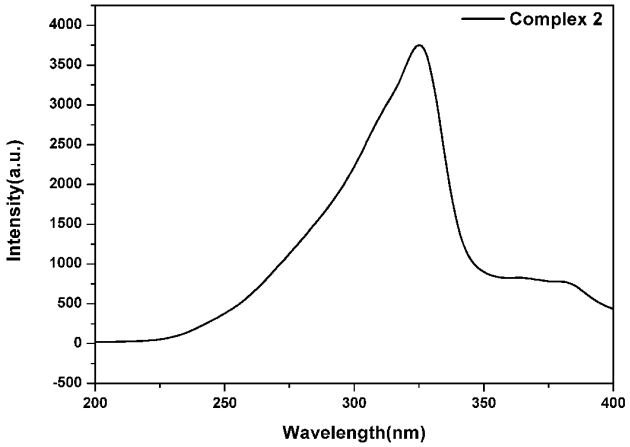

Figure S11. The photoluminescence excitation spectrum of complex **2** at 298 K

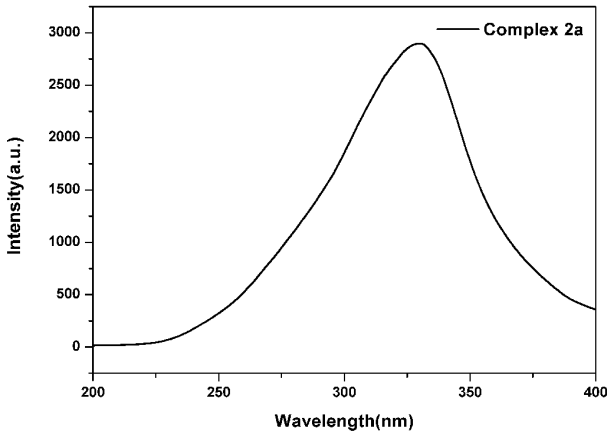

Figure S12. The photoluminescence excitation spectrum of complex **2a** at 298 K