Electronic Supplementary Material (ESI) for Dalton Transactions.

Framework Induced Deformation Modulates the Photophysical Properties of ZnTetra(4-pyridyl)Porphyrin Incorporated within a New Metal Organic Framework, RWLAA-1.

Abdulaziz A. Alanazia†, Lukasz Wojtasa, Jacob M. Mayersa, Jarolsava Miksovskab and Randy W. Larsena*

Supporting Information

1. FTIR

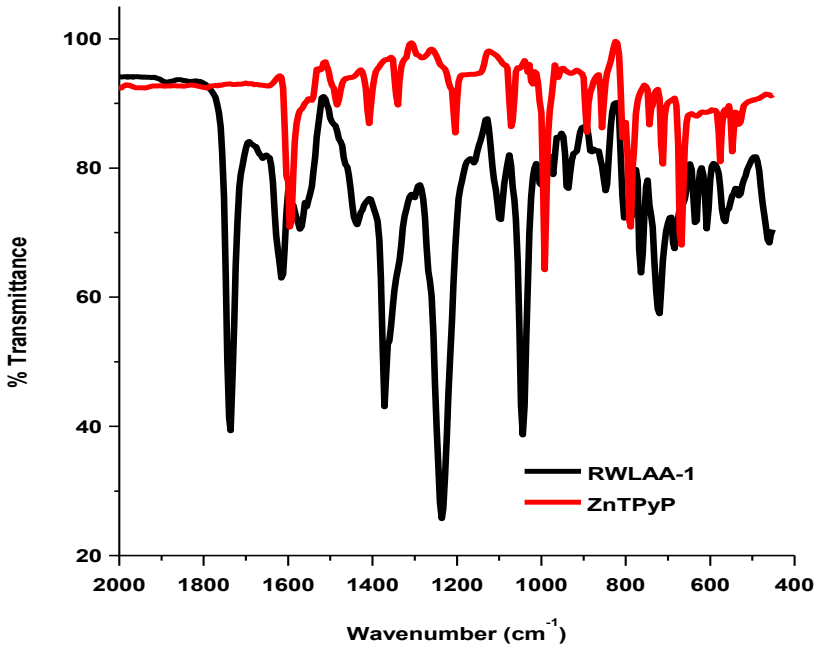


Figure S1: FTIR spectrum of RWLAA-1 and ZnTPyP.. The spectrum was obtained using a PerkinElmer Spectrum TWO instrument and was collected at 25°C. ~75 mg of air dried sample were used to obtain the spectrum.

2. X-Ray Powder Diffraction

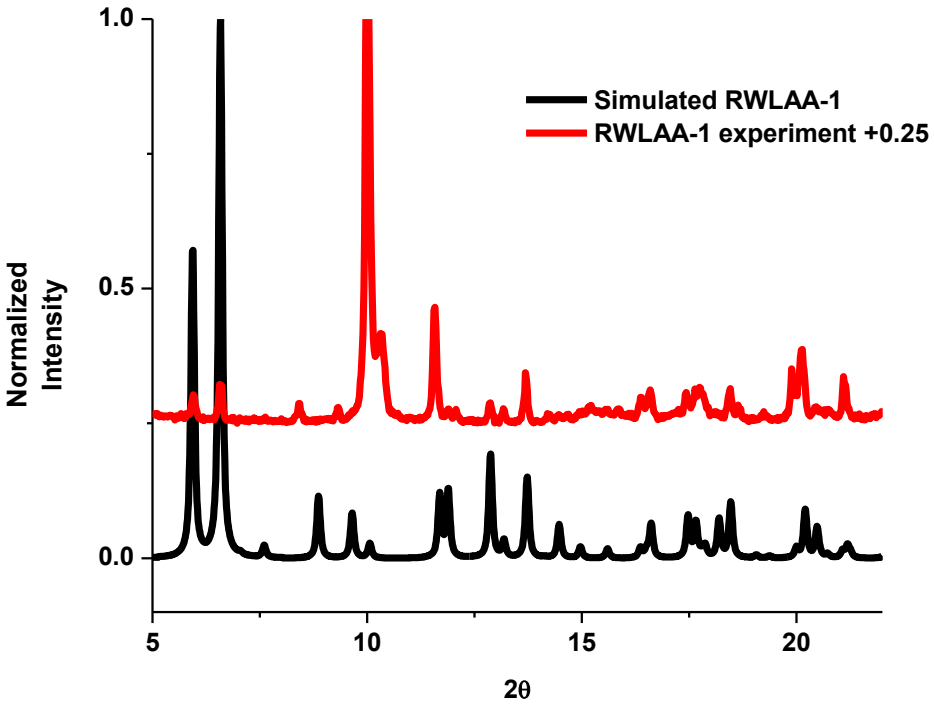
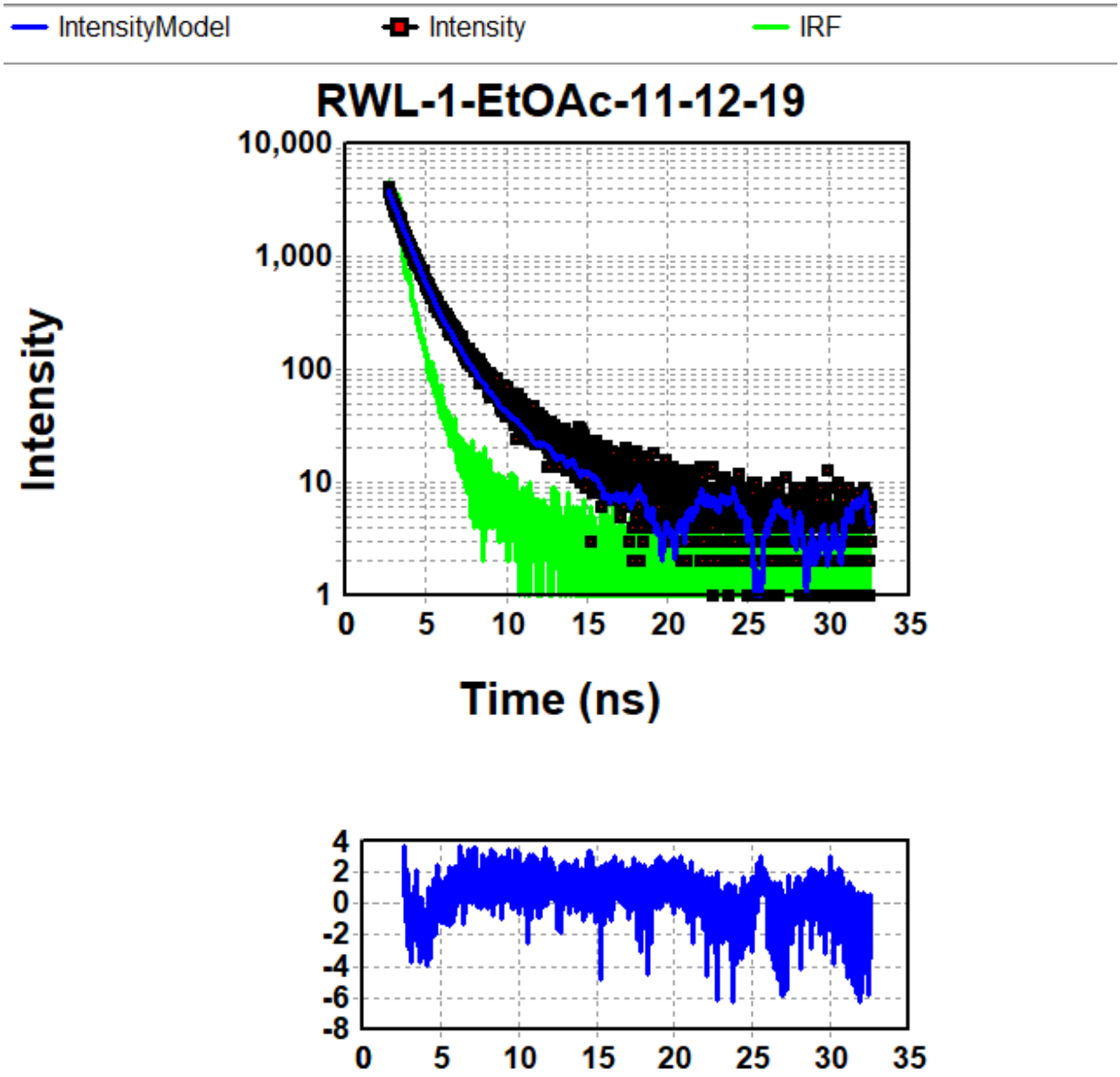
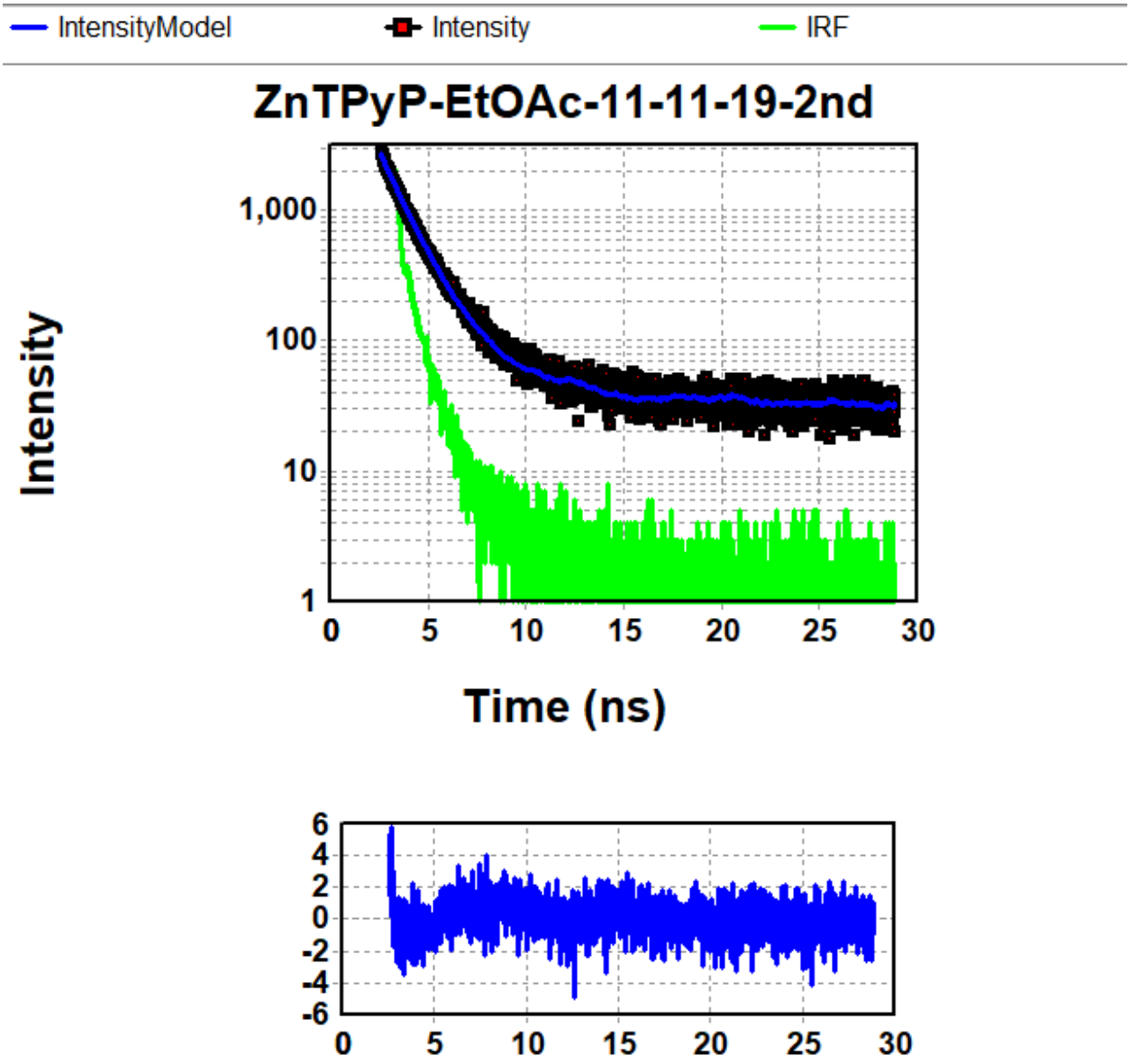


Figure S2: X-Ray powder diffraction data for RWLAA-1 (black trace) and data for RWLAA-1 simulated from single crystal parameters using Mercury software (red trace).

3. Emission Lifetime Fits

All fits were performed using Vinci software provided by ISS inc.




IntensityModel
Intensity
IRF
ZnTPyP-EtOAc-11-11-19-2nd
Intensity
1,000
100
10
1
0
5
10
15
20
25
30
Time (ns)
6
4
2
0
-2
-4
-6
0
5
10
15
20
25
30

4. Single-Crystal X-Ray Diffraction

Table 1 Crystal data and structure refinement for RWLAA-1.	
Identification code	RWLAA-1
Empirical formula	$C_{325.5}H_{217.5}N_{55.5}O_{55.5}Zn_{18}$
Moiety formula	[12Zn·7(C9H3O6)·6(C40H24N8Zn)]·3(anion$^-$)·xSOLV
Temperature/K	100
Crystal system	hexagonal
Space group	P6/m
a/Å	26.8343(9)
b/Å	26.8343(9)
c/Å	14.8769(5)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	9277.3(7)
Z	1
ρ_{calc}g/cm^3	1.248
μ/mm^{-1}	1.823
F(000)	3543.0
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.054 to 133.444
Index ranges	-31 ≤ h ≤ 31, -31 ≤ k ≤ 31, -17 ≤ l ≤ 17
Reflections collected	71805
Independent reflections	5721 [R_{int} = 0.0941, R_{sigma} = 0.0382]
Data/restraints/parameters	5721/1362/588
Goodness-of-fit on F^2	1.162
Final R indexes [I>=2σ (I)]	R_1 = 0.1024, wR_2 = 0.2904
Final R indexes [all data]	R_1 = 0.1112, wR_2 = 0.2974
Largest diff. peak/hole / e Å^{-3}	1.10/-0.93