

Supporting Information

Fixation of carbon dioxide by macrocyclic lanthanide(III) complexes under neutral condition producing self-assembled trimeric carbonato-bridged compounds with $\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^2$ bonding † ‡

Pradip Bag,^a Supriya Dutta,^a Papu Biswas,^b Swarup Kumar Maji,^b Ulrich Flörke^c and Kamalaksha Nag^{*a}

Fig. S1 ^1H NMR spectra of $[\{\text{Lu}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)](\text{ClO}_4)_4\cdot 7\text{H}_2\text{O}$ (**7**) in **(a)** CD_3CN and **(b)** $(\text{CD}_3)_2\text{SO}$. The solvent and water peaks are marked with asterisks.

Fig. S2 ^1H NMR spectra of $[\{\text{Nd}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)](\text{ClO}_4)_4\cdot \text{H}_2\text{O}$ (**2**) in **(a)** CD_3CN and **(b)** $(\text{CD}_3)_2\text{SO}$.

Fig. S3 The structural representating for the complex cations **(a)** $[\{\text{Nd}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)]^{4+}$ **(b)** $[\{\text{Tb}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)]^{4+}$.

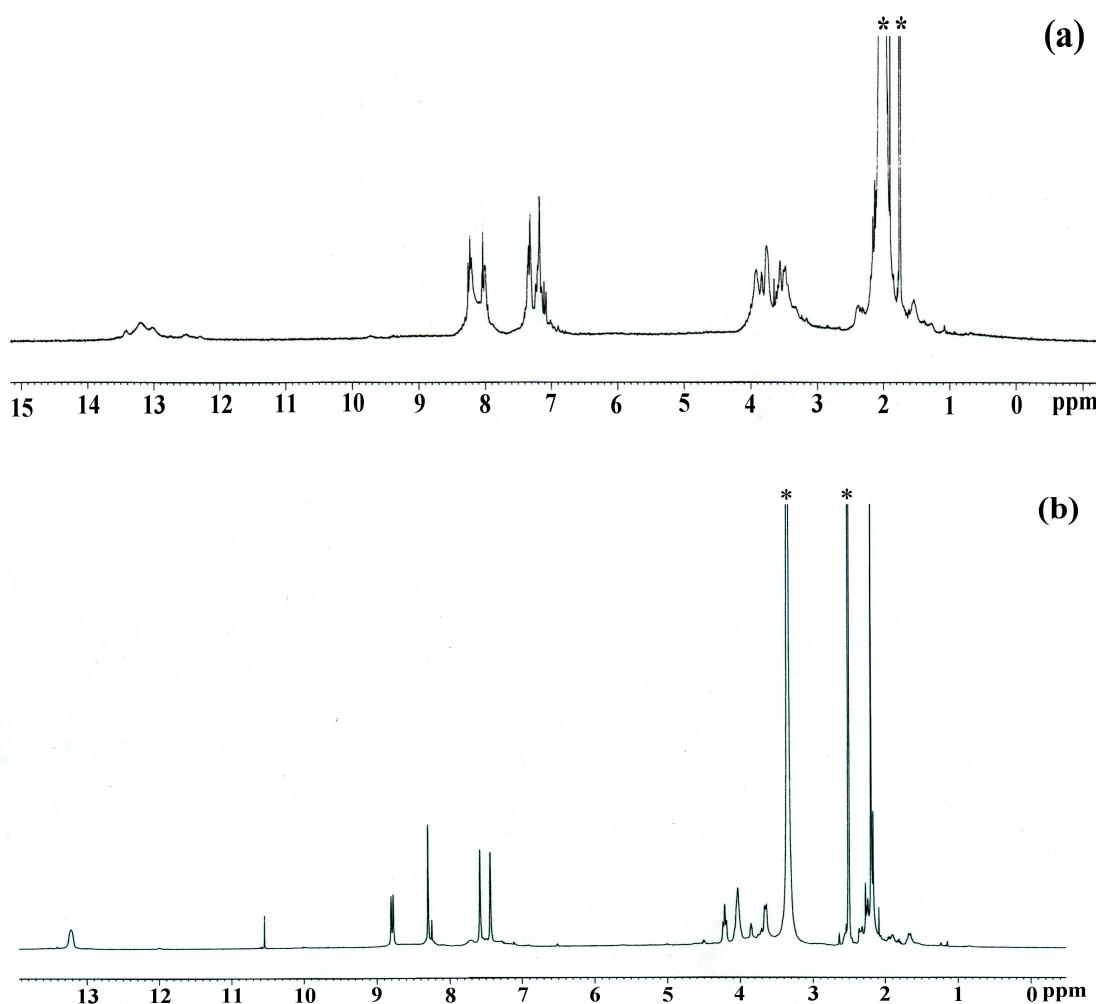


Fig. S1 ¹H NMR spectra of $[\{\text{Lu}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)](\text{ClO}_4)_4 \cdot 7\text{H}_2\text{O}$ (**7**) in (a) CD_3CN and (b) $(\text{CD}_3)_2\text{SO}$. The solvent and water peaks are marked with asterisks.

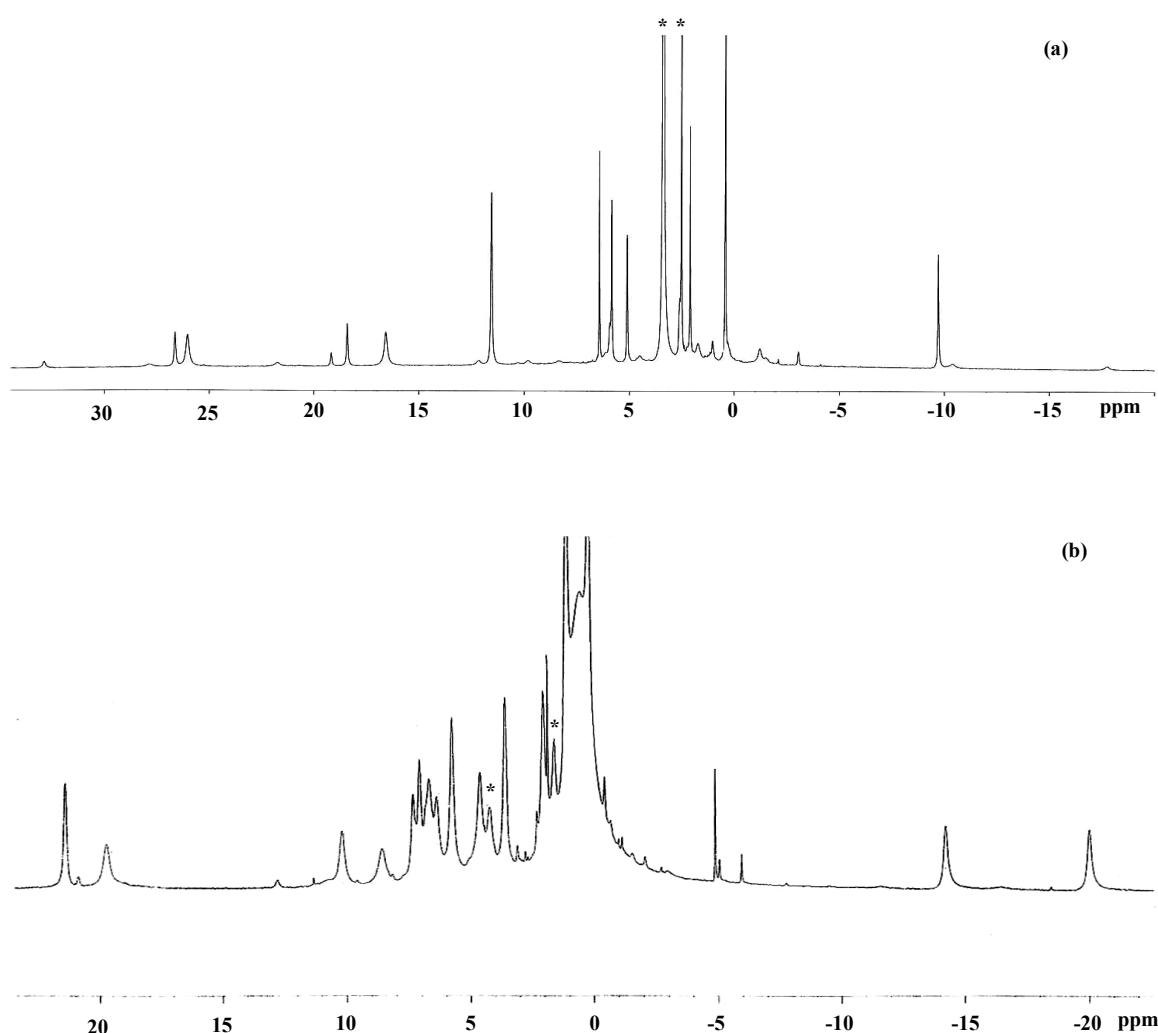


Fig. S2 ¹H NMR spectra of $[\{\text{Nd}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}\}_3(\mu_3\text{-CO}_3)](\text{ClO}_4)_4\cdot\text{H}_2\text{O}$ (**2**) in (a) CD_3CN and (b) $(\text{CD}_3)_2\text{SO}$.

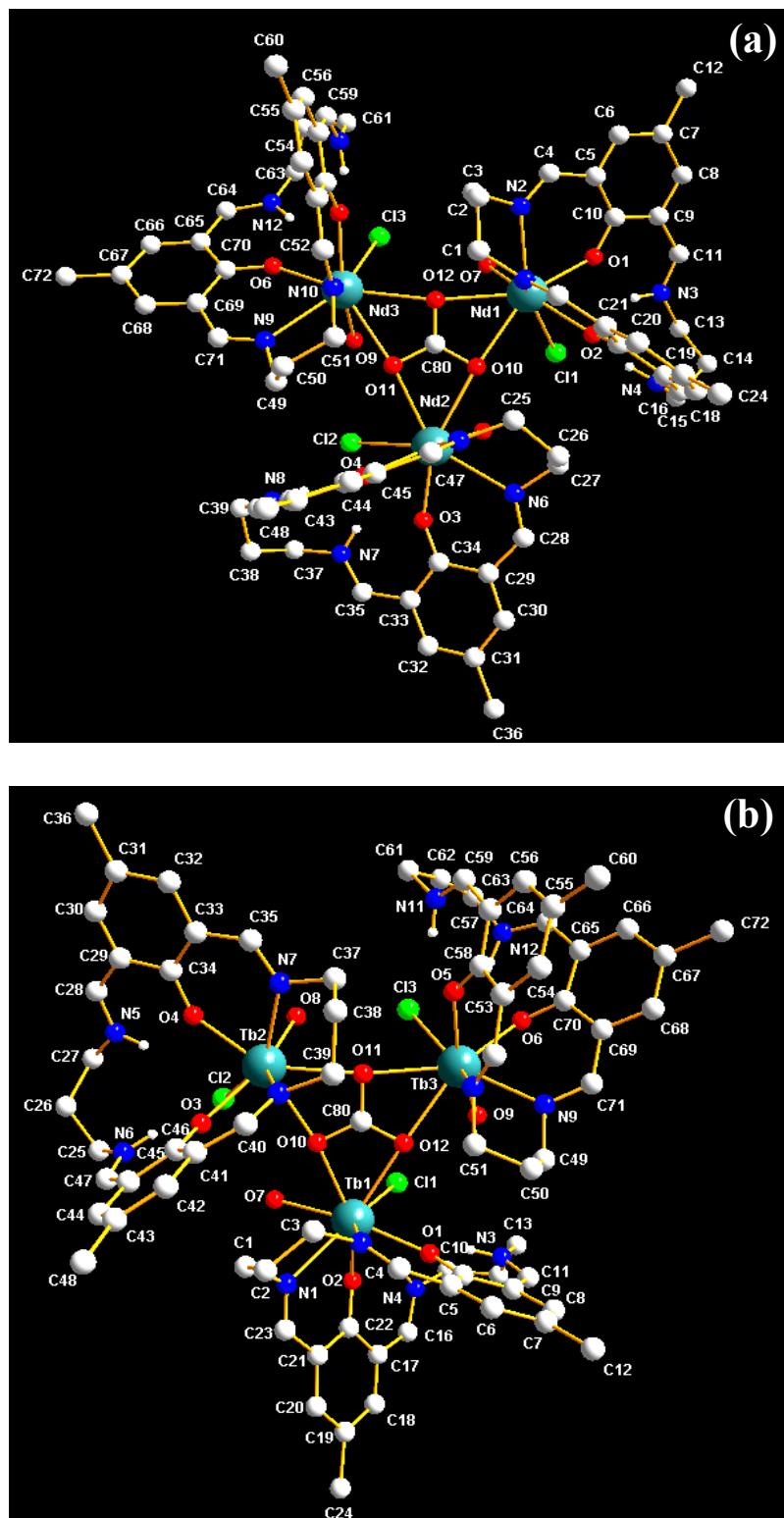


Fig. S3 The structural representing for the complex cations (a) $[\{Nd(LH_2)(H_2O)Cl\}_3(\mu_3\text{-CO}_3)]^{4+}$ (b) $[\{Tb(LH_2)(H_2O)Cl\}_3(\mu_3\text{-CO}_3)]^{4+}$.