Electronic Supplementary Material (ESI) for CrystEngComm

Mechanochemical interconversion between discrete complexes and coordination networks – formal hydration/dehydration by LAG

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Supplementary information: XRPD patterns, TGA curves.

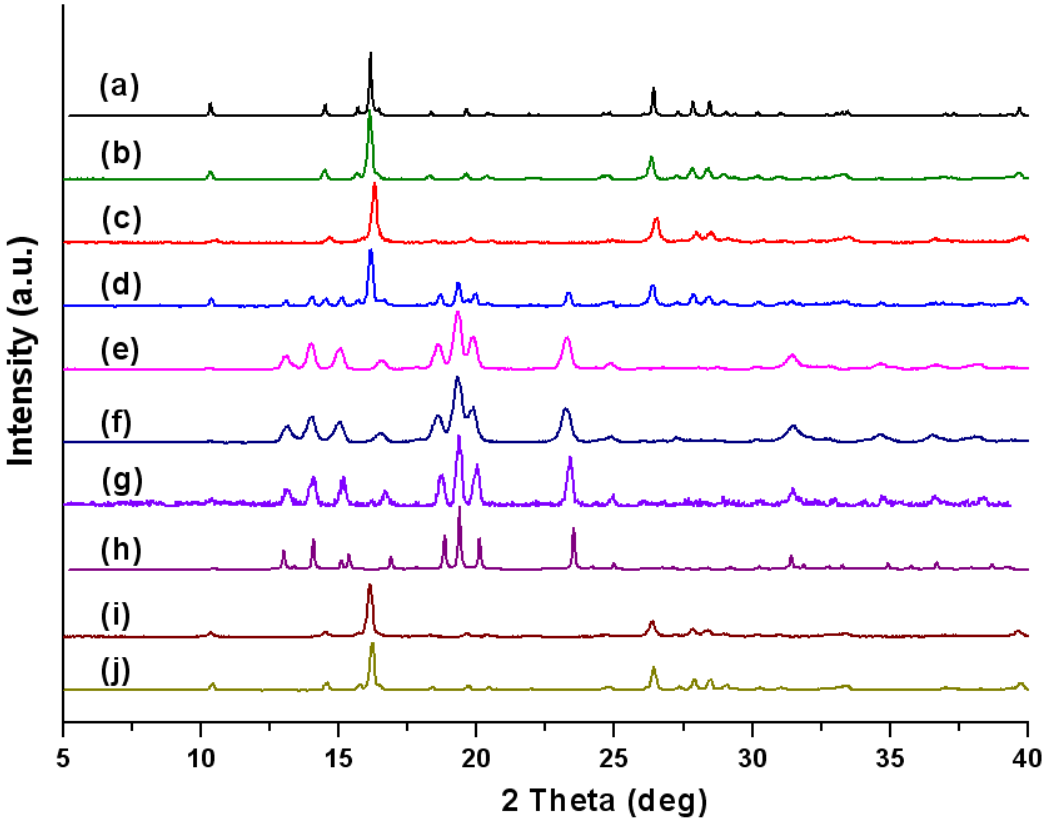

Figure S1 XRPD patterns for interconversions between **1** and **2**: (a) simulated pattern for **1** (CSD code INICZN); (b) submerging **1** in excess methanol for 24 hours; (c) grinding **1** with MeOH (100 μL) for 30 min at 650 rpm; (d) grinding **1** with MeOH (200 μL) for 60min at 750 rpm. (e) grinding **1** with MeOH (200 μL) for 90min at 20Hz in a shaking ball mill (QM-3B); (f) heating **1** at 200℃ for 12 hours; (g) submerging **1** in excess methanol for 3 days; (h) simulated pattern for **2 (**CSD code JUKVEQ**)**; (i) grinding **2** with H_2O (100 μL) for 30min at 650rpm/min; (j) submerging **2** in excess water for 24 hours.

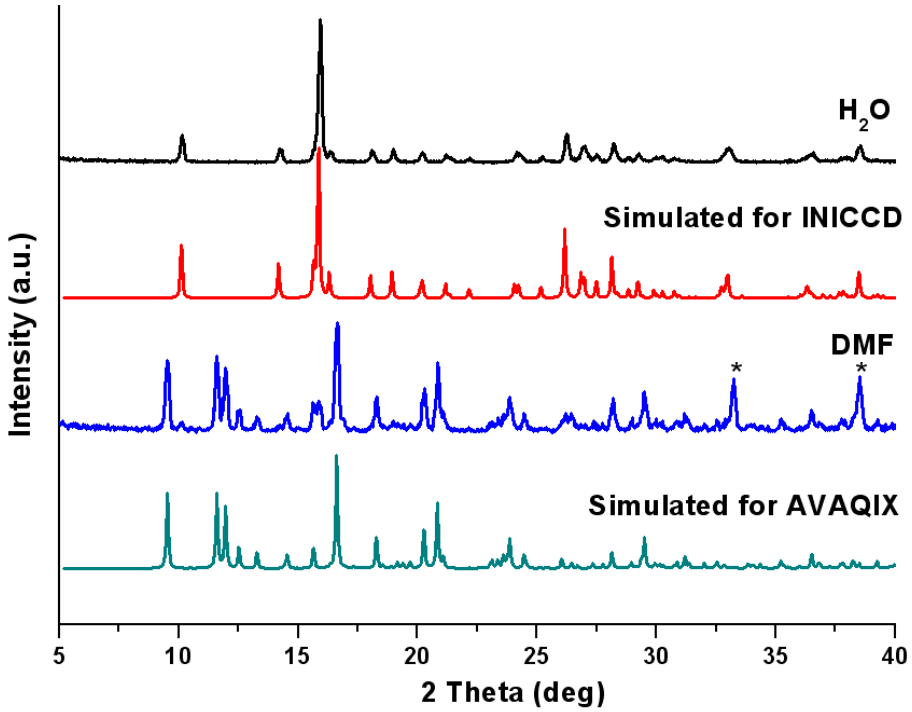

Figure S2 Comparison of XRPD patterns for products of mechanochemical reactions between CdO and HINA using LAG. The volume of the added solvent is 100μL. Peaks due to unreacted CdO are labelled *. INICCD and AVAQIX are CCD codes for $[Cd(INA)_2(OH_2)_4]$ (**3**) and $[Cd(INA)_2(OH_2)]\cdot DMF$ (**4**) respectively.

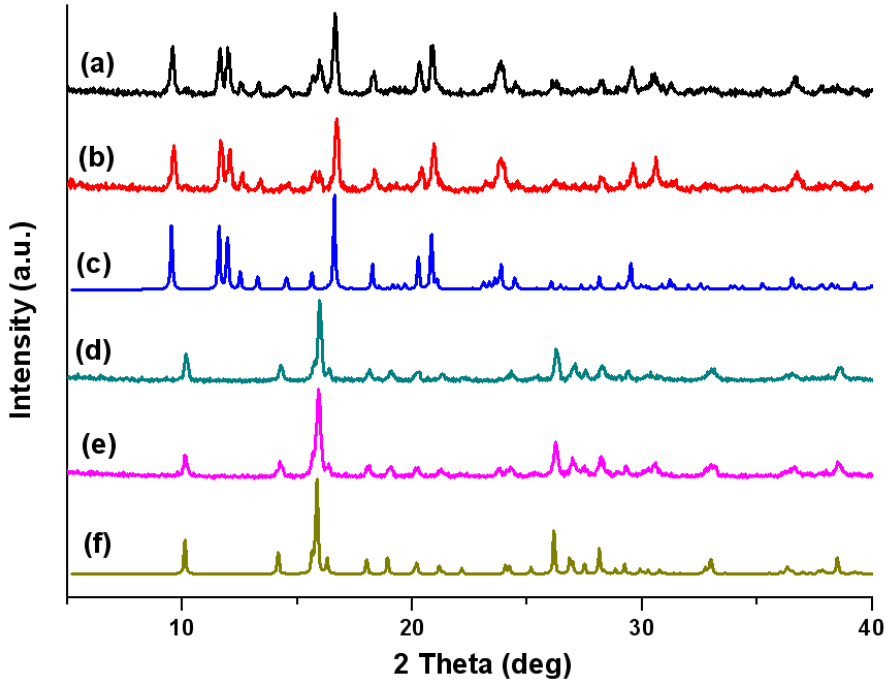

Figure S3 XRPD patterns for interconversions between **3** and **4**: (a) grinding **3** with DMF (100 μL) for 90min at 750 rpm; (b) submerging **3** in excess DMF for 24 hours; (c) simulated pattern for **4** (CSD code AVAQIX); (d) grinding **4** with H_2O (200 μL) for 90min at 750 rpm; (e) submerging **4** in excess H_2O for 24 hours; (f) simulated pattern for **3** (CSD code INICCD).

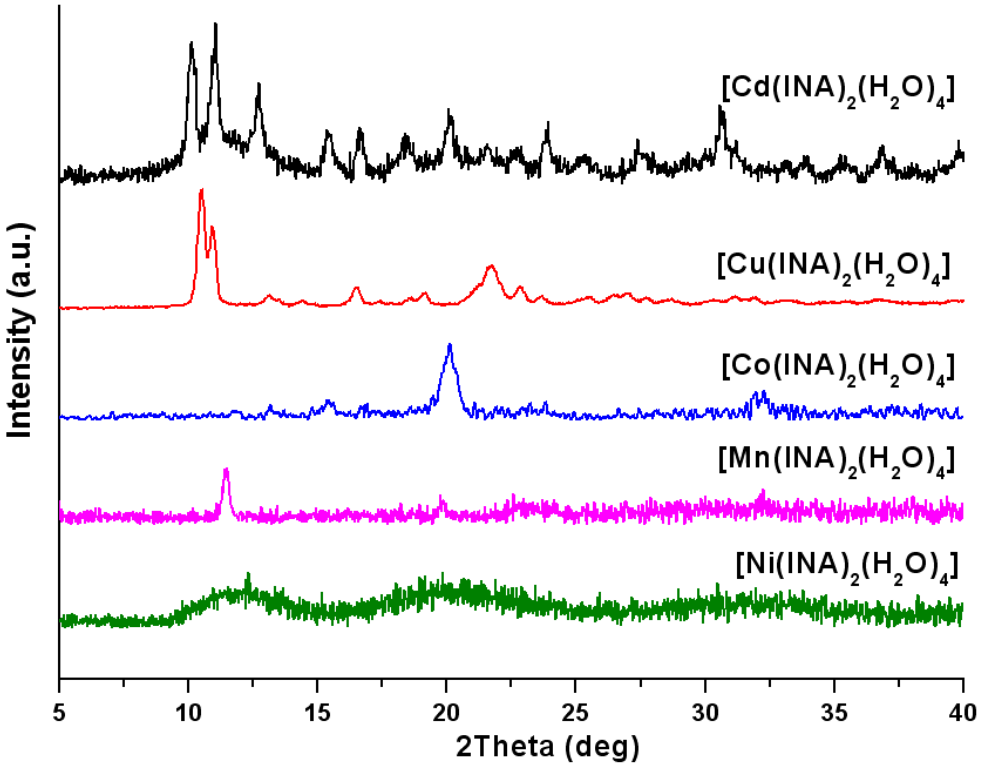

Figure S3. XRPD patterns for the products of heating $[M(INA)_2(H_2O)_4]$ (M = Cd, Cu, Co, Mn and Ni) at 150℃ for 12 hours (for Cd and Cu) and 2 hours (for Co, Mn and Ni).

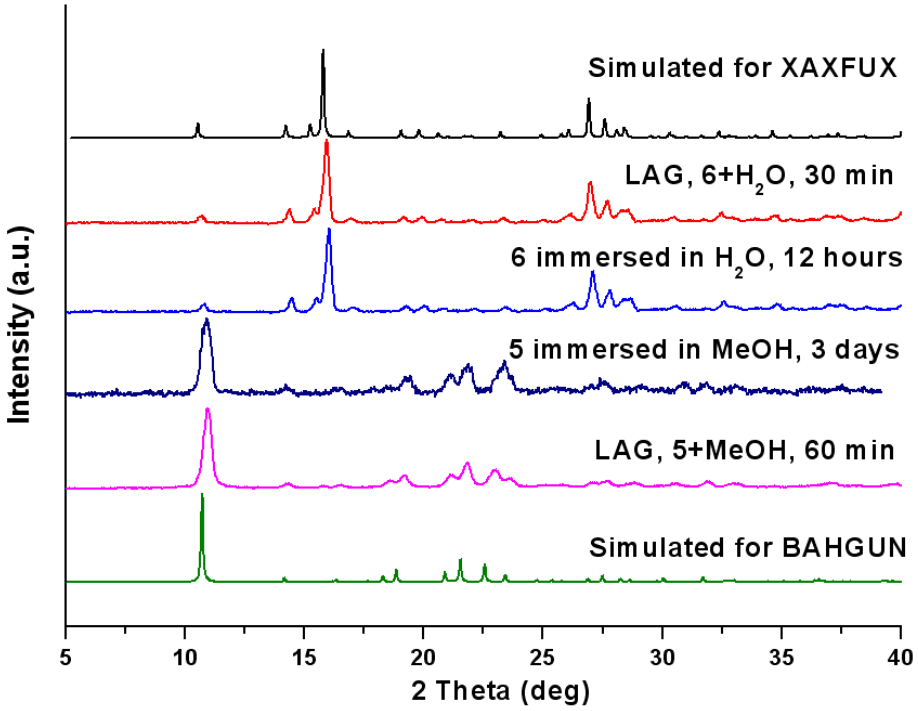

Figure S4. XPRD patterns for interconversions between compounds **5** and **6**. CSD codes XAXFUX and BAHGUN correspond to $[Cu(INA)_2(H_2O)_4]$ (**5**) and $[Cu(INA)_2]$ (**6**) respectively.