Electronic Supplementary Material (ESI) for CrystEngComm.

ESI

Photoluminescence of the First Examples of Metal-Organic-Frameworks with Two Novel Tetrazolatephenyl Acetic Acid Derivatives.An Experimental and Theoretical Study.

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1. Different rings formed in the structures.

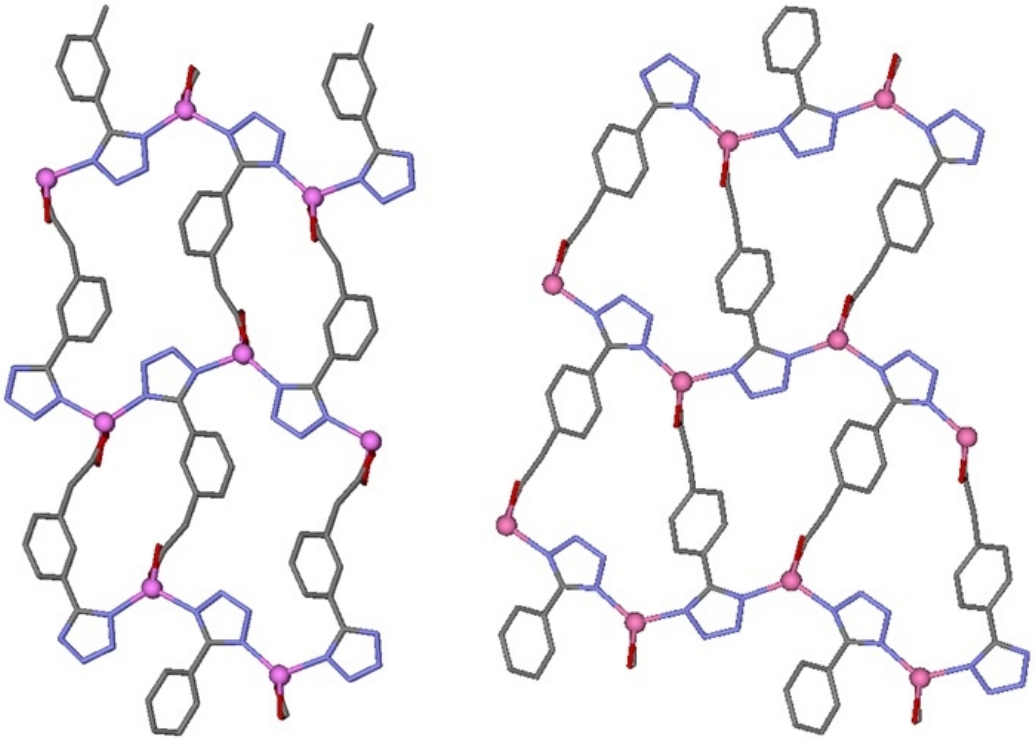

Figure S1. A view of the rings formed in the structures for **1** (left) and **2** (right), respectively.

2. Crystallographic Tables

Table S1. Bond distances (Å)

1	2
N1 Zn1 2.001(3)	N1 Zn1 1.991(5)
N2 N3 1.287(4)	N2 N3 1.285(5)
N3 N4 1.348(4)	N3 N4 1.352(6)
N4 Zn1 1.965(3)	N4 Zn1 1.973(6)
O1 Zn1 1.972(3)	O1 Zn1 1.965(2)
O2 Zn1 1.962(3)	O2 Zn1 1.976(2)
Zn1 O2 1.962(3)	Zn1 O1 1.965(2)
Zn1 N4 1.965(3)	Zn1 O2 1.976(2)
Zn1 O1 1.972(3)	Zn1 N1 1.991(5)

Table S2. Bond angles (º)

1	2
O2 Zn1 N4 118.94(12)	O1 Zn1 N4 113.3(2)
O2 Zn1 O1 107.75(11)	O1 Zn1 O2 108.13(10)
N4 Zn1 O1 106.09(11)	N4 Zn1 O2 104.7(2)
O2 Zn1 N1 101.73(11)	O1 Zn1 N1 103.0(2)
N4 Zn1 N1 116.27(12)	N4 Zn1 N1 123.37(15)
O1 Zn1 N1 105.10(13)	O2 Zn1 N1 103.2(2)

3. XRPD Analysis of 1 and 2.

The powders were gently ground in an agate mortar and then deposited with care in the hollow of an aluminum holder equipped with a zero background plate. Diffraction data (CuKα, λ=1.5418 Å) were collected on a θ:θ Bruker AXS D8 vertical scan diffractometer equipped with primary and secondary Soller slits, a secondary beam curved graphite monochromator, a Na(Tl)I scintillation detector, and pulse height amplifier discrimination. The generator was operated at 40 kV and 40 mA. Optics used are the following: divergence 0.5°, antiscatter 0.5°, receiving 0.2 mm. A short scan was performed with $5 < 2\theta < 25°$. LeBail refinements was obtained with technique implemented in Topas-13. [Topas-R, Bruker AXS: General profile and structure analysis software for powder diffraction data.]

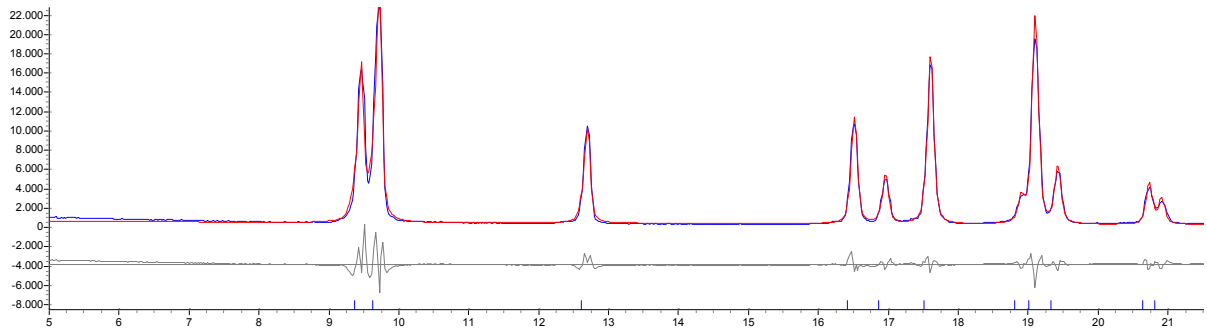

Figure S2. LeBail Refinement in **1**. a = 10.5058 Å, b = 18.8568 Å, c = 4.8160 Å, V = 954.095 Å^3, Simple Axial Model = 8 mm (Fixed) and Sample displacement = -0.189 mm.

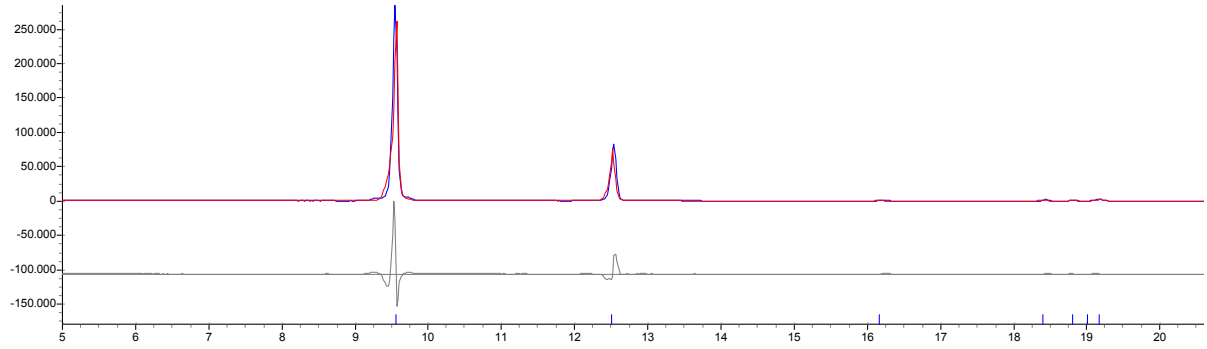

Figure S3. LeBail Refinement in **2**. a = 18.5777 Å, b = 4.7873 Å, c = 10.9274 Å, V = 971.864 Å^3, Simple Axial Model = 8 mm (Fixed) and Sample displacement = -0.03 mm.

4. TG measurements.

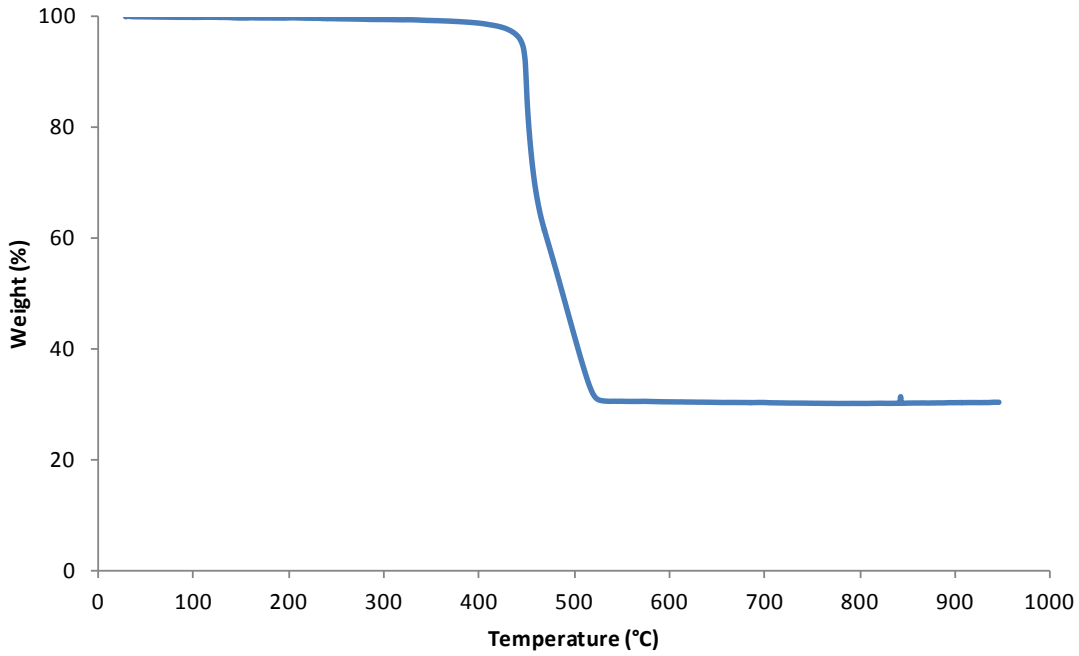

Figure S4. TG corresponding to **1**.

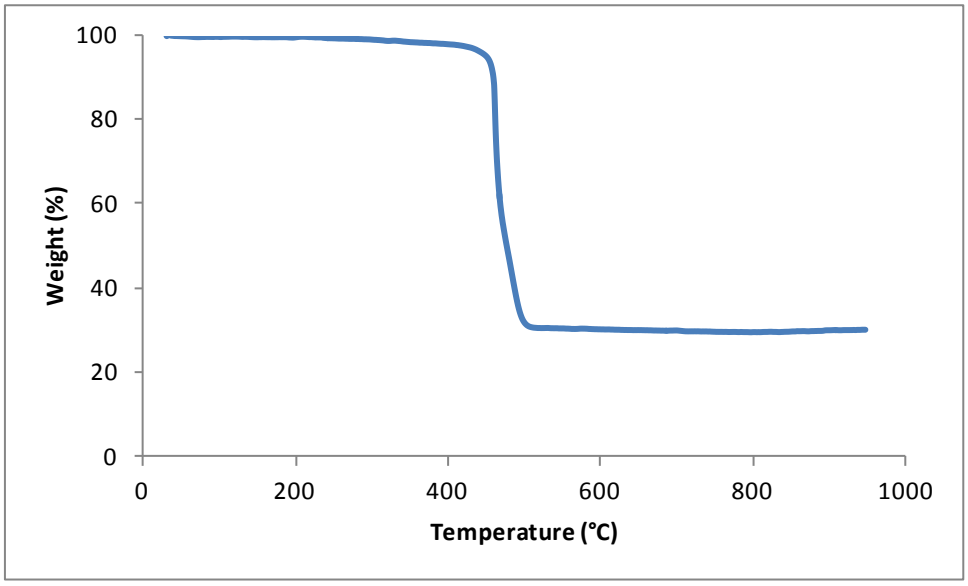

Figure S5. TG corresponding to **2**.

5. TDDFT calculation results for free ligands.

Table S3. Calculated emission maxima and corresponding transitions for free ligands 1,3-tzbaa^{-2} and 1,4-tzbaa^{-2}

	Calc. Emis (nm)	Cal. Transitions	Exp. Emis (nm)
1,3-tzbaa^{-2}	424	HOMO← LUMO	-
1,4-tzbaa^{-2}	352 502	HOMO← LUMO-1 HOMO← LUMO	-

Figure S6. Calculated emission spectra of free ligands 1,3-tzbaa^{-2} and 1,4-tzbaa^{-2}