Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supporting Information

Synthesis, structure, and luminescent properties of oligothiophene-containing metal-organic frameworks

Lyndsey D. Earl, Brian O. Patrick and Michael O. Wolf*

Table S1: Selected crystallographic data for **1-5**.

	1	**2**	**3**	**4**	**5**
Formula	$C_{57}H_{59}N_5O_{11}S_4Zn_2$	$C_{24}H_{35}NO_4S_2Zn$	$C_{16}H_9NO_4S_2Zn$	$C_{40}H_{36}N_4O_6S_2Zn$	$C_{201}H_{257}N_{15}O_{32}S_{12}Zn_6$
Crystal color, shape	Colorless, rod	Colorless, rod	Yellow, rod	Colorless, prism	Yellow, prism
Dimensions / mm	0.35 x 0.20 x 0.10	0.10 x 0.04 x 0.02	0.25 x 0.10 x 0.07	0.70 x 0.30 x 0.25	0.25 x 0.18 x 0.13
Temperature / K	100 (2)	100(2)	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space Group	P $2_1/n$	P $2_1/n$	C *2/c*	P-1	C *2/c*
a / Å	16.3642(6)	7.503(3)	17.1764(8)	8.6855(15)	31.138(2)
b / Å	17.0748(6)	18.281(6)	22.0141(12)	12.7109(18)	39.627(2)
c / Å	20.6230(7)	19.375(6)	9.9312(5)	18.183(3)	22.721(2)
α / deg	90.00	90.00	90.00	91.810(9)	90.00
β / deg	90.226(2)	100.470(15)	96.535(2)	102.910(9)	121.737(2)
γ / deg	90.00	90.00	90.00	106.455(8)	90.00
V / $Å^3$	5762.3(4)	2613.3(16)	3730.8(3)	1866.8(5)	23844(3)
Z	4	4	8	2	4
2θ (max) / deg	60.2	45.2	60.0	46.6	52.6
Exposure time / s	10	30	10	20	60
Total reflections	99492	11499	20371	19580	16035
Unique reflections	16899	3392	5427	5356	10893
ρ_{calc} / g cm^{-1}	1.44	1.35	1.455	1.420	1.162
μ (Mo kα) / mm^{-1}	1.041	1.128	1.557	0.823	0.761
R1[a] (I>2.00σ(I))	0.0525	0.0638	0.0420	0.0515	0.0542
ωR2[a] (I>2.00σ(I))	0.1425	0.1788	0.1102	0.1314	0.1611
Goodness of fit	1.101	0.952	0.962	1.017	1.078

[a]Function minimized. $\Sigma w(F_o^2-F_c^2)^2$, $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, $wR2 = [\Sigma (w (F_o^2 - F_c^2)^2)/ \Sigma w(F_o^2)^2]^{1/2}$

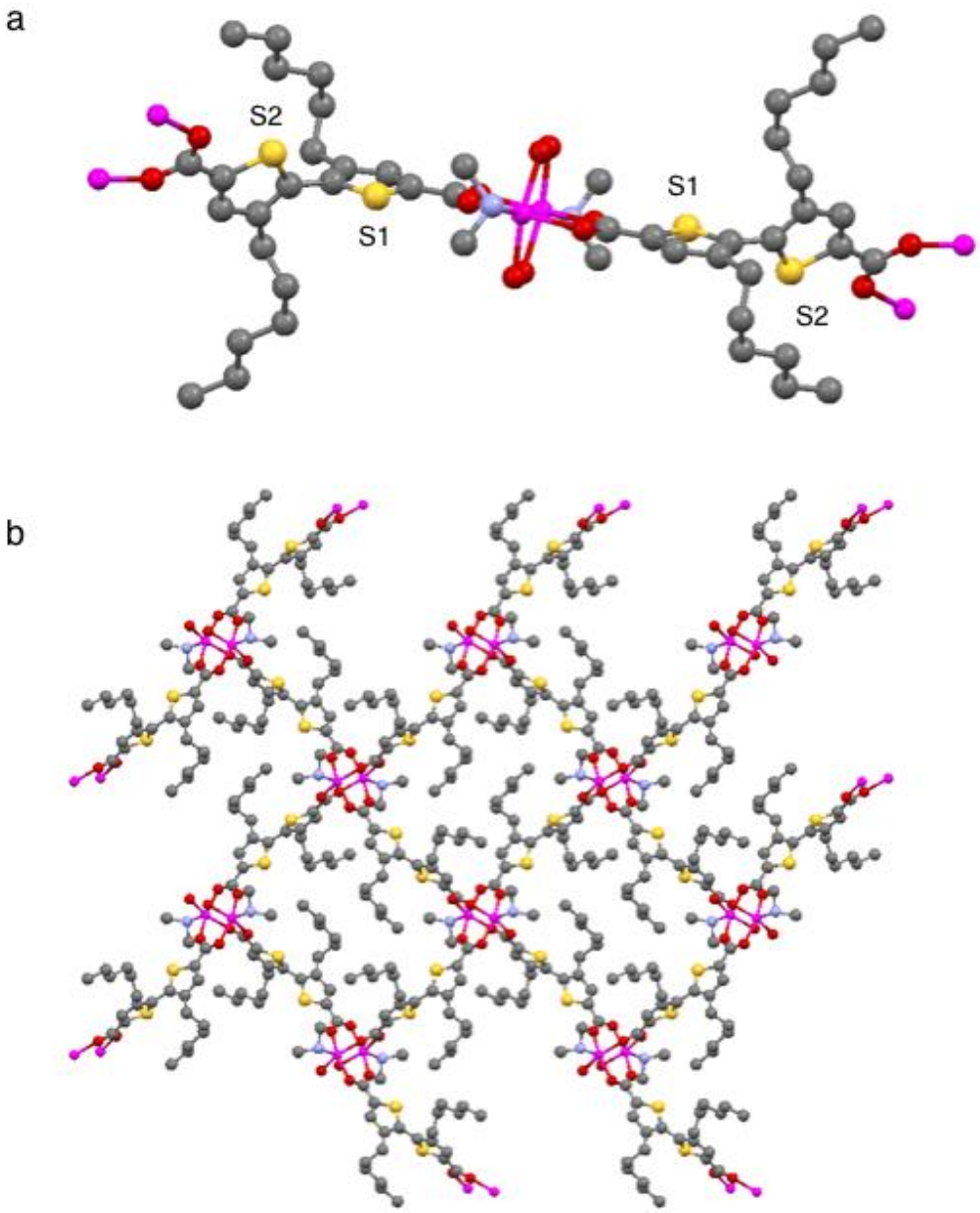

Figure S1. Solid state structure of **2**. Hydrogens have been removed for clarity. a) Metal coordination of **2**. b) 2D grid along the *bc* plane.

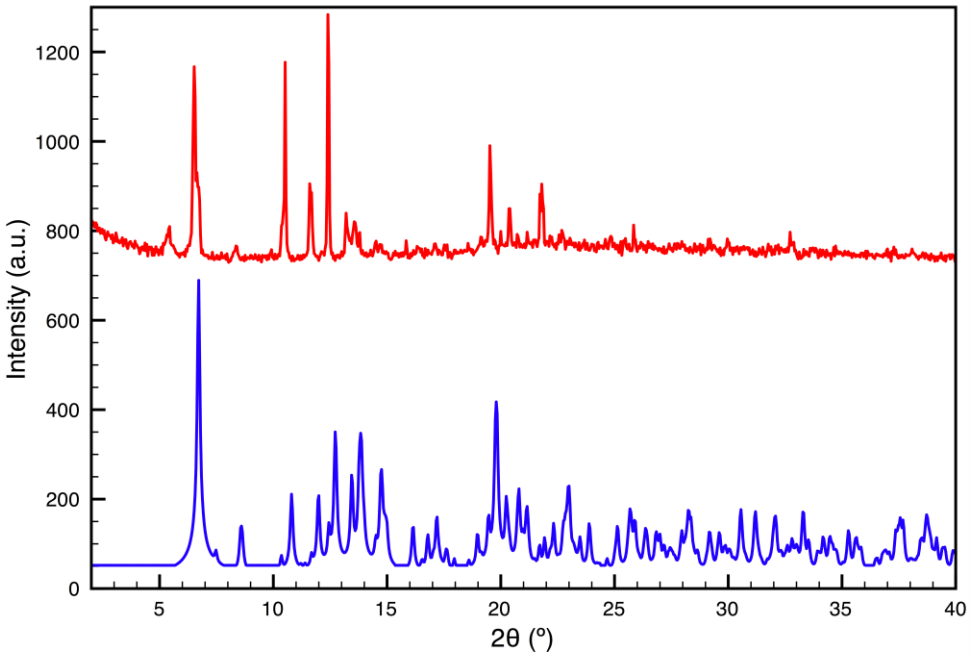

Figure S2. Powder X-ray diffraction patterns of **1**: experimental (red) and predicted (blue).

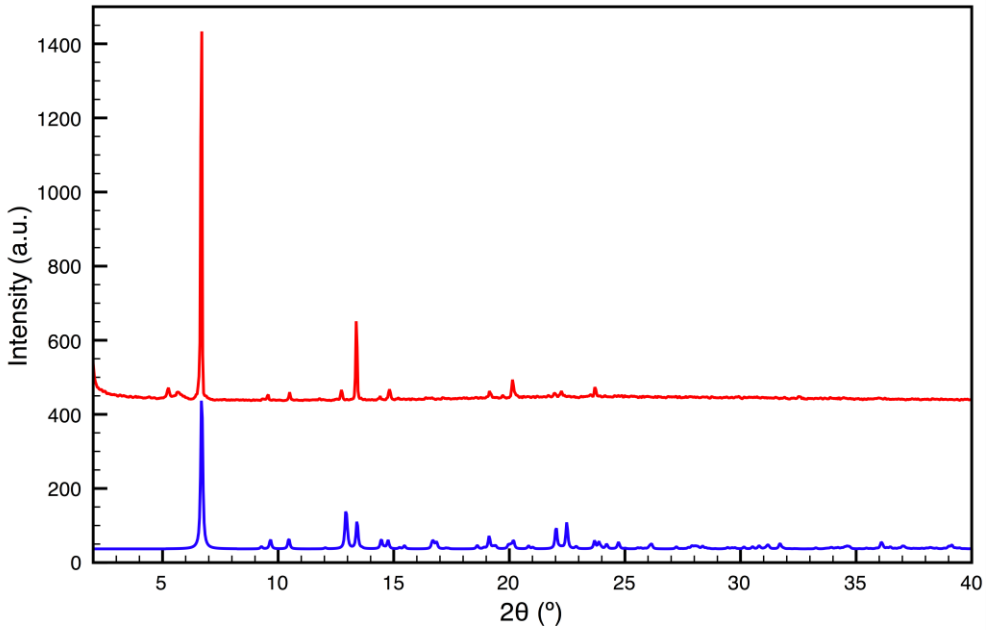

Figure S3. Powder X-ray diffraction patterns of **2**: experimental (red) and predicted (blue).

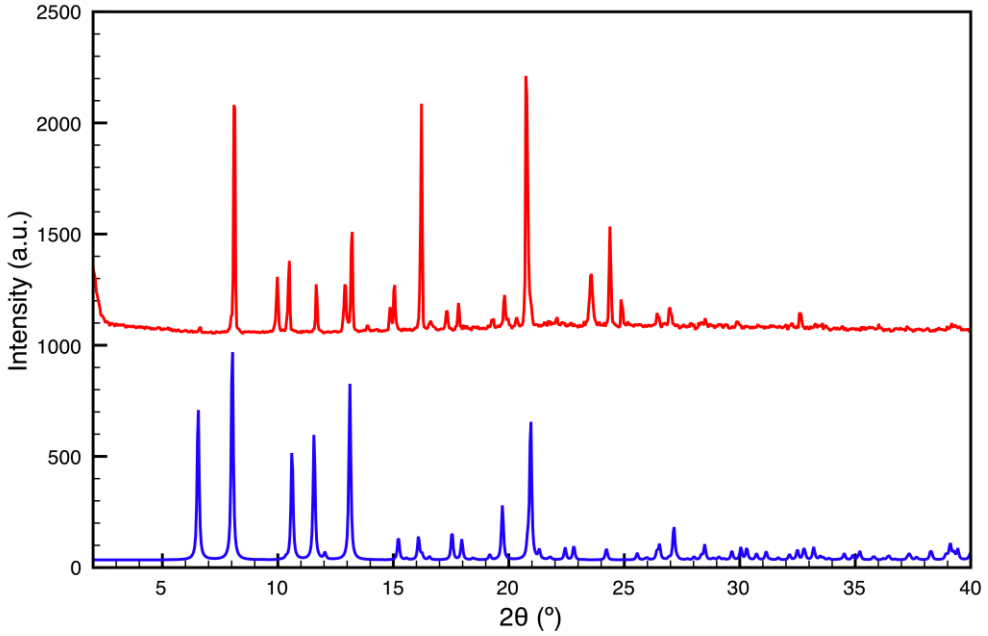

Figure S4. Powder X-ray diffraction patterns of **3**: experimental (red) and predicted (blue).

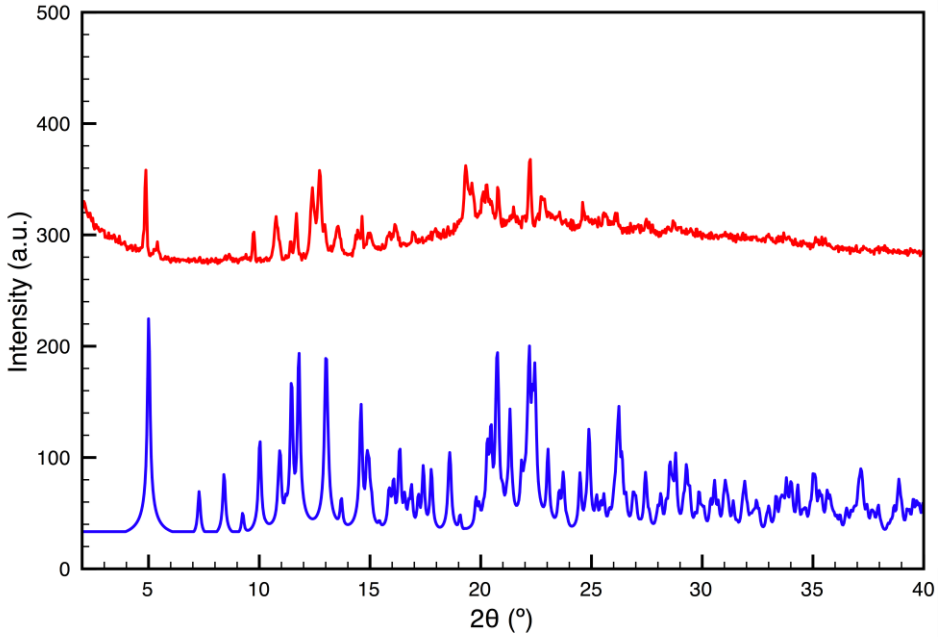

Figure S5. Powder X-ray diffraction patterns of **4**: experimental (red) and predicted (blue).

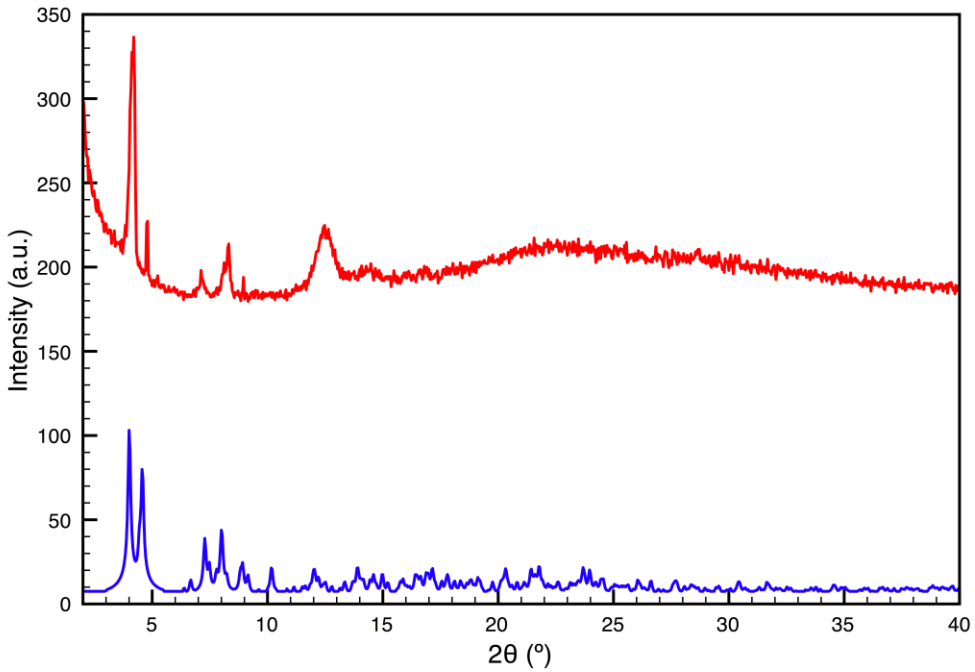

Figure S6. Powder X-ray diffraction patterns of **5**: experimental (red) and predicted (blue).

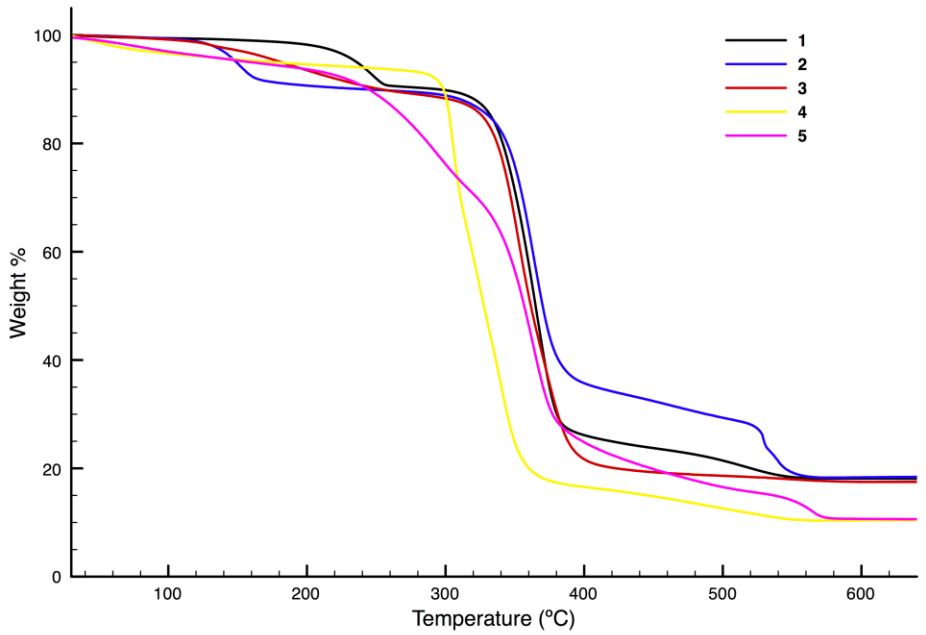

Figure S7. Thermogravimetric analyses of compounds **1-5**.

Table S2. Summary of thermogravimetric analyses data of compounds **1**-**5**.

	Initial temperature of major weight loss (°C)	Final weight (%) (experimental)	Final weight (%) (calculated)
1	220, 340	13.6	13.0
2	130, 315, 525	15.1	15.3
3	130, 320	16.2	14.5
4	300, 370	9.4	10.1
5	240, 400	10.7	11.5

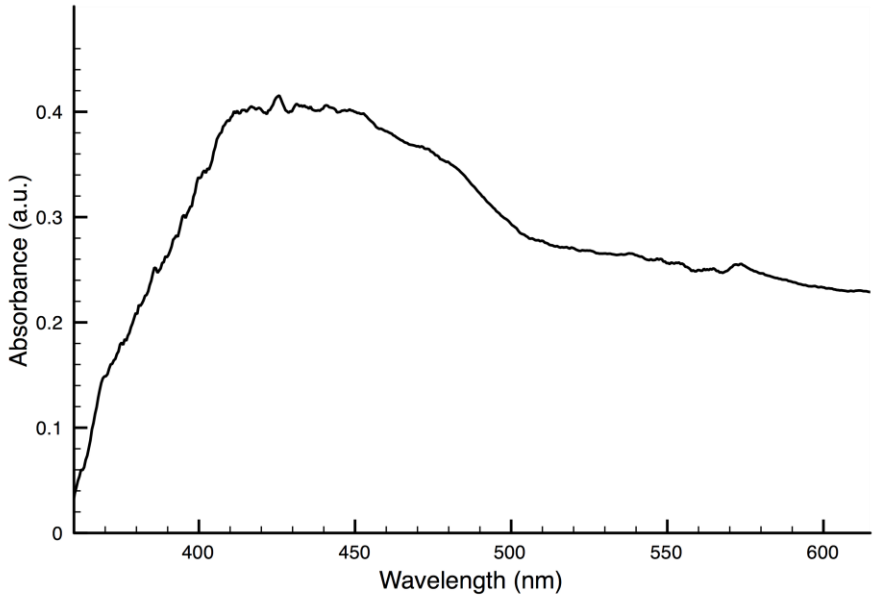

Figure S8. Solid state UV-Vis spectrum (derived from diffuse reflectance spectrum) of bpe.

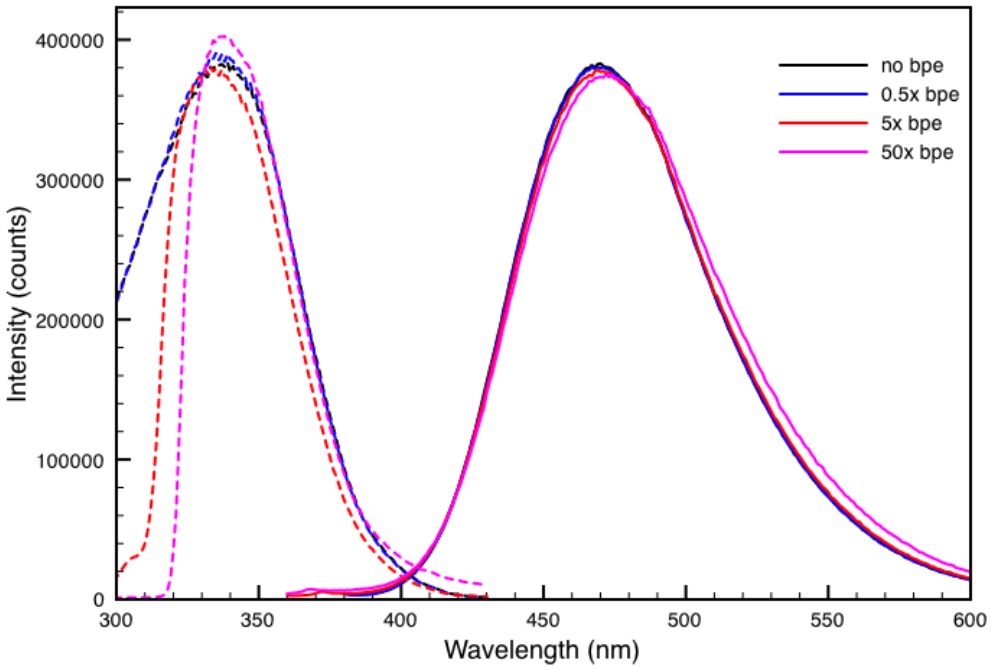

Figure S9. Excitation and emission spectra of H_2L1 and bpe in MeOH. $[H_2L1] = 1 \times 10^{-5}$ M.

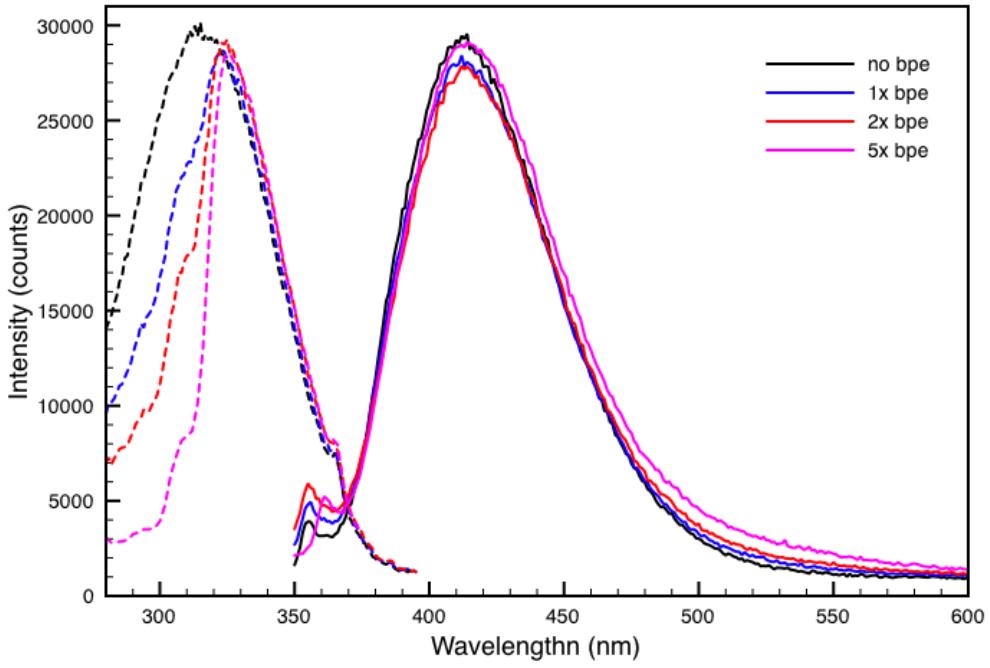

Figure S10. Excitation and emission spectra of H_2L2 and bpe in MeOH. $[H_2L2] = 1.25 \times 10^{-5}$ M.

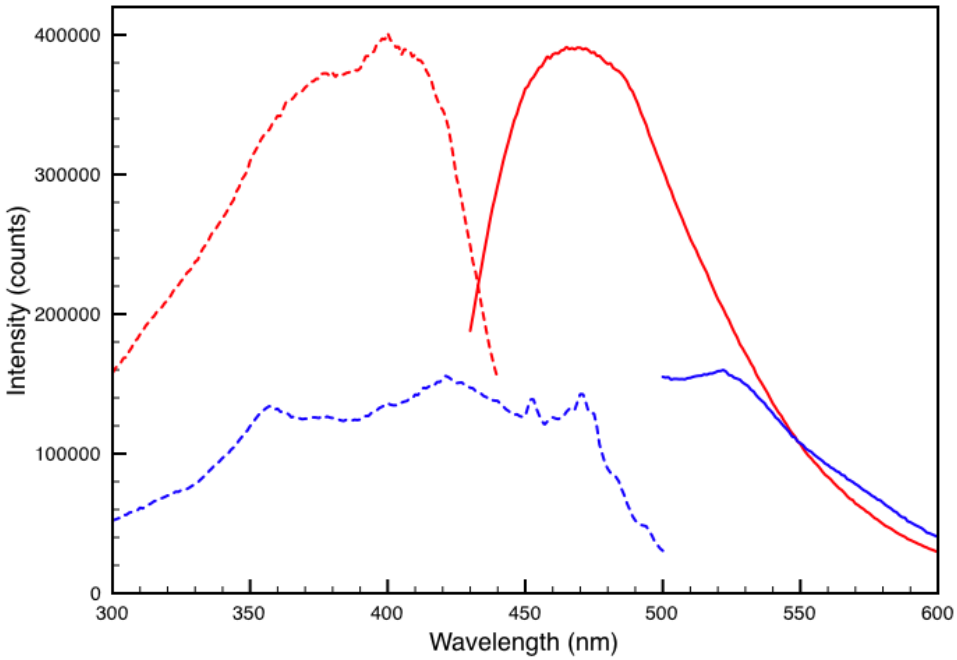

Figure S11. Excitation and emission spectra of 1:1 H_2L1 and bpe in the solid state. λ_{ex} 470 nm (dashed red), λ_{ex} 540 nm (dashed blue), λ_{em} 400 nm (solid red), λ_{em} 475 nm (solid blue).

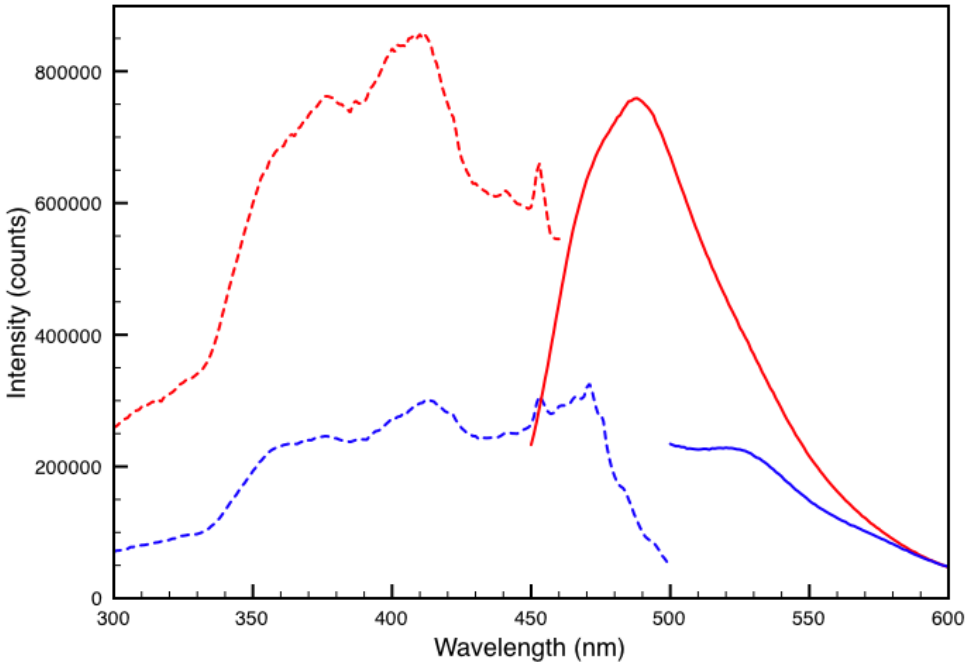

Figure S12. Excitation and emission spectra of 3:2 H_2L2 and bpe in the solid state. λ_{ex} 490 nm (dashed red), λ_{ex} 540 nm (dashed blue), λ_{em} 415 nm (solid red), λ_{em} 480 nm (solid blue).