

Fig. S1 Structure of  $1A \cdot 16H_2O$  with atom numbering; thermal elipsoids at 50% probability; water molecules and hydrogen atoms omitted for clarity.



Fig. S2 TG analysis for 1A·3.5H<sub>2</sub>O



Fig. S3 X-ray powder diffraction data for 1B (blue) and 2 (green) in comparison to calculated pattern for  $1A \cdot 16H_2O$  (red). The background and amorphous solvent signal were subtracted for clarity.



Fig. S4 TG analysis for 2.