

Supporting Information

Crystal-to-Crystal Structural Transformation of Hydrogen-Bonding Molecular Crystals of (Imidazolium)(3-Hydroxy-2- quinoxalinecarboxylate) through H₂O Adsorption–Desorption

Yuya Yoshii, Ken-ichi Sakai, Norihisa Hoshino, Takashi Takeda, Shin-ichiro Noro, Takayoshi Nakamura, and Tomoyuki Akutagawa

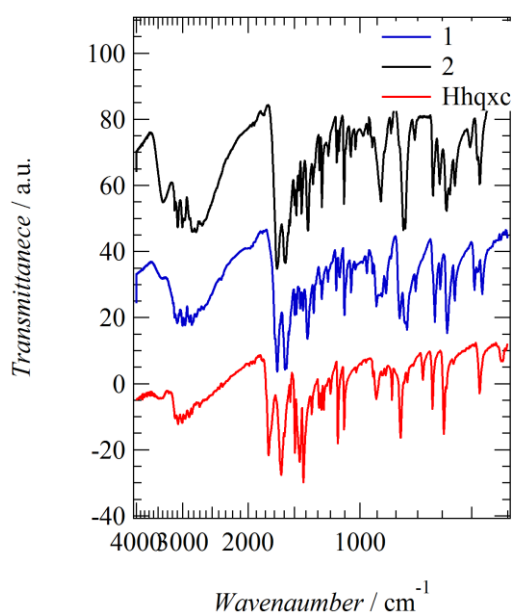


Figure S1. IR spectra of crystals **1** and **2** together with Hqxc on KBr pellets.

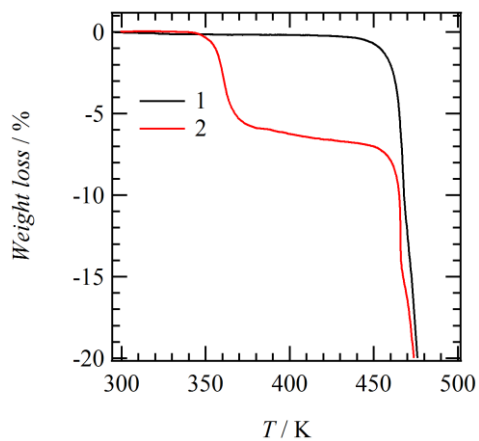


Figure S2. TG diagram of crystals **1** and **2**.

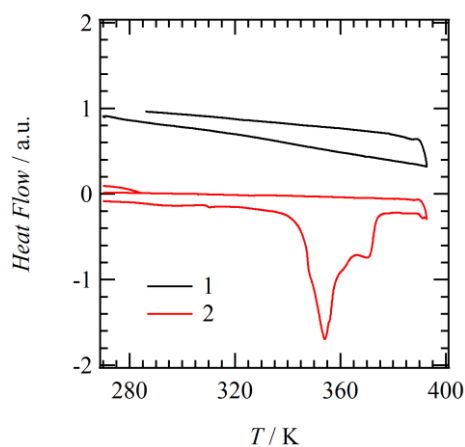


Figure S3. DSC diagram of crystals **1** and **2**.

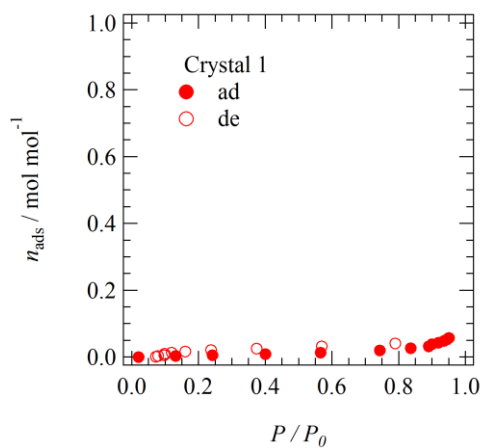


Figure S4. The adsorption-desorption isotherms of H₂O molecule in crystal **1** at 323 K. The number of H₂O molecules per (HIm⁺)(hqxc⁻) unit (n_{ads}) vs. relative pressure (P / P_0) of H₂O molecules.

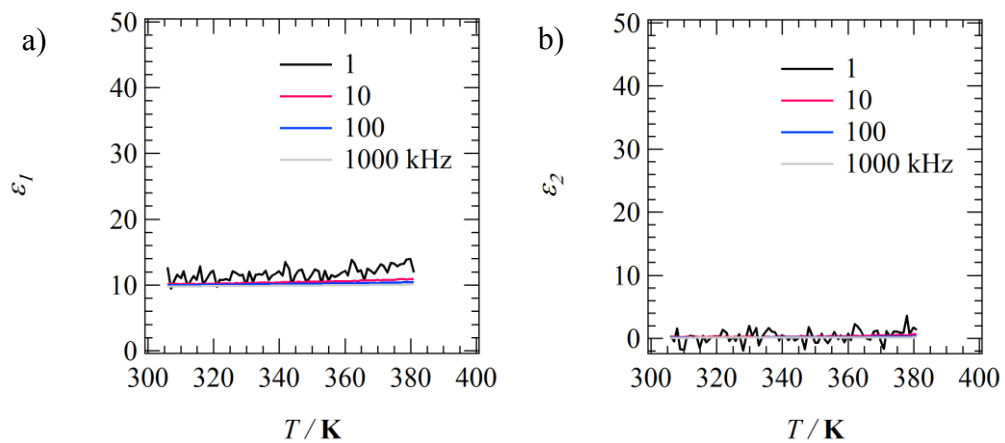


Figure S5. Temperature- and frequency-dependent a) real part ϵ_1 and b) imaginary part ϵ_2 of compressed pellet of crystal **1**.

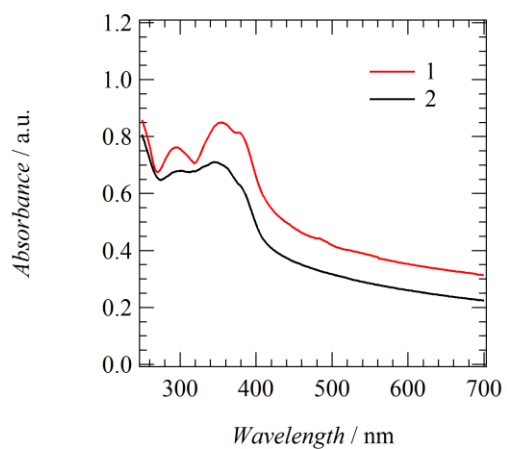


Figure S6. Solid state UV-vis spectra of crystals **1** and **2** on KBr pellets.

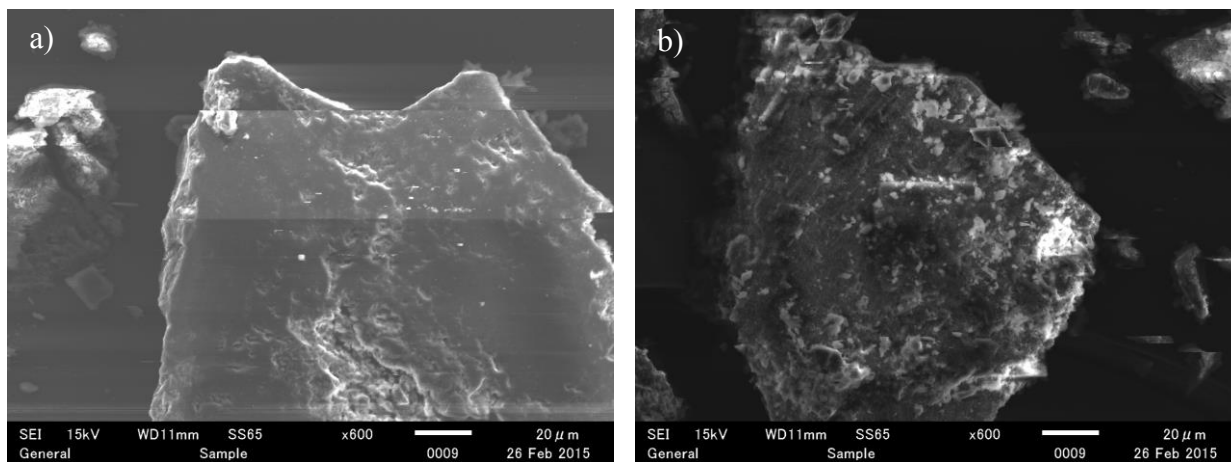


Figure S7. SEM images of grid crystal a) **1** and b) **2**. Both crystals were hold at 20 min at 373 K. Scale bar was 20 μm . The crystallinity of **1** was higher than that of crystal **2** after the thermal treatment at 373 K. Fine crystallites of unhydrated **2** were observed in Figure S7b.

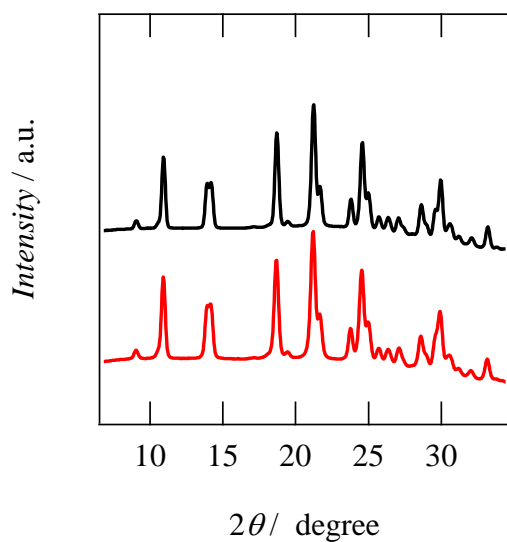


Figure S8. XRD profiles crystal **1**. The initial state of unhydrated **1** (red) and after the exposure to H₂O at 313 K. There was no changes in the XRD patterns, suggesting no structural transformation through the H₂O adsorption of crystals **1**.