Tunable, Ligand-Based Emission from Inorganic-Organic Frameworks: A New Approach to Phosphors for Solid State Lighting

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Supplementary Information

Thermal gravimetric analysis in air of **(1)** (Figure S1) shows removal of the two water molecules in two steps near 115°C and 200°C. An anhydrous phase is then present on heating until 450°C, where the compound decays to calcium oxalate and then finally to calcium hydroxide at 700°C. Analysis of **(2)** shows dehydration steps at 100°C and 150°C to an anhydrous structure that is stable to 400°C, followed by degradation to $SrCO_3$. The initial dehydration steps are unaffected

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by the choice of atmosphere, though the final thermal degradation characteristics are changed as expected. Additionally, luminescence studies showed a very slight decrease in luminescent intensity after holding the frameworks at 200°C for 1 day, with **(1)** decreasing from 7.4% to 6.8% and **(2)** decreasing from 2.8% to 2.5%. This behavior can been seen in Figure S3. Figure S4 and Figure S5 show Rietveld refinements of the structure determined by single crystal diffraction data to powder diffraction spectra of **(1)** and **(2)**, respectively. Data were collected at the Advanced Photon Source synchrotron X-ray beamline 11-BM at λ=0.589183Å for **(1)** and on a Bruker D8 with CuKα source for **(1)**. Models were refined to the data using GSAS and EXPGUI [1,2] to confirm purity of the bulk sample. Thermal ellipsoids and the atom numbering scheme for **(1)** and **(2)** are shown in Figure S6 and Figure S7, respectively.

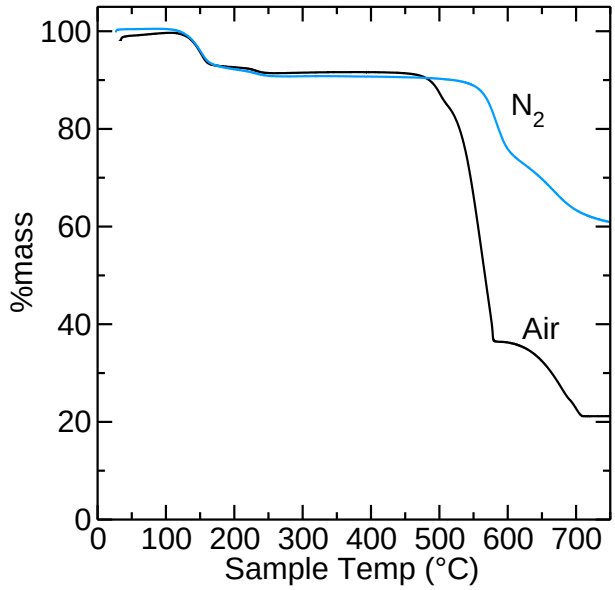

Figure S1: Thermogravimetric analysis of **(1)** in air (black) and N_2 (blue).

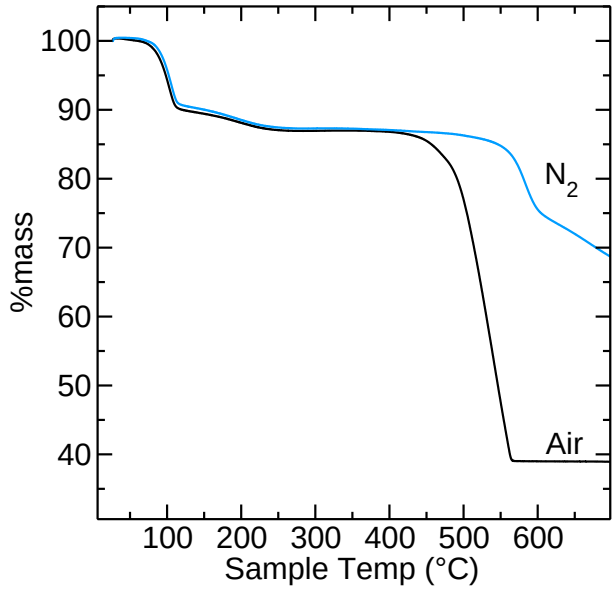

Figure S2: Thermogravimetric analysis of **(2)** in air (black) and N_2 (blue).

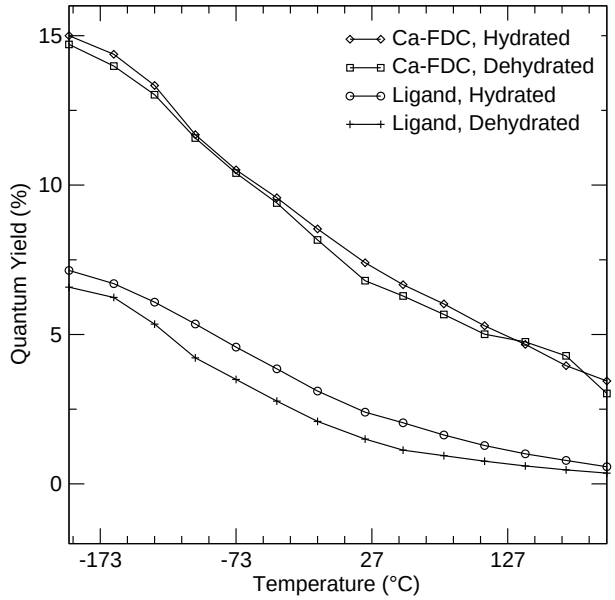

Figure S3: Temperature dependent QY of **(1)** and H_2FDC along both as prepared and dehydrated.

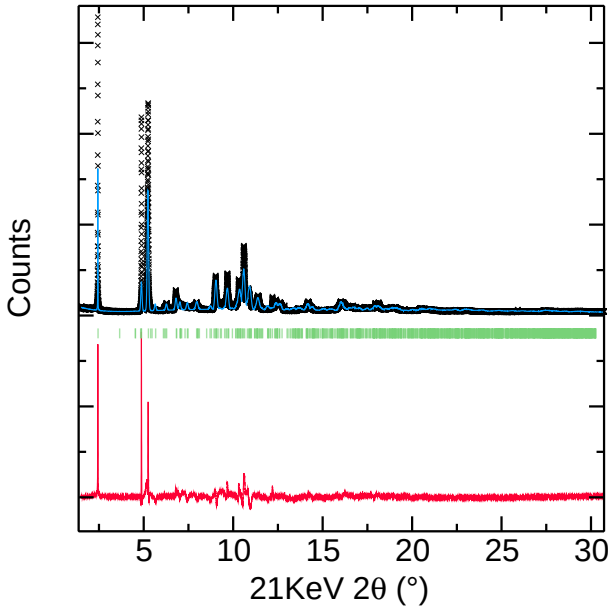

Figure S4: Synchrotron X-ray powder diffraction spectra (APS 11-BM) of bulk sample of **(1)** and Rietveld refinement of model determined by single crystal diffraction.

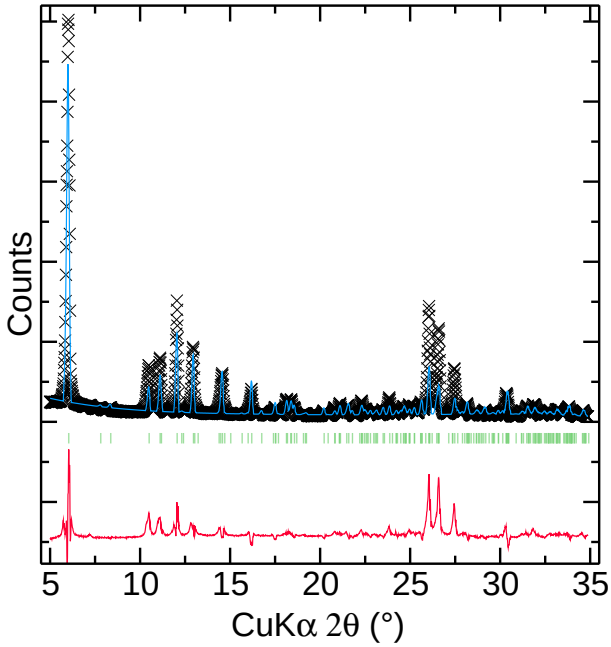

Figure S5: X-ray powder diffraction spectra of bulk sample of **(2)** and Rietveld refinement of model determined by single crystal diffraction.

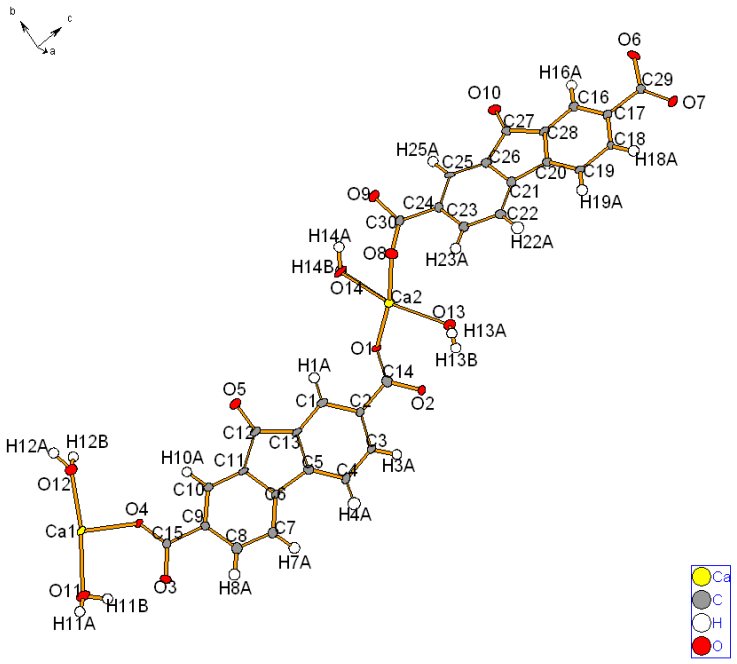

Figure S6: Thermal ellipsoid and atom numbering scheme of **(1)**

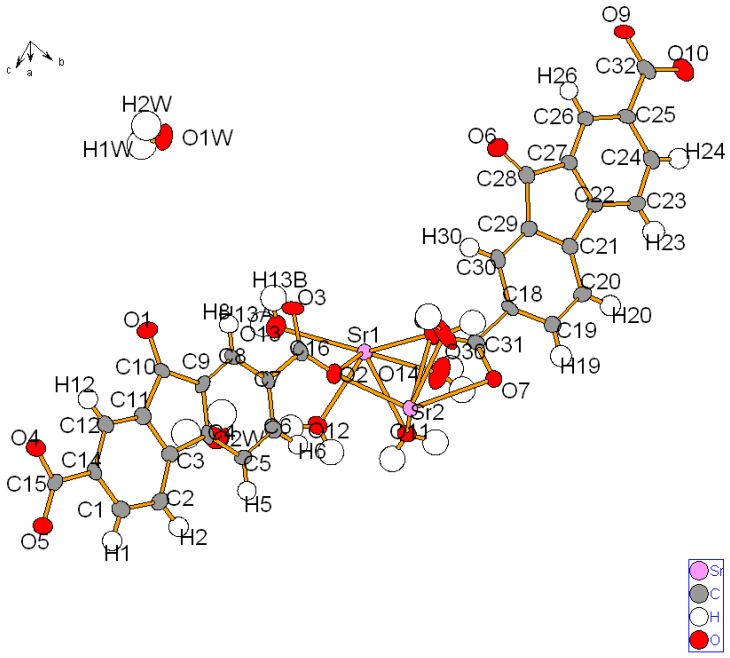

Figure S7: Thermal ellipsoid and atom numbering scheme of **(2)**

References

(1) Larson, A. C.; Von Dreele, R. B. *Los Alamos National Laboratory Report LAUR* **2000**, *86-748*, .

(2) Toby, B. H. *J. Appl. Cryst.* **2001**, *34*, 210–213.