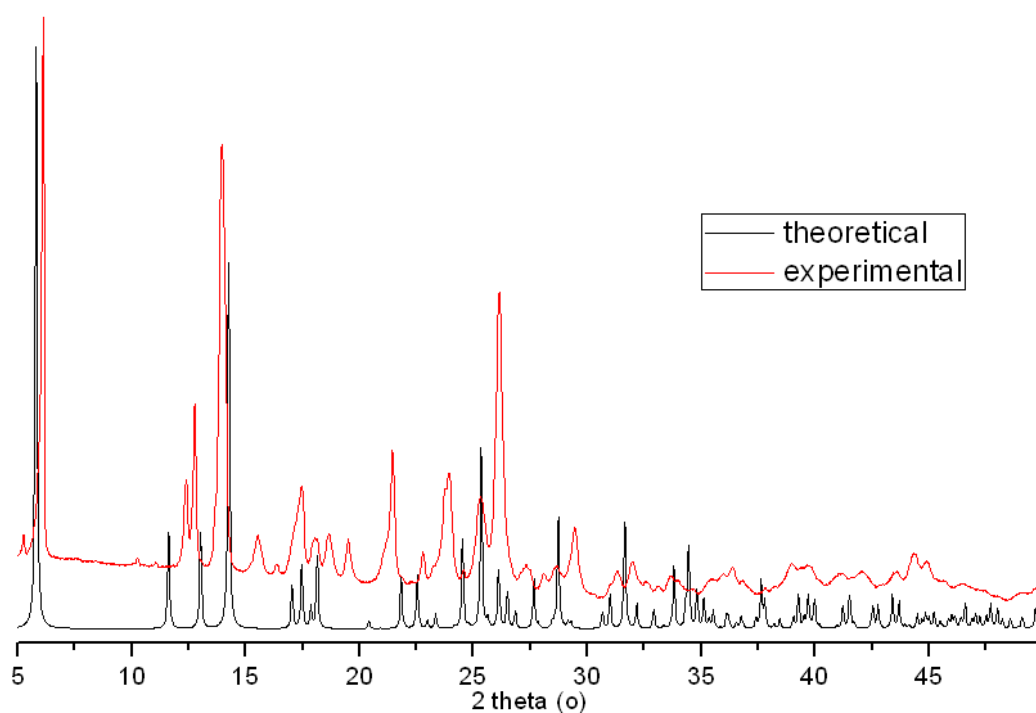
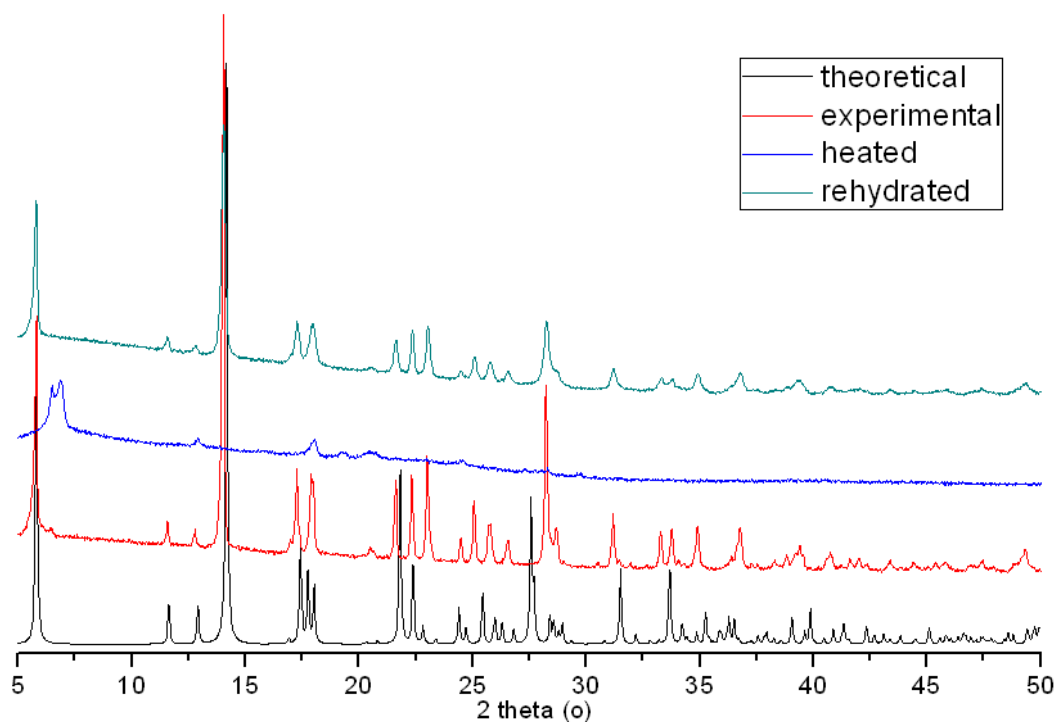


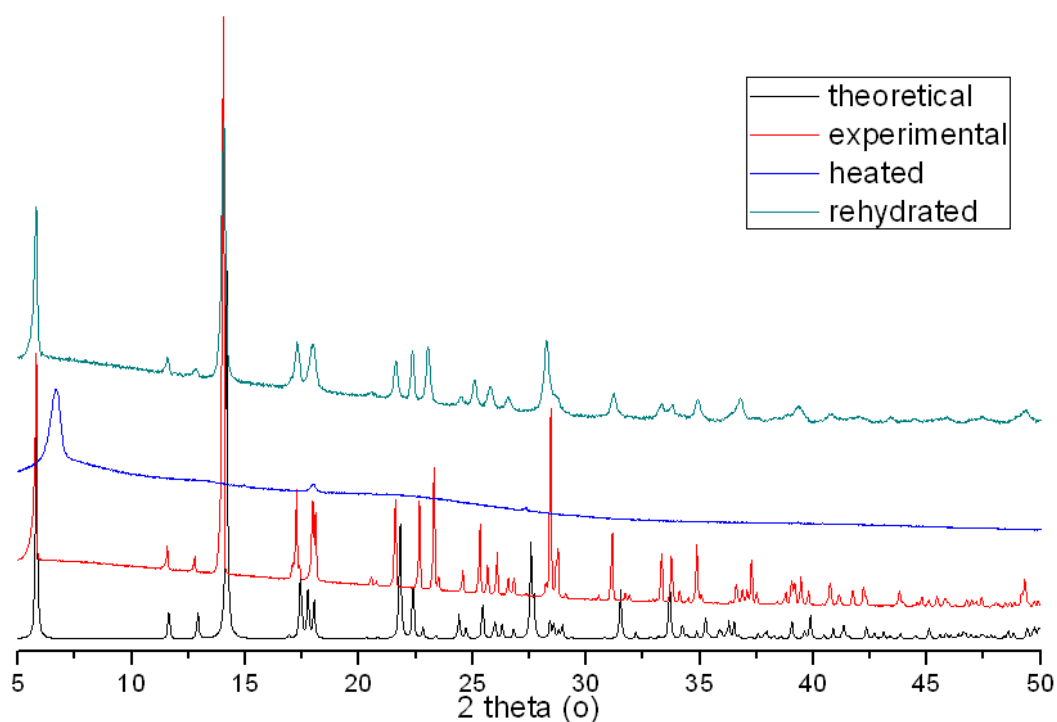
**Fig. S1** The powder XRD pattern of compound **3** (experimental) and the simulation of the powder pattern of **3** from the crystal structure.



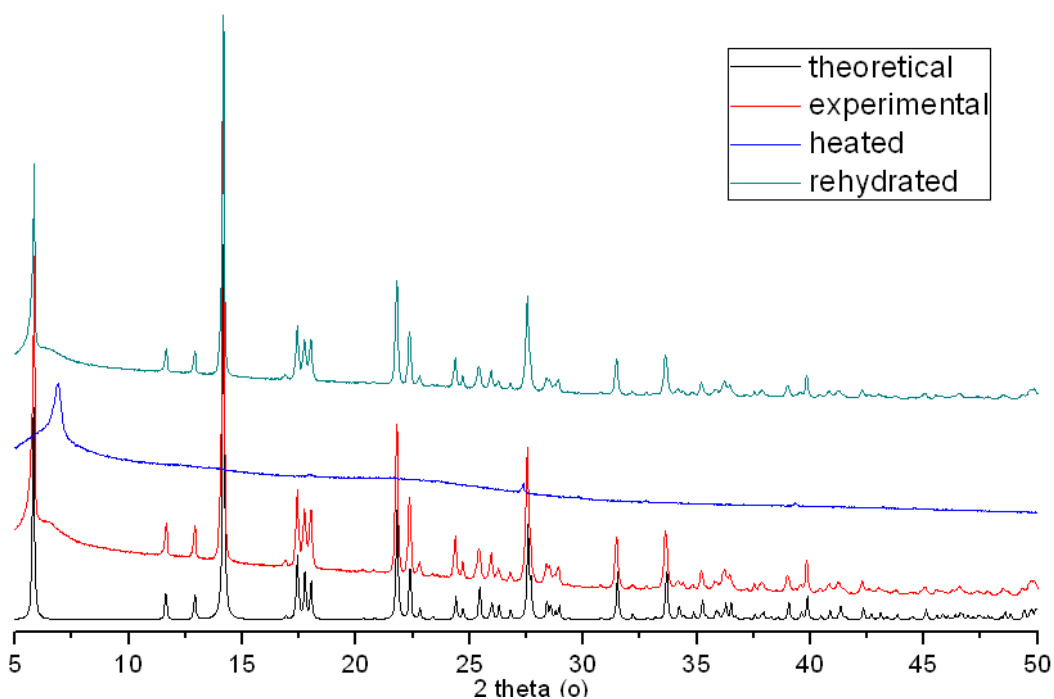
**Fig. S2** The powder XRD pattern of compound **4** (experimental) and the simulation of the powder pattern of **4** from the crystal structure.



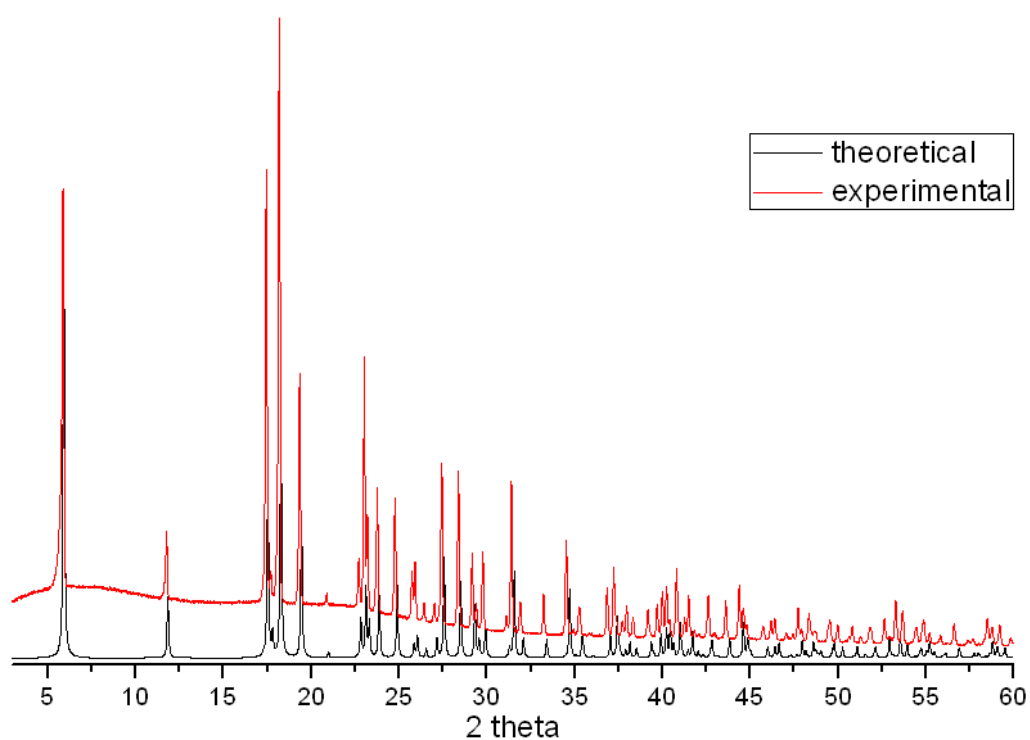
**Fig. S3** The powder XRD pattern of compound **6** (experimental), the rehydrated analogue of **6** and the simulation of the powder pattern of **6** from the crystal structure.



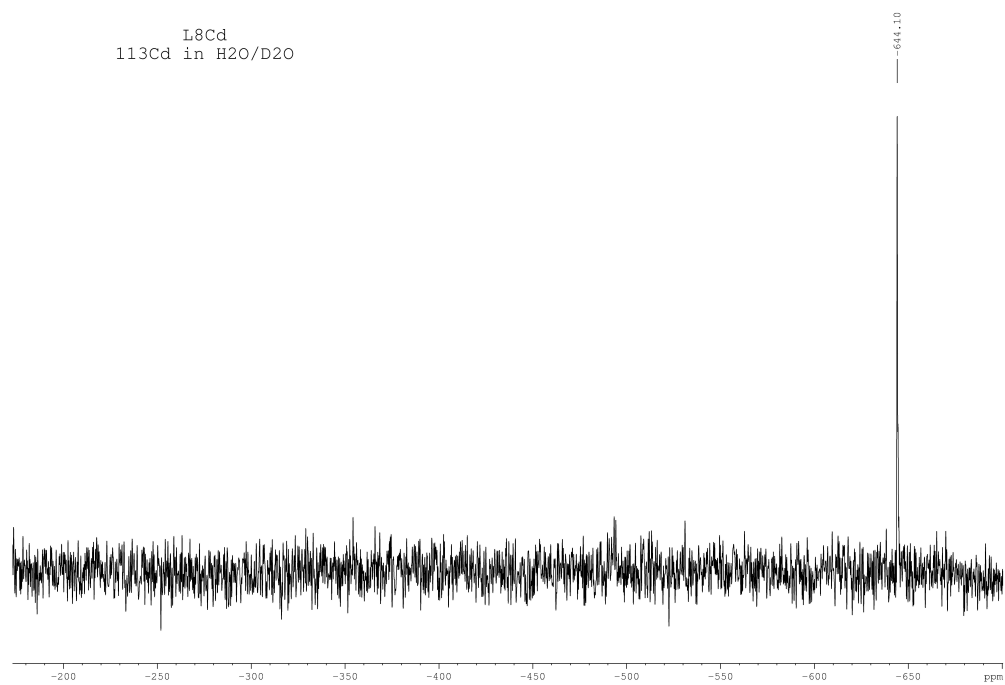
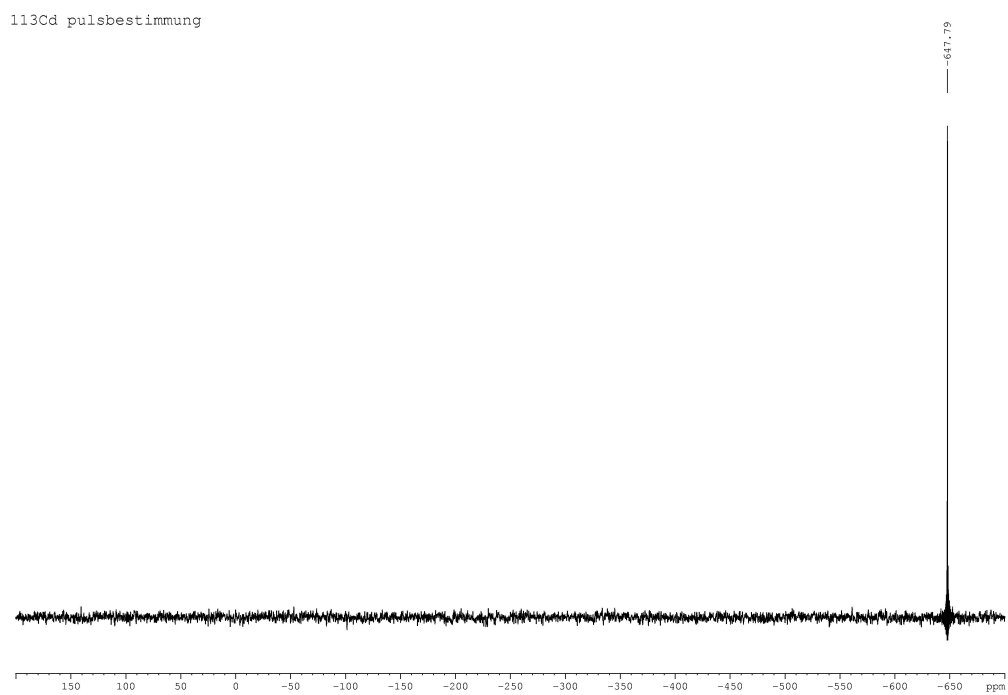
**Fig. S4** The powder XRD pattern of compound **7** (experimental), the rehydrated analogue of **7** and the simulation of the powder pattern of **7** from the crystal structure.



**Fig. S5** The powder XRD pattern of compound **8** (experimental), the rehydrated analogue of **8** and the simulation of the powder pattern of **8** from the crystal structure.



**Fig. S6** The powder XRD pattern of compound **9** (experimental) and the simulation of the powder pattern of **9** from the crystal structure



**Fig. S7.** (up)  $^{113}\text{Cd}$  NMR spectra of the reference and (down)  $^{113}\text{Cd}$  NMR spectra of compound **9**.

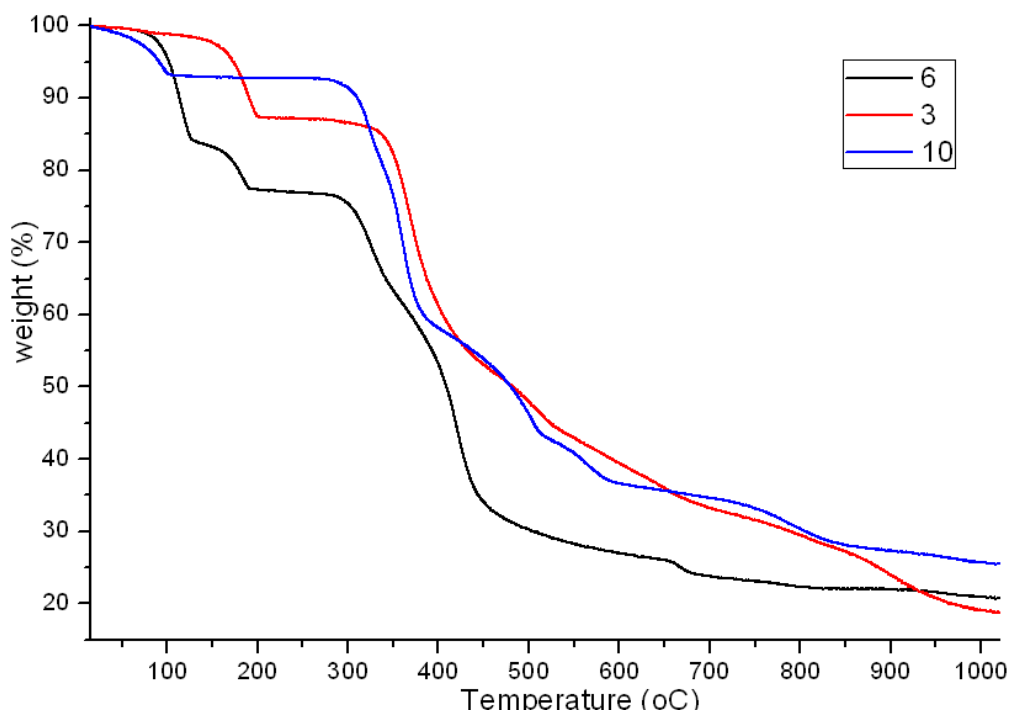


Fig. S8 TGA curves for compounds **3**, **6** and **10**.

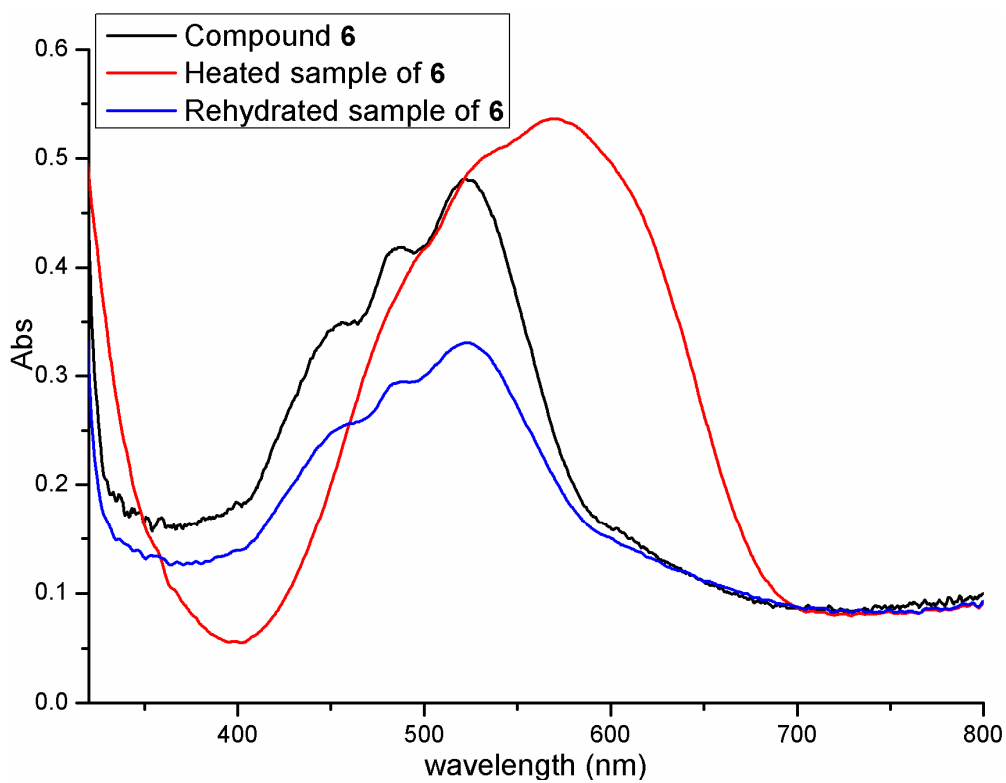
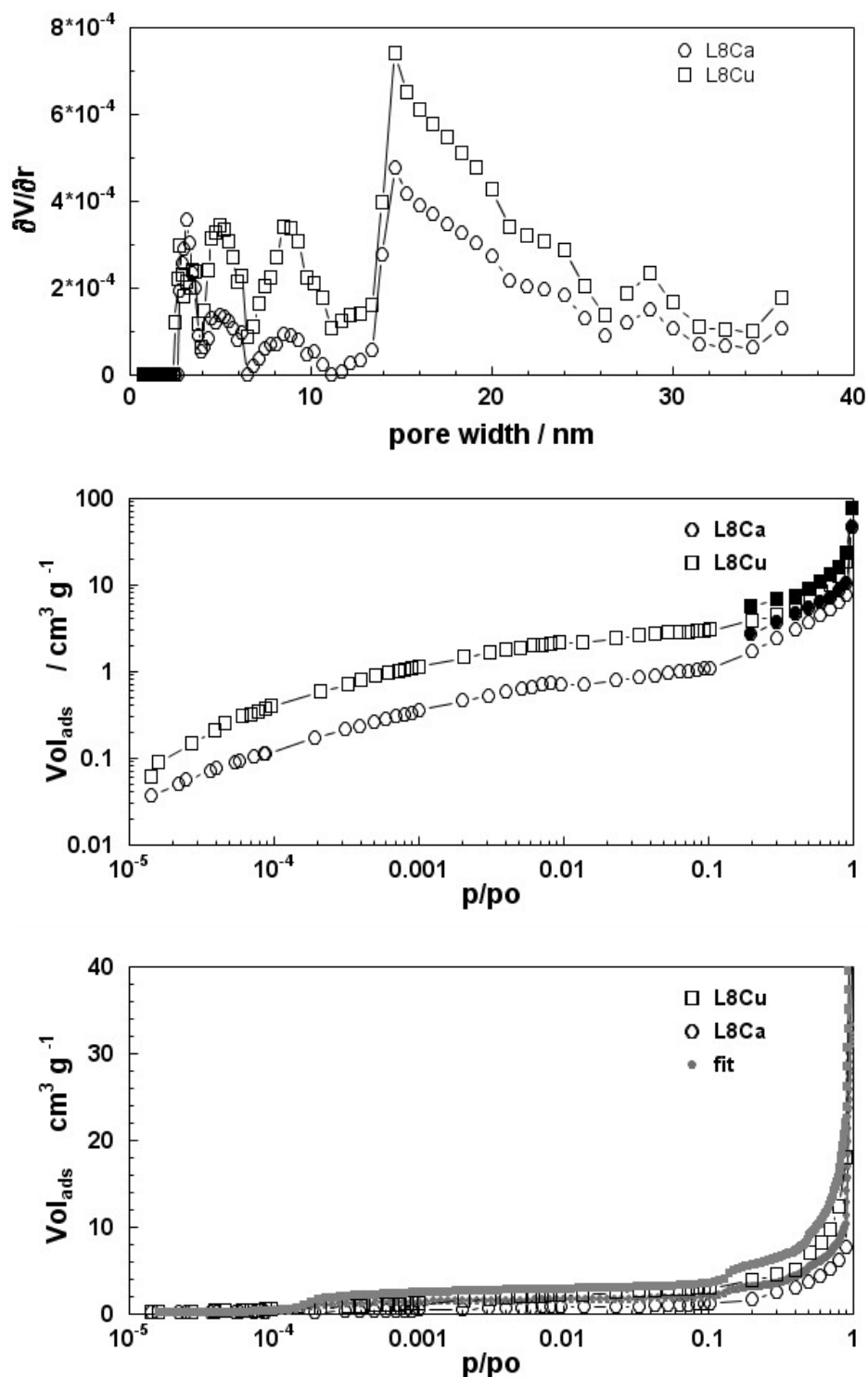
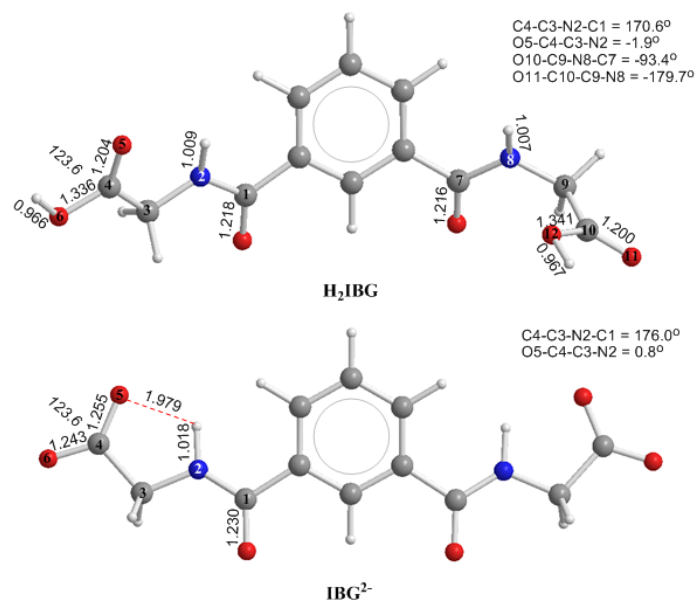


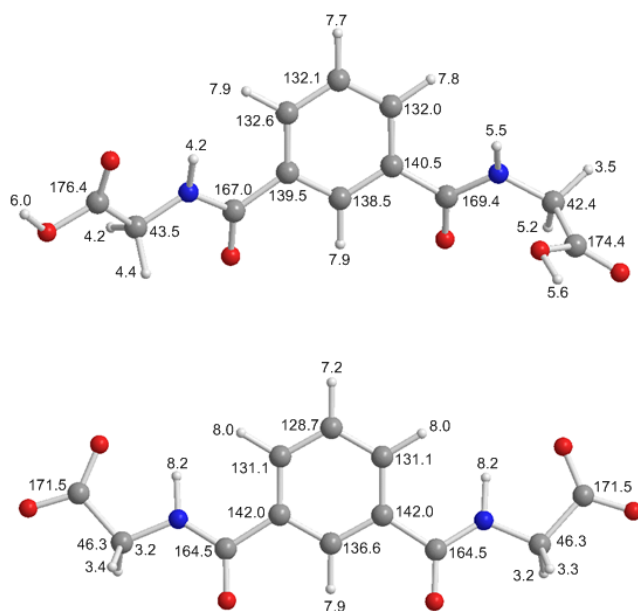
Fig. S9 DRS spectra for compound **6**



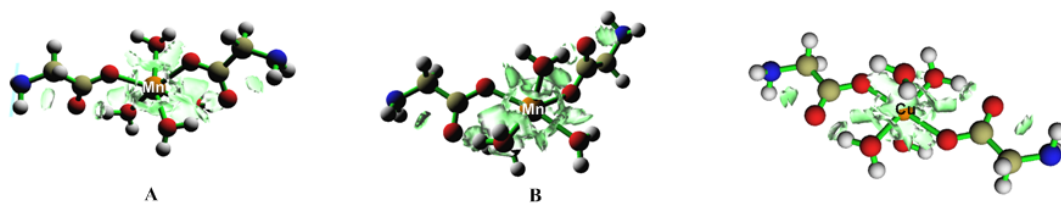
**Fig. S10** (upper) Pore width distribution (middle) Isotherm vs partial pressure (lower) Isotherms Fitting



**Fig. S11** Equilibrium geometries of the free-standing  $\text{H}_2\text{IBG}$  (1) ligand and its deprotonated dianionic conjugate base  $\text{IBG}^{2-}$  calculated at the PBE0/6-311+G(d,p) level.



**Fig. S12**  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts ( $\delta$ , ppm) of the free-standing  $\text{H}_2\text{IBG}$  and  $\text{IBG}^{2-}$  species calculated at the GIAO-PBE0/6-311+G(d,p) level.



**Fig. S13** 3D plots of the Reduced Density Gradient (RDG) (isosurface = 0.700) for the  $\text{Mn}(\text{glycine})_2(\text{H}_2\text{O})_4$  and  $\text{Cu}(\text{glycine})_2(\text{H}_2\text{O})_4$  complexes calculated at the DSD-PBEP86/Def2-TZVP level