Electronic Supplementary Material (ESI) for Dalton Transactions.

ESI

Encapsulation of Ni Salen Complex in Zeolite Y: An Experimental and DFT Study

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Figure S1

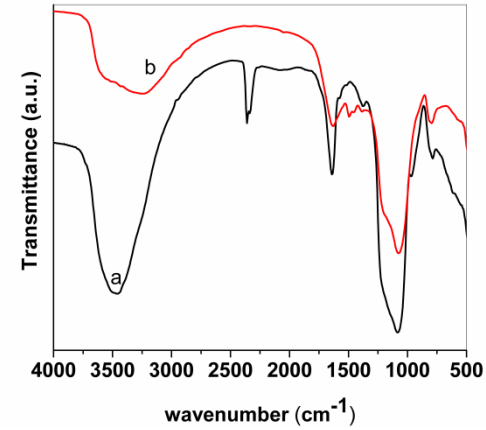

Figure S1. FTIR spectra in the range of 500 cm^{-1} to 4000 cm^{-1} of (a) pure MCM-41, (b) encapsulated 5-OH-NL5 in MCM-41

Figure S2

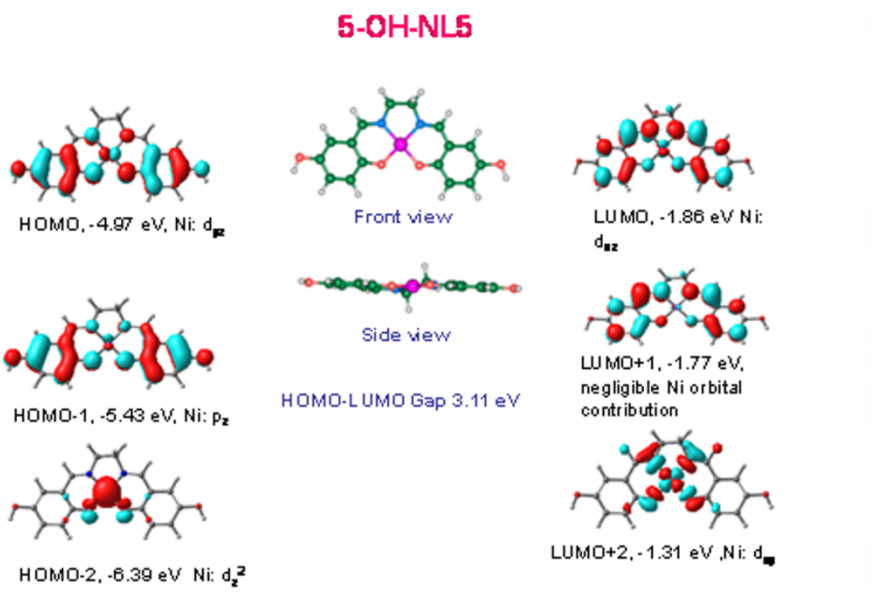

Figure S2. The structure and important molecular orbitals for 5-OH-NL5. The frontier orbitals with clear metal orbital characters are shown.

Figure S3

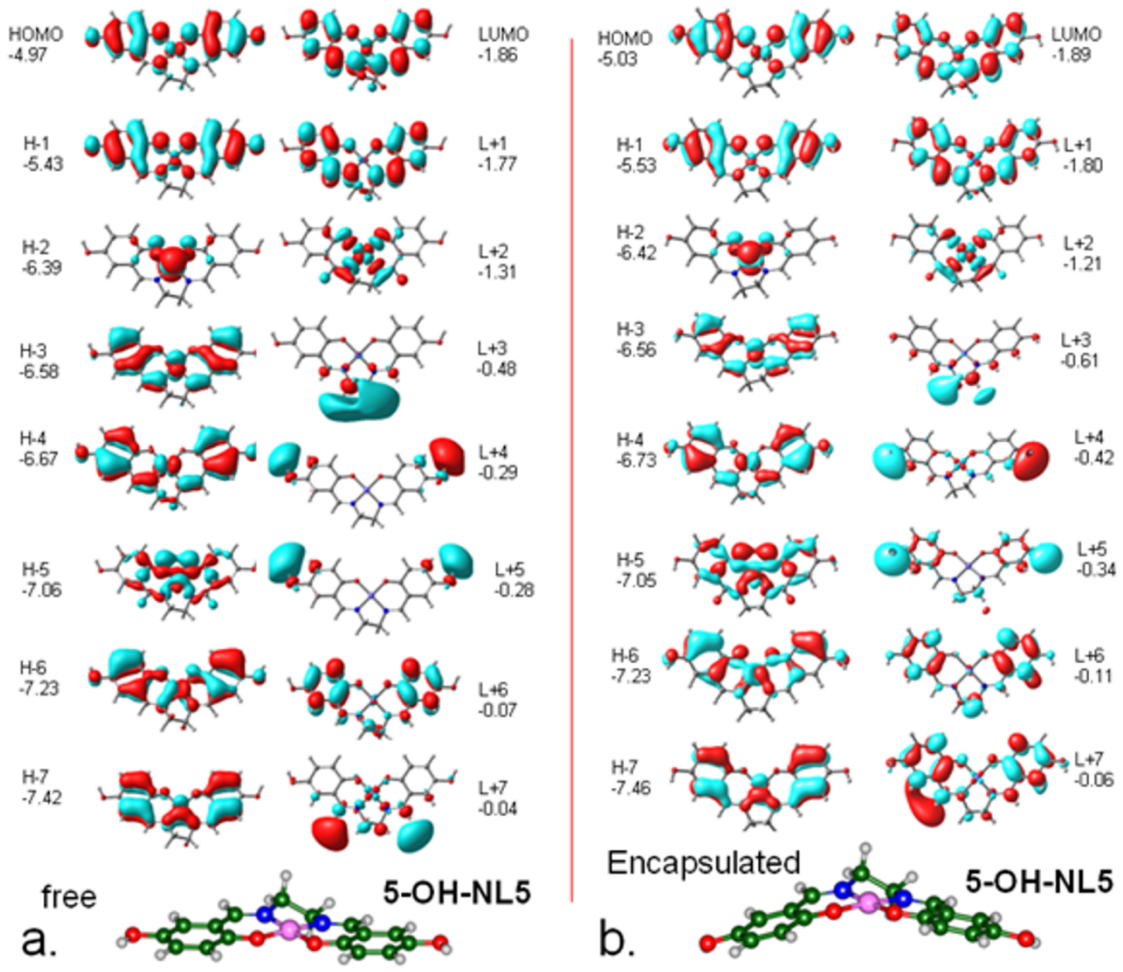

Figure S3. (a) The molecular orbitals of 5-OH-NL5 in free state, including the HOMO, LUMO. The orbitals lower in energy than HOMO are marked as H-n (n = 0 being HOMO) and LUMO+n (n =0 being LUMO). (b) The molecular orbitals of 5-OH-NL5 in encapsulated singlet state, including the HOMO, LUMO. Corresponding molecular structures are shown for reference.

Figure S4

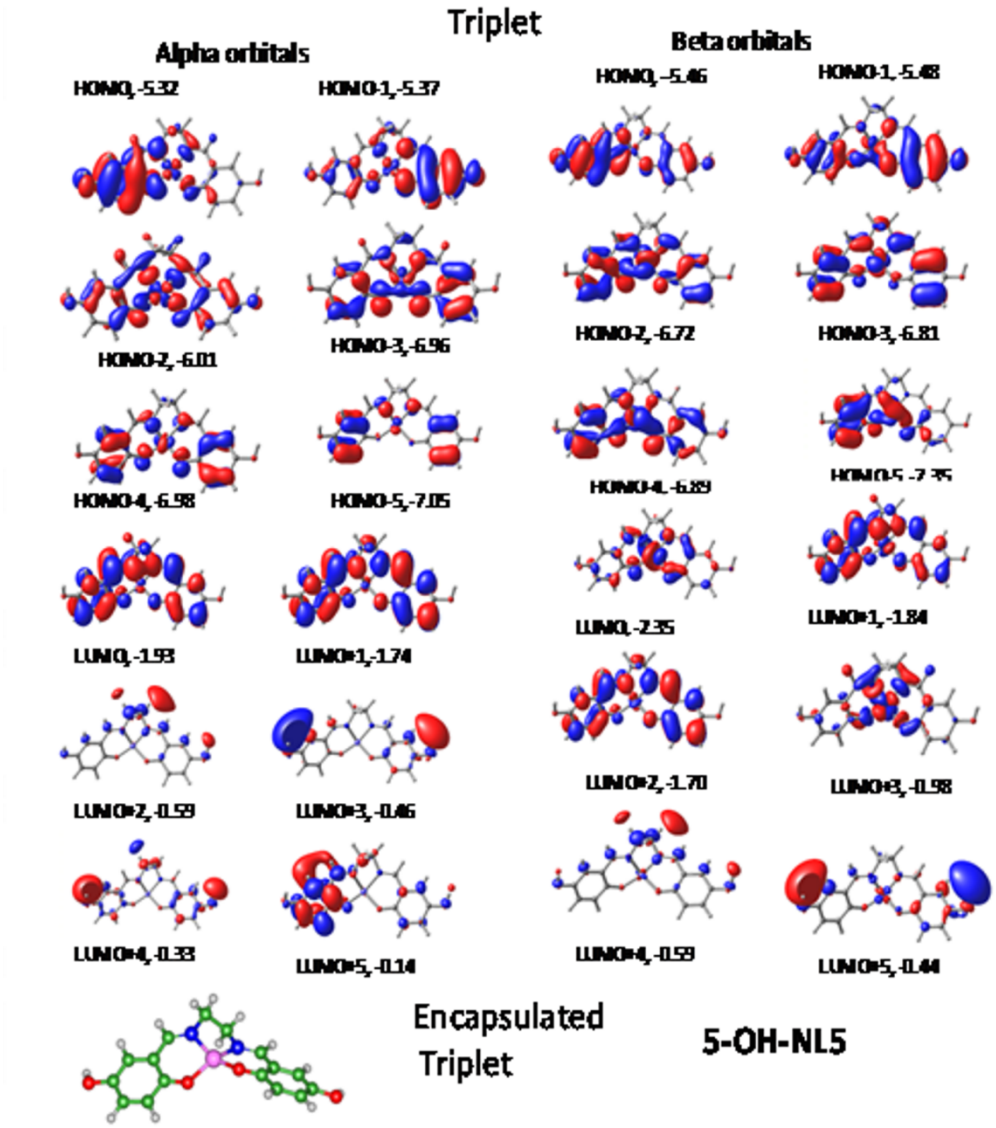

Figure S4. The molecular orbitals of 5-OH-NL5 in encapsulated triplet state, including the HOMO, LUMO. The orbitals lower in energy than HOMO are marked as HOMO-n (n = 0 being HOMO) and LUMO+n (n =0 being LUMO). Corresponding molecular structure is shown for reference.

Figure S5

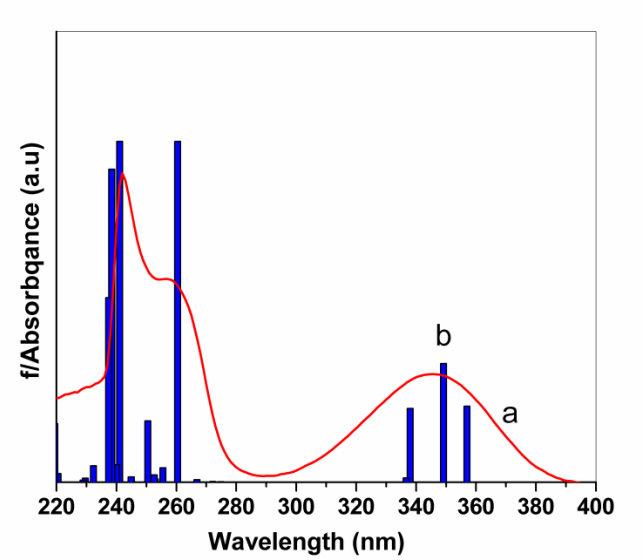

Figure S5. UV-Vis spectra of (a) 5-OH salen ligand in chloroform (b) TD- DFT simulated UV-Vis spectra of 5-OH salen.