Supplementary Material (ESI) for CrystEngComm

Novel Quadridentate Salen Type Triple-decker Sandwich Ytterbium Complexes with Near Infrared Luminescence

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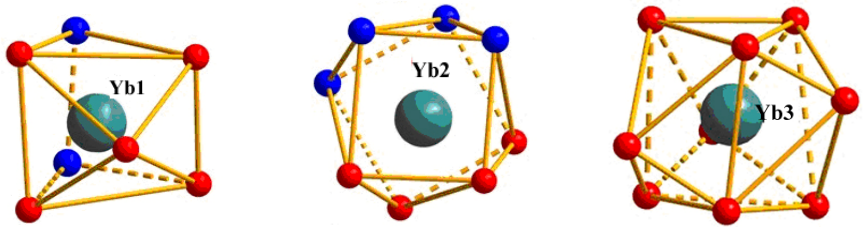
§ Electronic supplementary information (ESI):



(a) (b) (c)

Figure S1. Coordination geometries of Yb(III) ions in **1** and **2**. (a) seven-coordinated geometry of mono-capped trigonal prism; (b) eight-coordinated geometry of square antiprism; (c) nine-coordinated geometry of tri-capped trigonal prism).

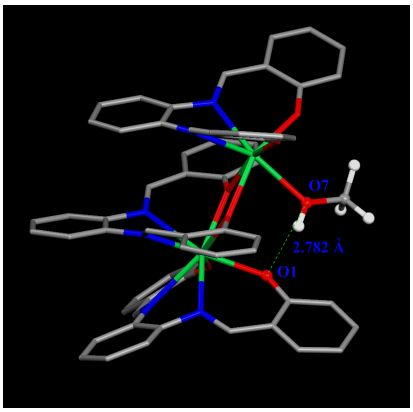


Figure S2. Intramolecular H-bonding between the CH_3OH group and the ligand in **1**.

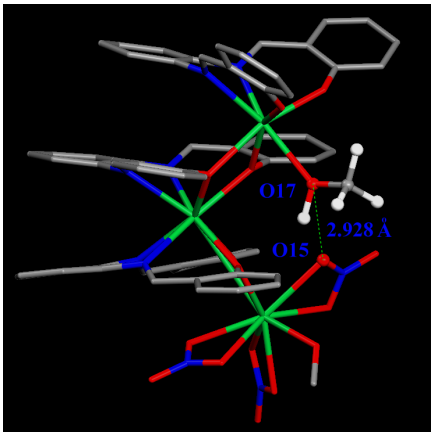


Figure S3. Intramolecular H-bonding between the CH_3OH group and the nitrate group in **2**.

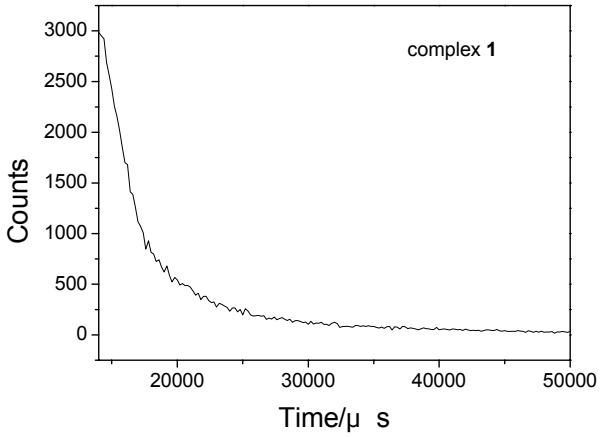


Figure S4. The decay curves of excited states in single exponential way for lifetime values of **1** in CH_3OH at room temperature.

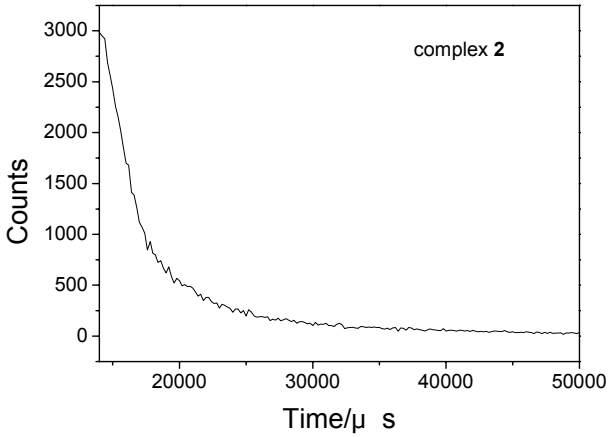


Figure S5. The decay curves of excited states in single exponential way for lifetime values of **2** in CH_3OH at room temperature.

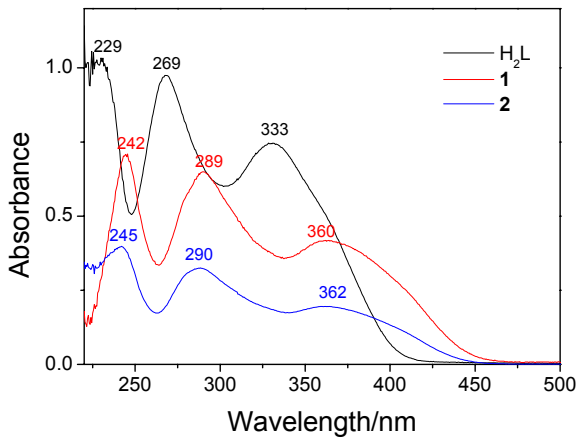


Figure S6. Uv-Vis spectra of free H_2L and complexes **1** and **2** in CH_3OH (1×10^{-5} M). The photophysical properties of complexes **1** and **2** were studied in CH_3OH. The free ligand (H_2L) exhibits absorption bands at 229, 269 and 333 nm, which become red-shifted upon coordination to the metals in **1** and **2**.

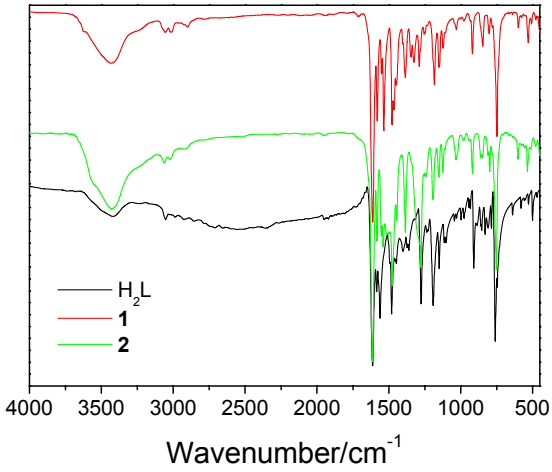


Figure S7. Infrared spectra of complexes **1, 2** and H_2L recorded from a KBr pellet. IR (KBr, cm^{-1}) for **1**: 3429(s), 1612(s), 1581(m), 1535(m), 1477(m), 1464(m), 1403(m), 1289(s), 1183(m), 1027(m), 919(w), 749(s), 530(m). IR (KBr, cm^{-1}) for **2**: 3428(s), 1614(s), 1582(m), 1552(m), 1540(m), 1476(s), 1385(m), 1277(s), 1193(m), 918(m), 798(m), 752(s), 536(m).

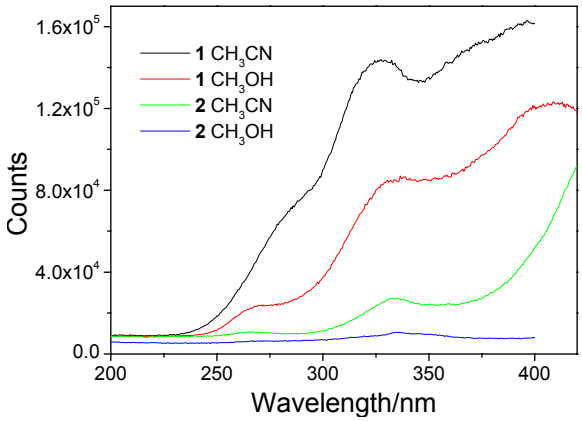


Figure S8. NIR excitation spectra of complexes **1** and **2** in CH_3CN and CH_3OH.