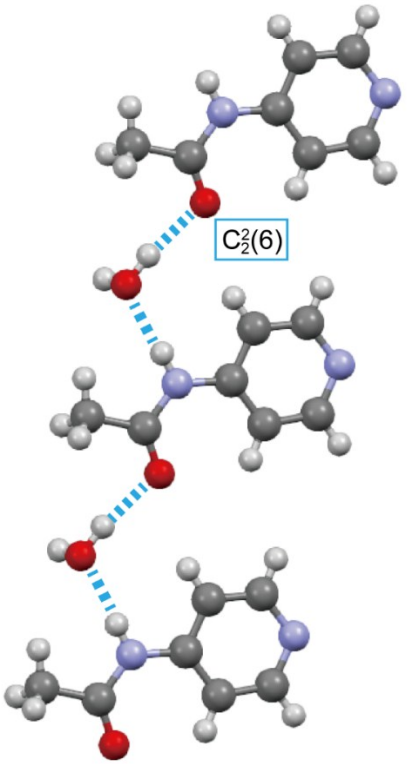

Figure S1 Chain hydrogen-bond motif of $C_2^2(6)$ between water and co-former molecules in **1H**.

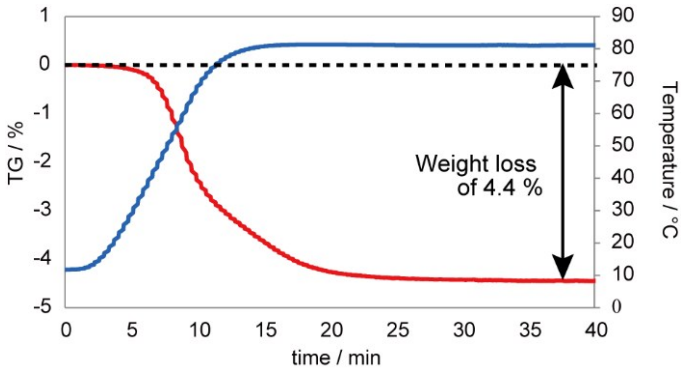

Figure S2 TG analysis data of the monohydrated co-crystal **1H**. The blue line represents temperature and the red line shows the change in sample weight. The weight loss of 4.4 wt.% agrees with the theoretical value of 4.6 wt.% for one water molecule.

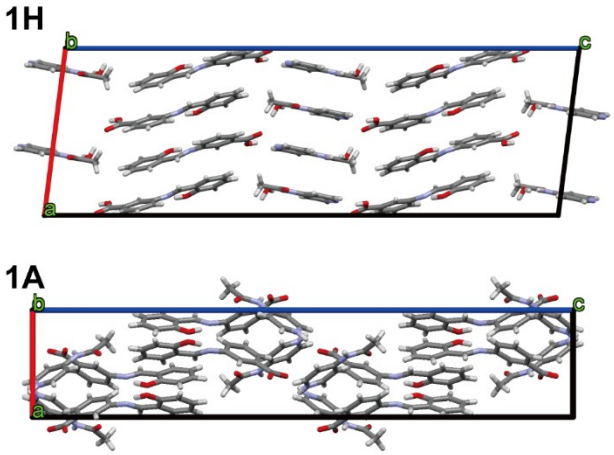

Figure S3 Crystal packing of **1H** (top) and **1A** (bottom).

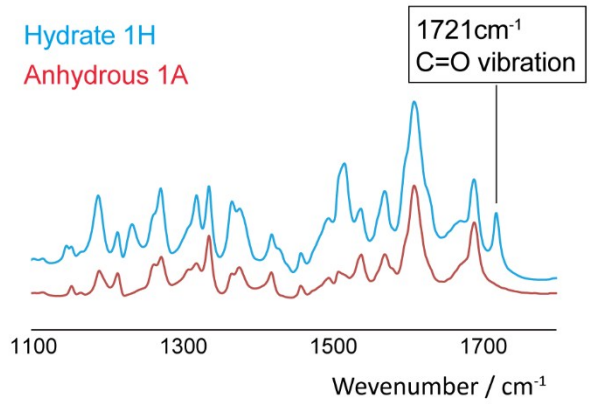

Figure S4 IR spectra of **1H** and **1A**. The absorption peak related to C=O vibration was observed in **1H**.