Supporting Information

Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al^{3+} Sensing

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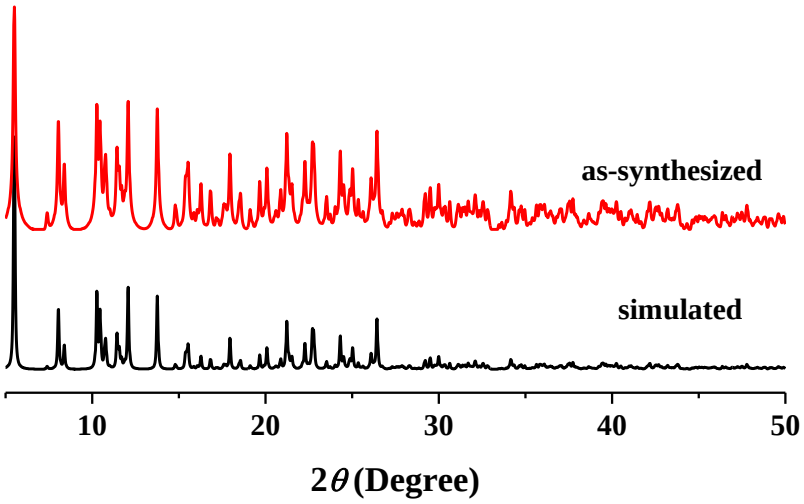

Figure S1. Simulated and as-synthesized PXRD patterns of compound **1**.

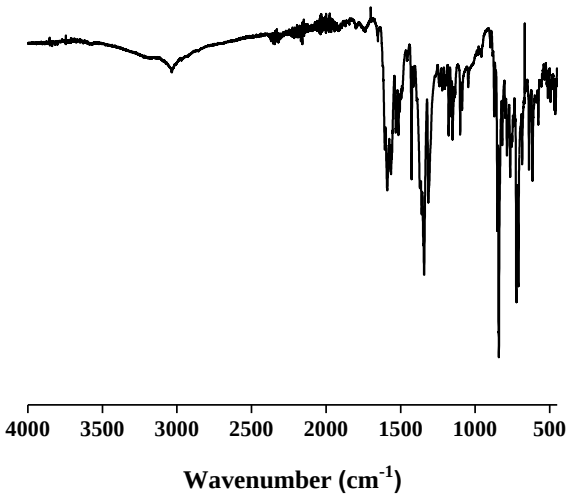

Figure S2. FT-IR spectrum of **1**.

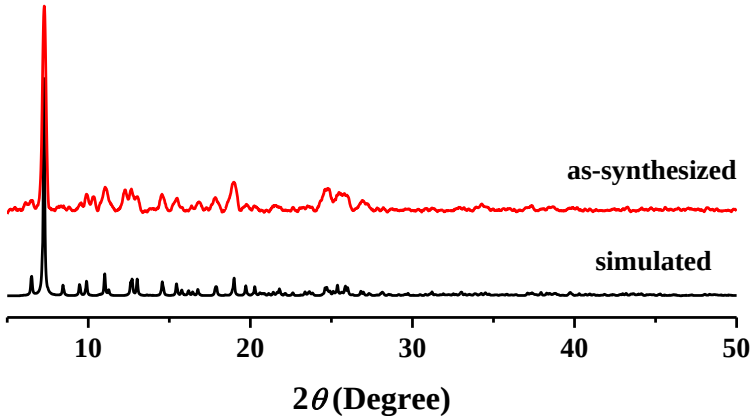

Figure S3. Simulated and as-synthesized PXRD patterns of compound **2**.

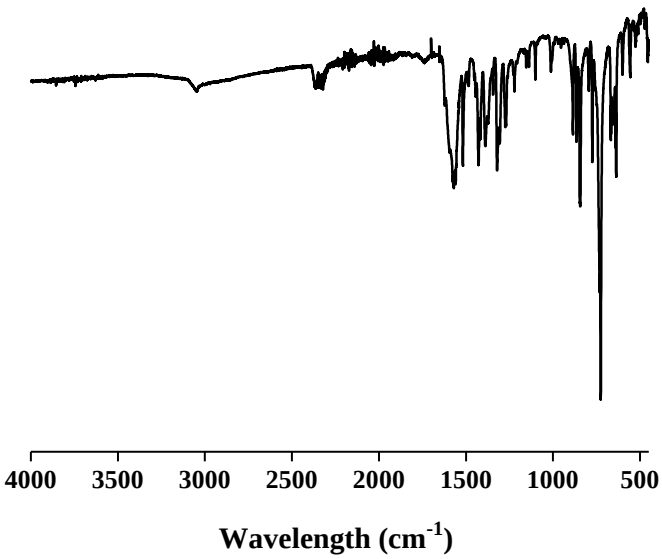

Figure S4. FT-IR spectrum of **2**.

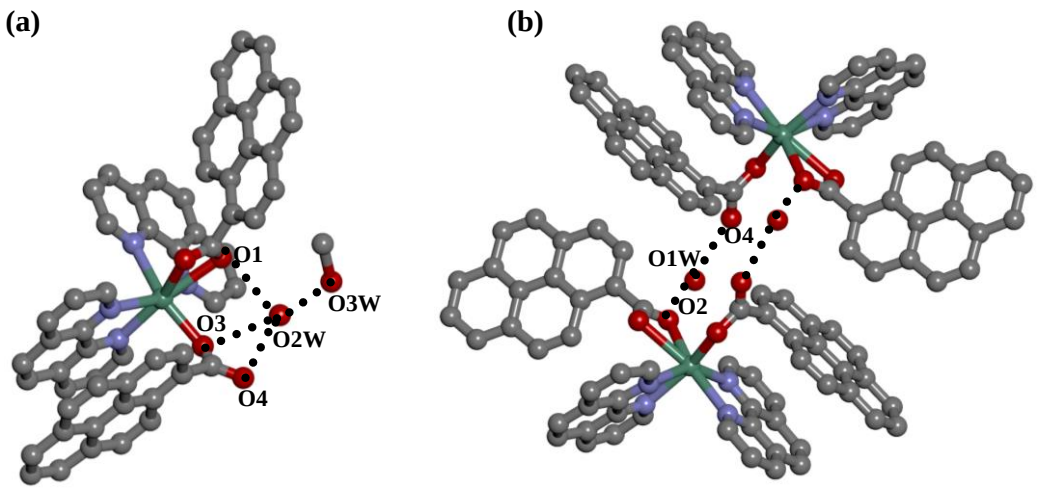

Figure S5. Hydrogen bonds (dotted black lines) in **1**: (a) O3···O2W, O4···O2W, O1···O2W and O2W···O3W hydrogen bonds keep the guest solvents attached; (b) O4···O1W and O2···O1W hydrogen bonds hold two monomer complexes.

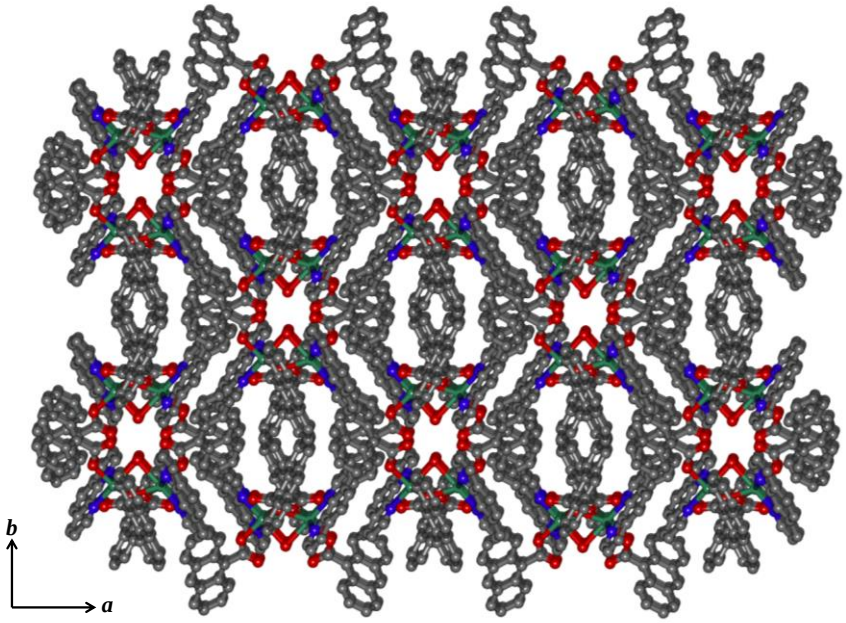

Figure S6. View of the 3D close packed structure of complex **2** along *c*-direction.

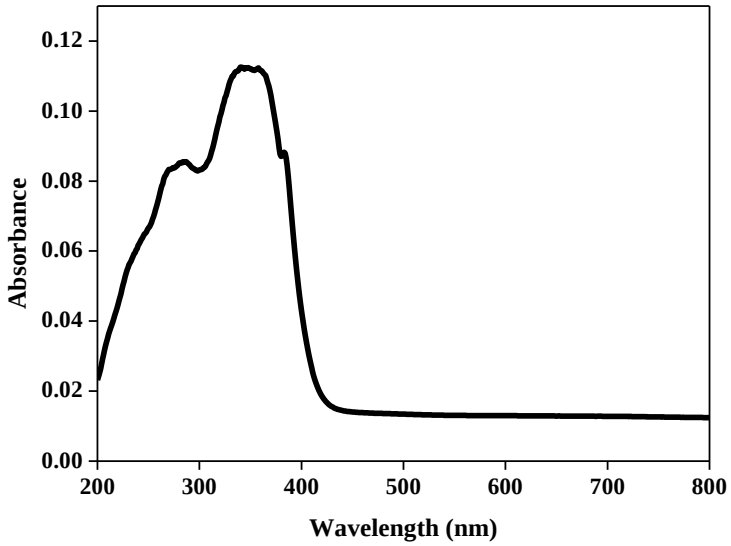

Figure S7. UV-vis spectrum of **1**.

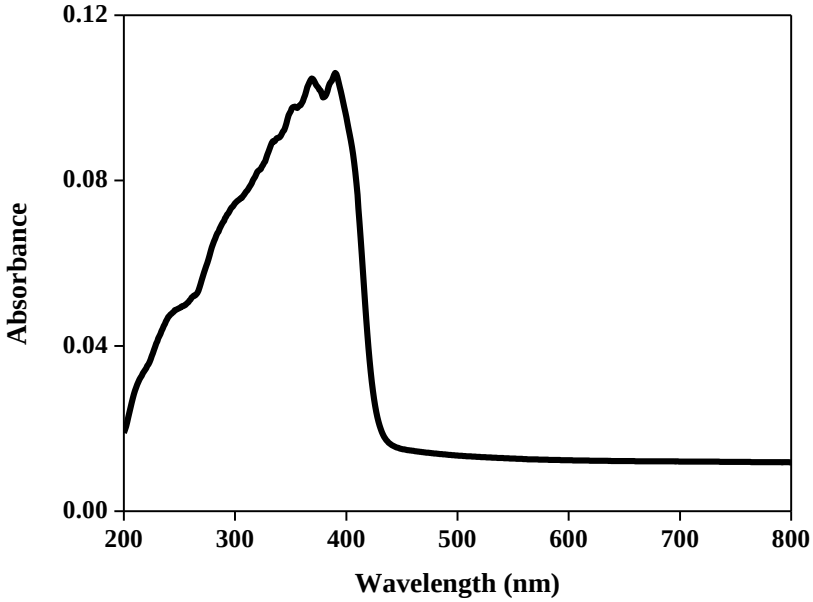

Figure S8. UV-visible spectrum of **2**.

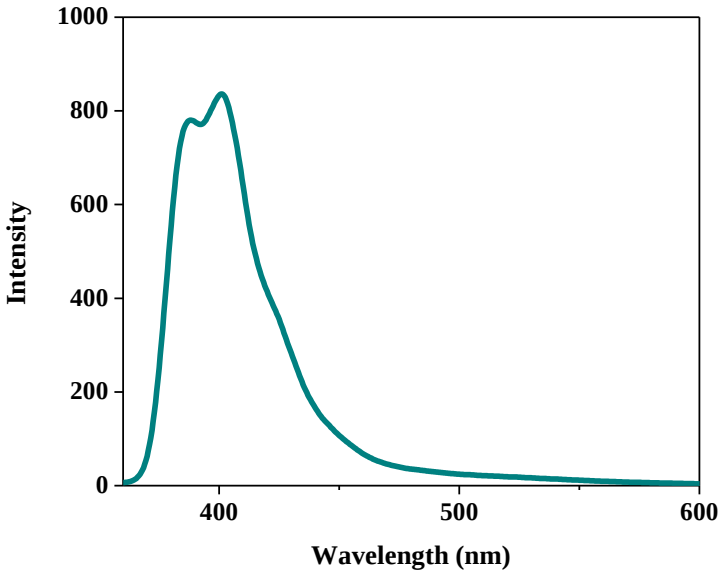

Figure S9. Emission spectrum of compound **1** in methanol upon excitation at 350 nm.

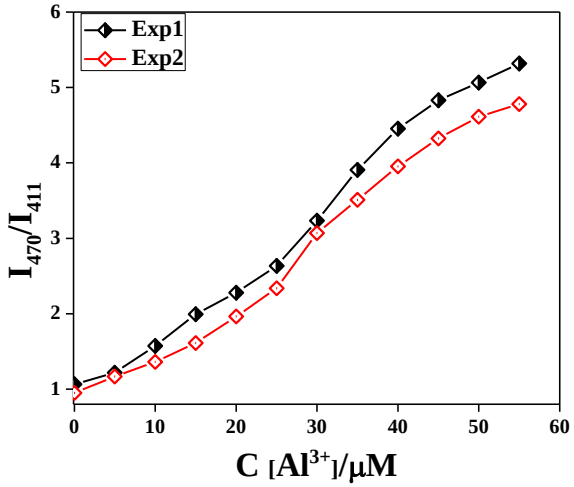

Figure S10. Ratiometric fluorescence intensity [I_{470}/I_{411}] as a function of Al^{3+} concentration in methanol solution of compound **2**.

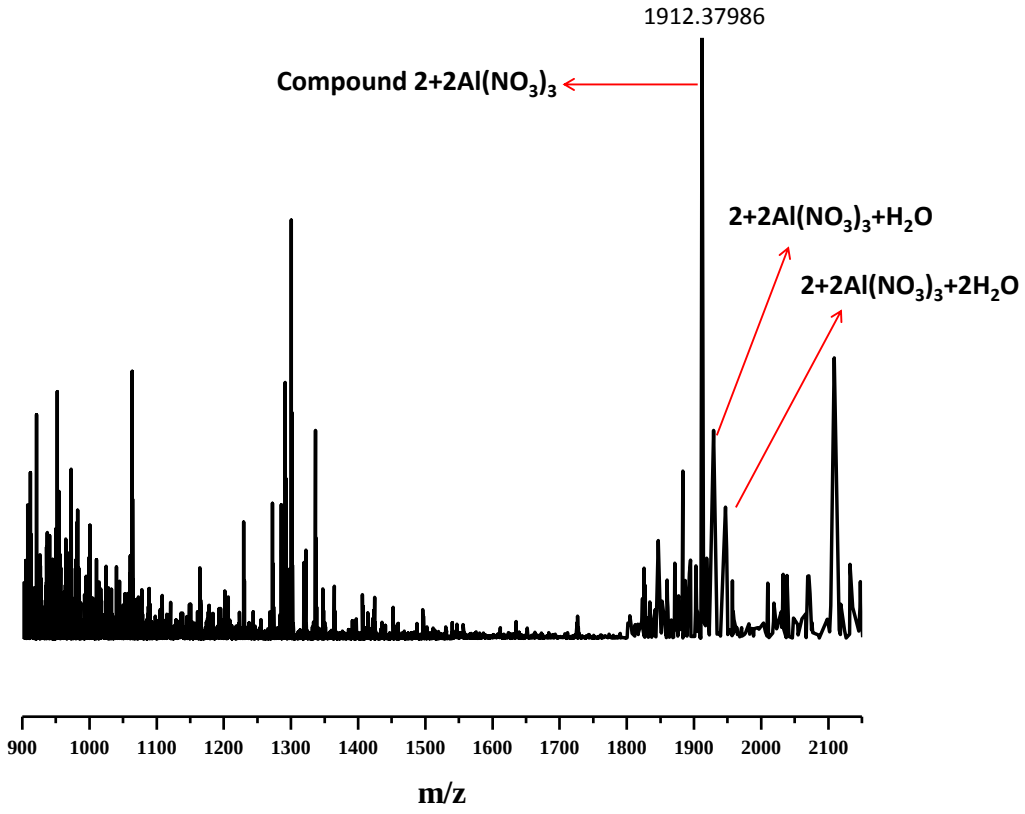

Figure S11. High Resolution Mass spectrum of Al^{3+} added compound **2** in methanol.

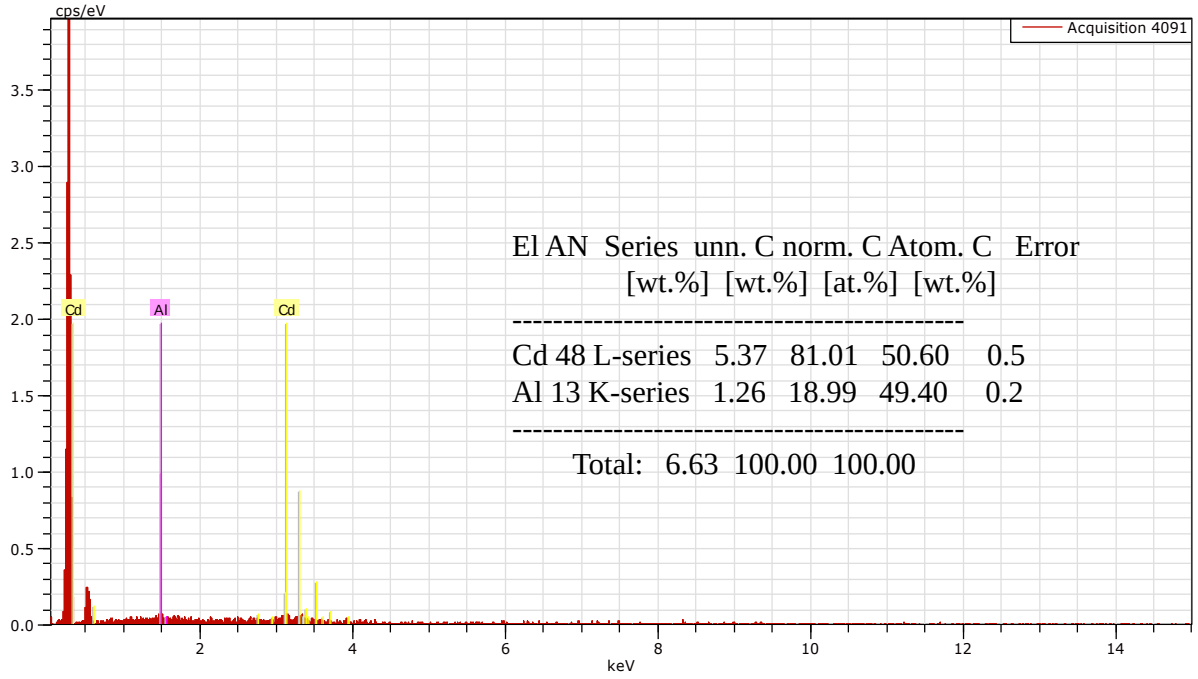

Figure S12. EDAX spectrum showing the Al^{3+} and Cd^{2+} abundancy in **2** after Al^{3+} addition.

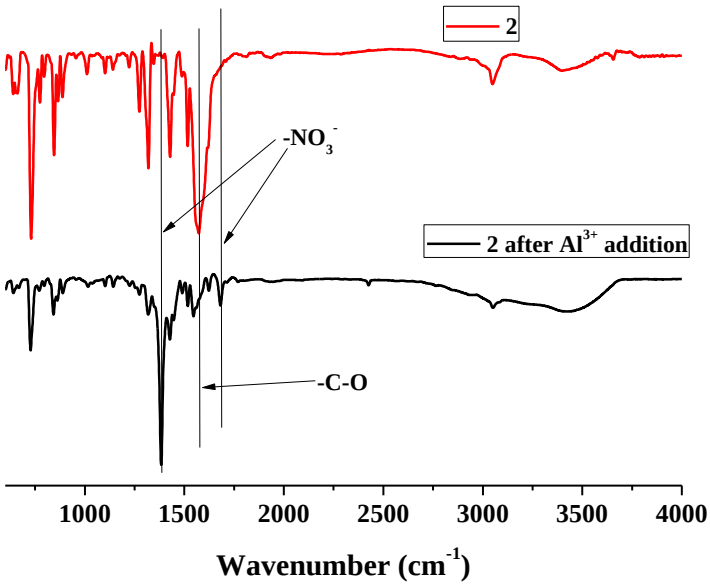

Figure S13. FT-IR spectrum of **2** and **2** after Al^{3+} addition.

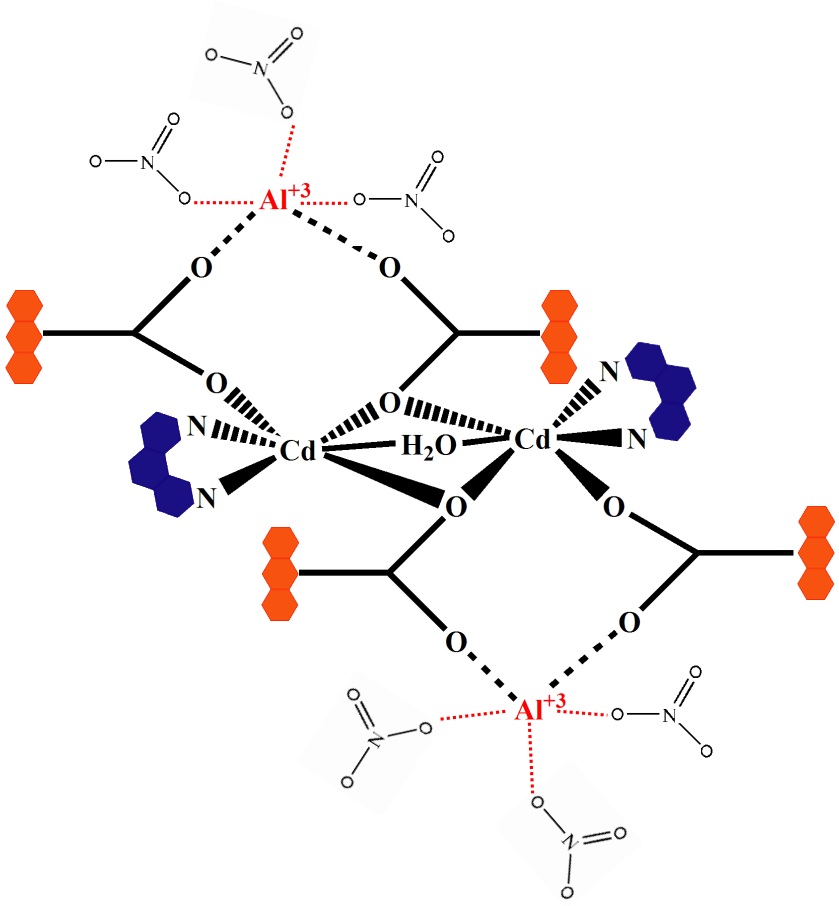

Figure S14. Possible interactions of Al^{3+} with the pendant oxygens in complex **2**.

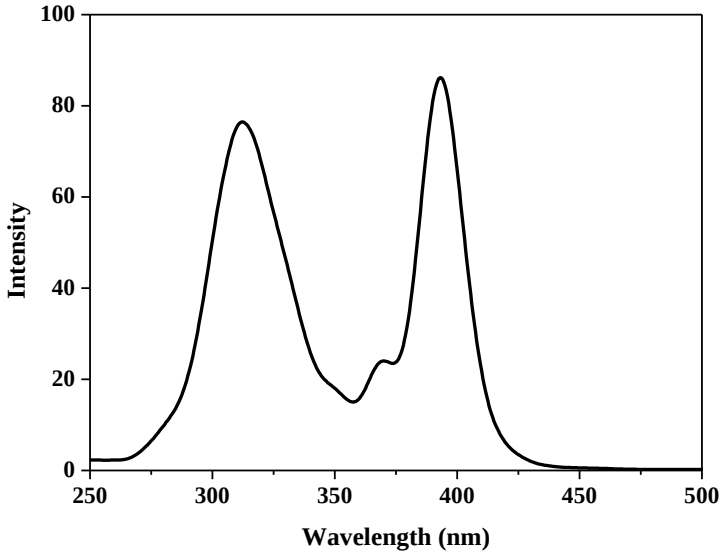

Figure S15. Excitation spectrum of methanol solution of compound **2** after addition of Al^{3+}, monitored at 510 nm.

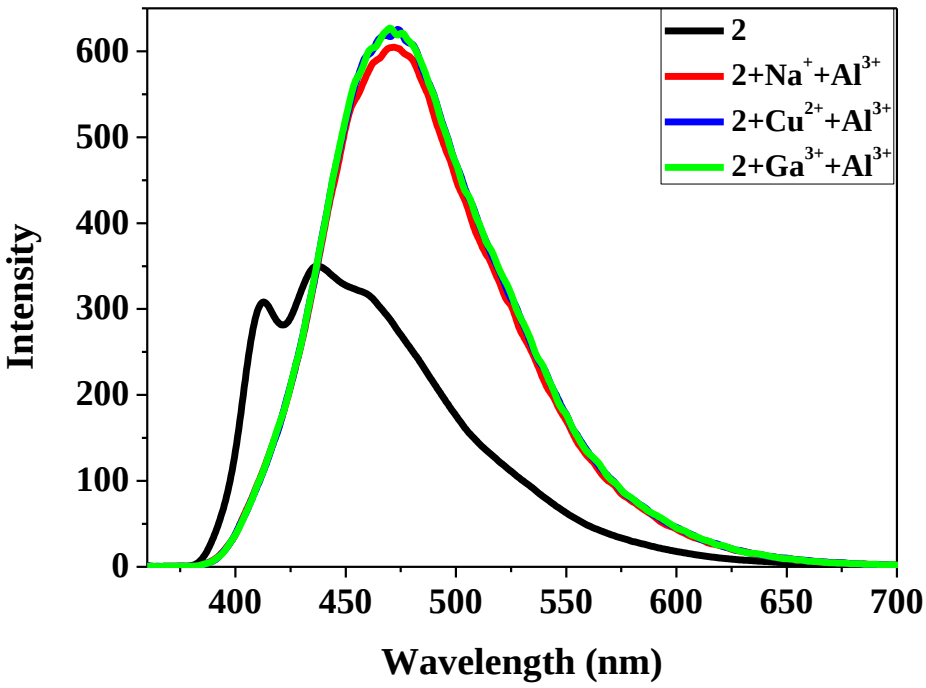

Figure S16. Emission spectra of methanol solution of compound **2** after addition of Na^{+}+Al^{3+}, Cu^{2+}+Al^{3+} and Ga^{3+}+Al^{3+} in 1:1 ratio upon excitation at 350 nm.

Table S1: Calculated CT transfer spectra (in nm) of compound **1** and compound **2** using different exchange correlation energy functional. Oscillator strengths are written in bracket.

System	CAM-B3LYP			B97XD			B3LYP		
	CT	**π -π***	**π -π***	**CT**	**π -π***	**π -π***	**CT**	**π -π***	**π -π***
pyrene	381.50 (0.03)	343.64 (0.28)	314.39 (0.24)	365.08 (0.04)	339.97 (0.29)	312.84 (0.29)	-	354.89 (0.18)	342.60 (0.09)
anthracene	356.70 (0.09)	333.21 (0.23)	323.61 (0.14)	349.91 (0.12)	331.78 (0.29)	316.31 (0.09)	-	378.46 (0.14)	370.49 (0.18)

The charge transfer (CT) spectrum was not observed using B3LYP exchange correlation energy functional. These results indicate the important of consideration of long-range corrected exchange correlations energy functional, CAM-B3LYP and B97XD in our study.

Table S2: Metal ion concentrations obtained by ICP analysis in metal bound compound **2** via dissolution of the compounds in water.

Metal ions	Concentrations mg/L
Na^{+}	3.705
Fe^{3+}	1.598
Zn^{2+}	1.159
Ga^{3+}	2.569
Cu^{2+}	2.177
Mn^{2+}	1.218
Eu^{3+}	5.136

Table S3: Cd^{2+} and Al^{3+} concentrations obtained by ICP analysis in compound **2** and metal bound compound **2** via dissolution of equal amount of compound **2** in water. Concentrations were measured in two different batches of experiments.

Compounds	**Batch**	**Al^{3+} mg/L**	**Cd^{2+} mg/L**
Compound **2**	i	--------	2.850
	ii	--------	2.902
Al^{3+} bound compound **2**	i	2.635	2.795
	ii	2.560	2.817