Comparison of Homoleptic Indium-Quinolato Monomeric and Dimeric Complexes: Synthesis, Structure, Photoluminescence and Photo-Degradation

Supplementary Information (SI)

For

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Figure SI1: Solid state ¹H-NMR of [In(Ox)₃] 2H₂O (1) indicating a meridional monomer.

Figure SI2 depicts the solution state ¹H-NMR spectra of **1** and **2** indicating *fac*-In(Ox)₃ and the conformation of the $[In_2(Ox)_2Cl_2-\mu-[\kappa^2-O,O'-(Ox)_2]$ dimer.



Figure SI2: The ¹H-NMR exhibition of **1** and **2**.

The spectrum of **1** in **Figure SI2** exhibits six resonance environments integrating for three protons each for three 8-quinolato ligands in the monomer. The ligand resonance environments in a facial isomer are the same, hence only six are observed and not more,

whereas more resonance environments are expected in a meridional counterpart. There are also clustered/overlapping six (supposedly 12) resonance environments in **2**, however, integrating for four protons (*there are four 8-quinolato ligands in the dimer*) due to the symmetry therein.



Figure SI3: Solution state ¹H-NMR of [In(Ox)₃] 2H₂O (1).





Figure SI5: Solution state ¹H-NMR of {[In2(Ox)2Cl2- μ -[κ 2-O,O'-(Ox)2] C7H8 } (2)



Figure SI6: Solution state ¹³C-NMR of {[In2(Ox)2Cl2-μ-[κ2-O,O'-(Ox)2] C7H8 } (2)



Figure SI7: Crystal structure of 1 with two aqua molecules in an asymmetric unit cell.



Figure SI8: Crystal structure of 1 exhibiting inter-molecular hydrogen interaction.



Figure SI9: Symmetry generated crystal structure of 2 with the toluene solvent in the unit cell.



Figure SI10: Crystal structure of 2 with half toluene molecule in an asymmetric unit cell.