Novel Photo-Active Cd:1,4-Benzene Dicarboxylate Metal Organic Framework Templated by $[Ru(II)(2,2'\text{-bipyridine})_3]^{2+}$: Synthesis and Photophysics of RWLC-5

Randy W. Larsen*, Jacob M. Mayers and Lukasz Wojtas

Supporting Information

FTIR

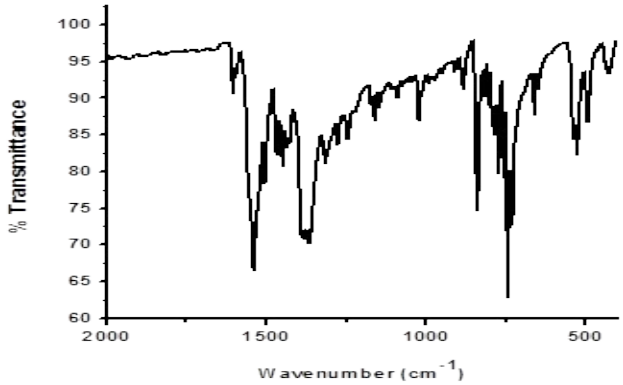

Figure S1: FTIR spectrum of RWLC-5. The spectrum was obtained using a PerkinElmer Spectrum TWO instrument and was collected at 25°C after ethanol exchange. ~75 mg of air dried sample were used to obtain the spectrum.

TGA Analysis

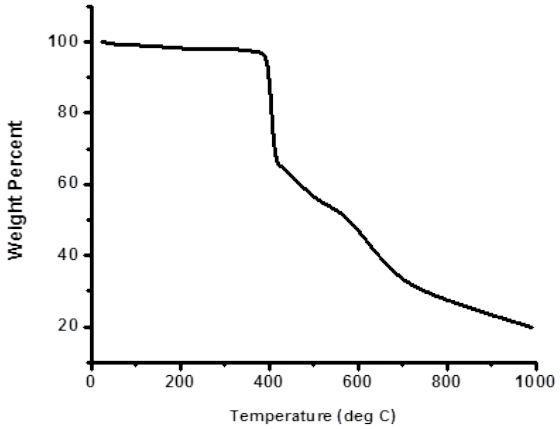

Figure S2: Thermal gravimetric analysis (TGA) shows that the compound is stable to ~500C. The first weight loss of 4% from 50 to 200 C is likely due to the loss non-coordinated solvent. The second weight loss of ~40% from 400 to 550 C is consistant with the loss of additional coordinated solvent molecules. The BTC ligand starts to decompose from 530 to 1000C.

X-Ray Powder Diffraction

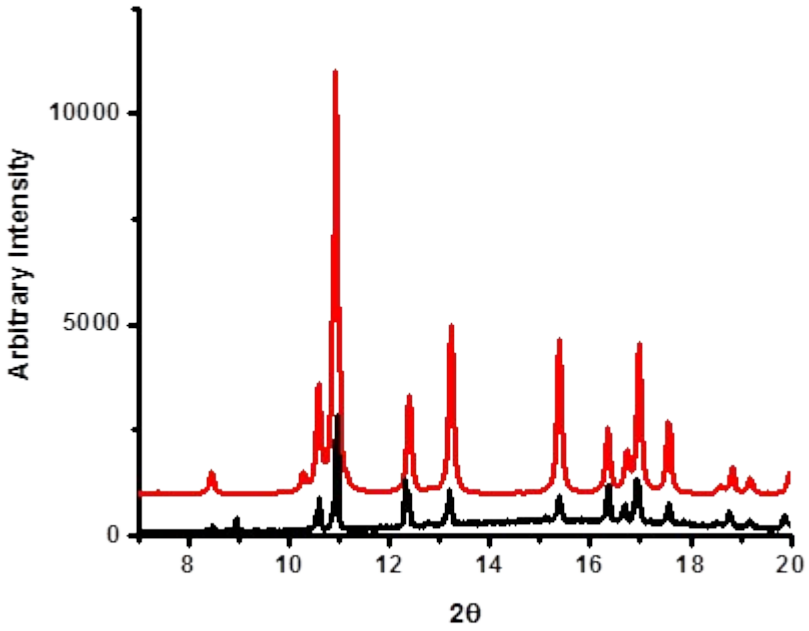

Figure S3: X-Ray powder diffraction data for RWLC-5 (black trace) and data for RWLC-5 simulated from single crystal parameters using Mercury software (red trace).

X-ray Crystallography

The X-ray diffraction data was measured on Bruker D8 Venture PHOTON 100 CMOS system equipped with a Cu K_α INCOATEC ImuS micro-focus source (λ = 1.54178 Å). Indexing was performed using *APEX3* [1] (Difference Vectors method). Data integration and reduction were performed using SaintPlus 6.01 [2]. Absorption correction was performed by multi-scan method implemented in SADABS [3]. Space groups were determined using XPREP implemented in APEX3 [1]. Structures were solved using SHELXT and refined using SHELXL-2014 [4-7] (full-matrix least-squares on F^2) through OLEX2 interface program [8]. All non-hydrogen atoms were refined anisotropically. The occupancy of disordered water was initially refined free and fixed at converged value during the final step of the refinement. Crystal data and refinement conditions are shown in Table 1.

[1] Bruker (2016). *APEX3* (Version 2015.9). Bruker AXS Inc., Madison, Wisconsin, USA.
[2] Bruker (2016) SAINT V8.35A. Data Reduction Software.
[3] Sheldrick, G. M. (1996). *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany.
[4] G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst.,

C71, 3-8
[5] Sheldrick, G.M. (1990) Acta Cryst. A46, 467-473
[6] Sheldrick, G. M. (2008) Acta Cryst. A64, 112-122.
[7] Sheldrick, G. M. (2015) Acta Cryst..A71, 3-8
[8] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341.

Table 1 Crystal data and structure refinement for RWLC5.

Identification code	RWLC5
Empirical formula	$C_{46}H_{32.68}Cd_2Cl_2N_6O_{8.34}Ru$
Moiety formula	$[Cd_2(C_8H_4O_4)_2Cl_2]^{2-}(C_{30}H_{24}N_6Ru)^{2+}\cdot 0.34H_2O$
Formula weight	1198.98
Temperature/K	100
Crystal system	monoclinic
Space group	C2/c
a/Å	18.4093(5)
b/Å	16.6908(4)
c/Å	14.8012(4)
α/°	90
β/°	111.1042(8)
γ/°	90
Volume/Å^3	4242.86(19)
Z	4
ρ_{calc}g/cm^3	1.877
μ/mm^{-1}	12.511
F(000)	2363.0
Crystal size/mm^3	0.28 × 0.246 × 0.207
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.386 to 154.354
Index ranges	$-23 \leq h \leq 22$, $-21 \leq k \leq 20$, $-17 \leq l \leq 18$
Reflections collected	31004
Independent reflections	4437 [R_{int} = 0.0428, R_{sigma} = 0.0246]
Data/restraints/parameters	4437/0/301
Goodness-of-fit on F^2	1.119
Final R indexes [I>=2σ (I)]	R_1 = 0.0247, wR_2 = 0.0622
Final R indexes [all data]	R_1 = 0.0251, wR_2 = 0.0624
Largest diff. peak/hole / e Å^{-3}	0.78/-1.10