## Supplementary information for

## Synthesis, Crystal Structures and Nonlinear Optical Properties of β-RbCdI<sub>3</sub>·H<sub>2</sub>O and CsCdI<sub>3</sub>·H<sub>2</sub>O

Qi Wu<sup>a\*</sup>, Xian Liu<sup>a</sup>, Siran Xu<sup>a</sup>, Hongbing Pi<sup>a</sup>, Xue Han<sup>a</sup>, Yang Liu<sup>a</sup>, Yanjun Li<sup>b\*</sup>

a. Hubei Normal Univ, Hubei Collaborat Innovat Ctr Rare Met Chem, Hubei Key Lab Pollutant Anal & Reuse Technol, Dept Chem, Huangshi, 435002, China.
b. Hubei Province Key Laboratory of Coal Conversion and New Carbon Materials, School of Chemistry and Chemical Engineering, Wuhan University of Science and Technology, Wuhan, 430081, China.

## Captions of the figures

**Figure S1.** X-ray diffraction powder patterns for  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O: Calculated and experimental

**Figure S2.** X-ray diffraction powder patterns for  $CsCdI_3 \cdot H_2O$ : Calculated and experimental.

**Figure S3.** ATR-FTIR spectrum for  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O and CsCdI<sub>3</sub>·H<sub>2</sub>O.

**Figure S4.** The UV-vis reflectance spectrum of  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O and CsCdI<sub>3</sub>·H<sub>2</sub>O.

**Figure S5**. Thermogravimetric analysis curve for  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O.

**Figure S6**. Thermogravimetric analysis curve for  $CsCdI_3 \cdot H_2O$ .



**Figure S1.** X-ray diffraction powder patterns for β-RbCdI<sub>3</sub>·H<sub>2</sub>O: Calculated and experimental. (The impurity peaks marked with red asterisks come from a very small amount of CdI<sub>2</sub>)



**Figure S2.** X-ray diffraction powder patterns for CsCdI<sub>3</sub>·H<sub>2</sub>O: Calculated and experimental.



**Figure S3**. ATR-FTIR spectrum for  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O and CsCdI<sub>3</sub>·H<sub>2</sub>O.



Figure S4. The UV-vis reflectance spectrum of  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O and CsCdI<sub>3</sub>·H<sub>2</sub>O.



**Figure S5.** The TGA-DSC spectra for  $\beta$ -RbCdI<sub>3</sub>·H<sub>2</sub>O.



**Figure S6.** The TGA-DSC spectra for  $CsCdI_3 \cdot H_2O$ .