A New Photoactive Ru(II)tris(2,2'-bipyridine) Templated Zn(II)- 1,4 Benzene Dicarboxylate Metal Organic Framework: Structure and Photophysical Properties

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Supporting Information

X-ray Crystallography

The X-ray diffraction data for **RWLC-3** were measured on a 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 *APEX2* [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 APEX2 [1]. The structure was solved using SHELXS-97 (direct methods) and refined using SHELXL-97 [7] (full-matrix least-squares on F^2) contained in APEX2 [1,7], WinGX v1.70.01 [4,5,6,7] and OLEX2 [7,8]. All non-H atoms have been found from difference Fourier map and majority of them were refined anisotropically. Disordered atoms with low occupancies as well as disordered nitrogen atoms N7 and N1 have been refined isotropically. Restraints have been used to refine disordered 1,4-bdc ligand and disordered DMF molecules (DFIX, DANG, FLAT, SIMU). The RuBpy is disordered over two positions across the inversion center (1:1 ratio). One of benzene dicarboxylate ligand is disordered over two positions with 0.91:0.09 occupancy ratio. The sum of chemical occupancies of all parts of disordered DMF molecule has been restrained to 1. No SIMU restraints have been used for disordered DMF molecule. Hydrogen atoms of –CH groups were placed in geometrically calculated positions and included in the refinement process using riding model with isotropic thermal parameters: Uiso(H) = 1.2Ueq(-CH). Crystal data and refinement conditions are shown in Table 1.

[1] Bruker (2013). *APEX2* (Version 2013.6-2). Bruker AXS Inc., Madison, Wisconsin, USA.
[2] Bruker (2013). SAINT-V8.32A. Data Reduction Software.
[3] Sheldrick, G. M. (1996). *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany.
[4] Farrugia L.J. Appl. Cryst. (1999). 32, 837±838
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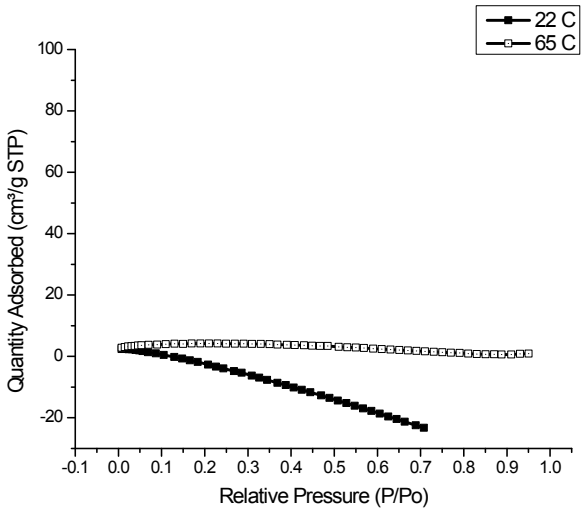
[6] Sheldrick, G.M. (1990) Acta Cryst. A46, 467-473
[7] Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
[8] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341

Table 1 Crystal data and structure refinement for RWLC-3.	
Identification code	**RWLC-3**
Empirical formula	$C_{76}H_{58}N_8O_{22.16}RuZn_4$
Formula weight	1800.40
Moiety formula	Zn4(C8H4O4)5,Ru(C10H8N2)3, 2(C3H7NO), 0.16(H2)O
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.7838(4)
b/Å	12.3757(4)
c/Å	13.6009(4)
α/°	95.7503(12)
β/°	93.7677(11)
γ/°	109.0329(9)
Volume/Å^3	1855.35(10)
Z	1
ρ_{calc}g/cm^3	1.611
μ/mm^{-1}	3.754
F(000)	911.0
Crystal size/mm^3	0.29 × 0.21 × 0.19
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	7.98 to 144.76
Index ranges	-14 ≤ h ≤ 14, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16
Reflections collected	71553
Independent reflections	7122 [R_{int} = 0.0294, R_{sigma} = 0.0143]
Data/restraints/parameters	7122/109/748
Goodness-of-fit on F^2	1.122
Final R indexes [I>=2σ (I)]	R_1 = 0.0291, wR_2 = 0.0712
Final R indexes [all data]	R_1 = 0.0307, wR_2 = 0.0720
Largest diff. peak/hole / e Å^{-3}	0.55/-0.37

Gas Sorption

Gas adsorption isotherms were collected using the surface area analyzer ASAP-2020. Before the measurements, the freshly prepared sample was exchanged with HPLC-grade methanol for 3 days, and then activated with the "degas" port under vacuum at 25°C overnight. The N_2 adsorption isotherm was measured at 77K using a liquid nitrogen bath. A second isotherm was collected after the sample was activated with the "degas" port under vacuum at 65°C overnight.



FTIR

The solid sample infrared spectrum (PerkinElmer Spectrum TWO) was collected at 25°C after methanol exchange. ~75 mg of sample were used to obtain the spectrum.