

Novel isomorphism of two hexagonal non-centrosymmetric hybrid crystals of $M(en)_3Ag_2I_4$ ($M =$ transition metal Mn^{2+} or main-group metal Mg^{2+} ; en = ethylenediamine)

Xin Chen,^a Zhi-Yuan Yao,^a Chen Xue,^a Zhu-Xi Yang,^a Jian-Lan Liu^a and Xiao-Ming Ren^{*a,b,c}

^aState Key Laboratory of Materials-Oriented Chemical Engineering and College of Chemistry & Molecular Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

^bCollege of Materials Science and Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

^cState Key Laboratory of Coordination Chemistry, Nanjing University 210093, P. R. China

Tel.: +86 25 58139476

Fax: +86 25 58139481

Email: xmren@njtech.edu.cn

Contents

Fig. S1 (a, b) Photos of crystals of **2** (c) An asymmetric unit in **2** with non-hydrogen atom labeling, where the ellipsoids are drawn at the 50% probability level (d) $\text{Mg}(\text{en})_3^{2+}$ coordination polyhedron with the symmetry of D_3 point group.

Fig. S2 Packing diagrams, which shows hexagonal channels built from AgI_4 tetrahedra and $\text{Mn}(\text{en})_3^{2+}$ polyhedra residual in the channels viewed along (a) c -axis (b) a -axis directions in **2**.

Fig. S3 (a) Experimental and simulated PXRD patterns and (b) TG plot of **2**.

Fig. S4 IR spectra of **1** and **2**.

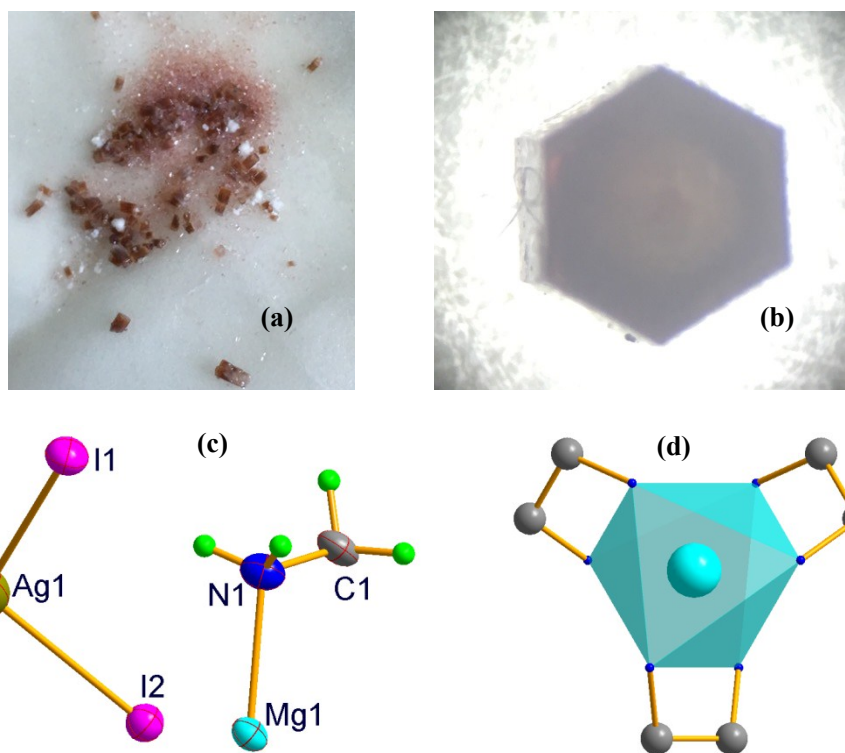


Fig. S1 (a, b) Photos of crystals of **2** (c) An asymmetric unit in **2** with non-hydrogen atom labeling, where the ellipsoids are drawn at the 50% probability level (d) $\text{Mg}(\text{en})_3^{2+}$ coordination polyhedron with the symmetry of D_3 point group.

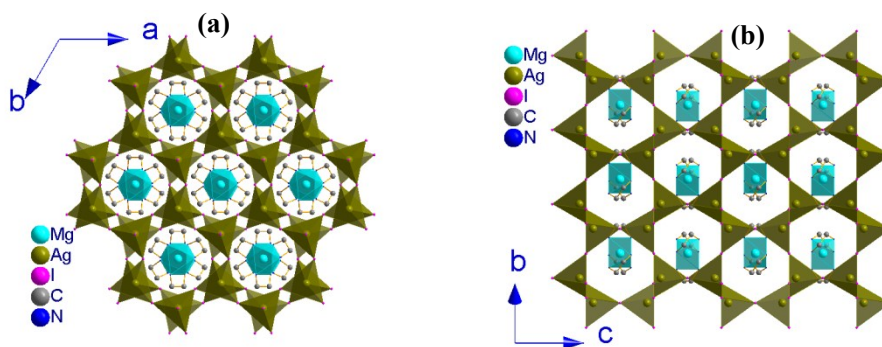


Fig. S2 Packing diagrams, which shows hexagonal channels built from AgI_4 tetrahedra and $\text{Mn}(\text{en})_3^{2+}$ polyhedra residual in the channels viewed along (a) c -axis (b) a -axis directions in **2**.

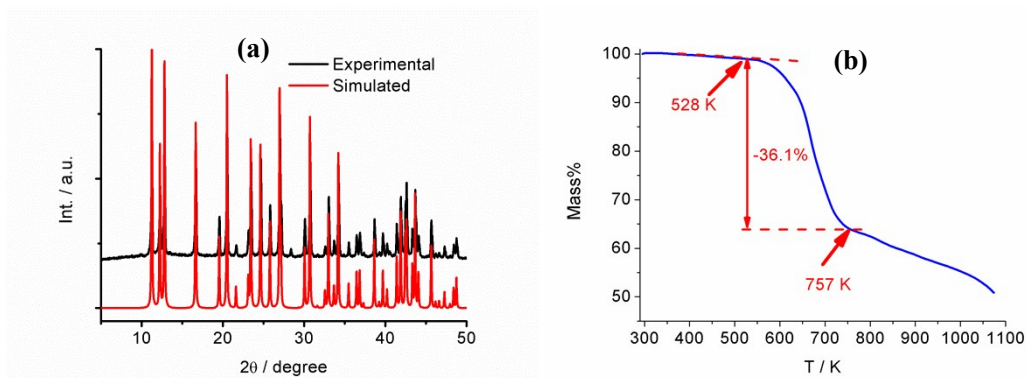


Fig. S3 (a) Experimental and simulated PXRD patterns and (b) TG plot of **2**.

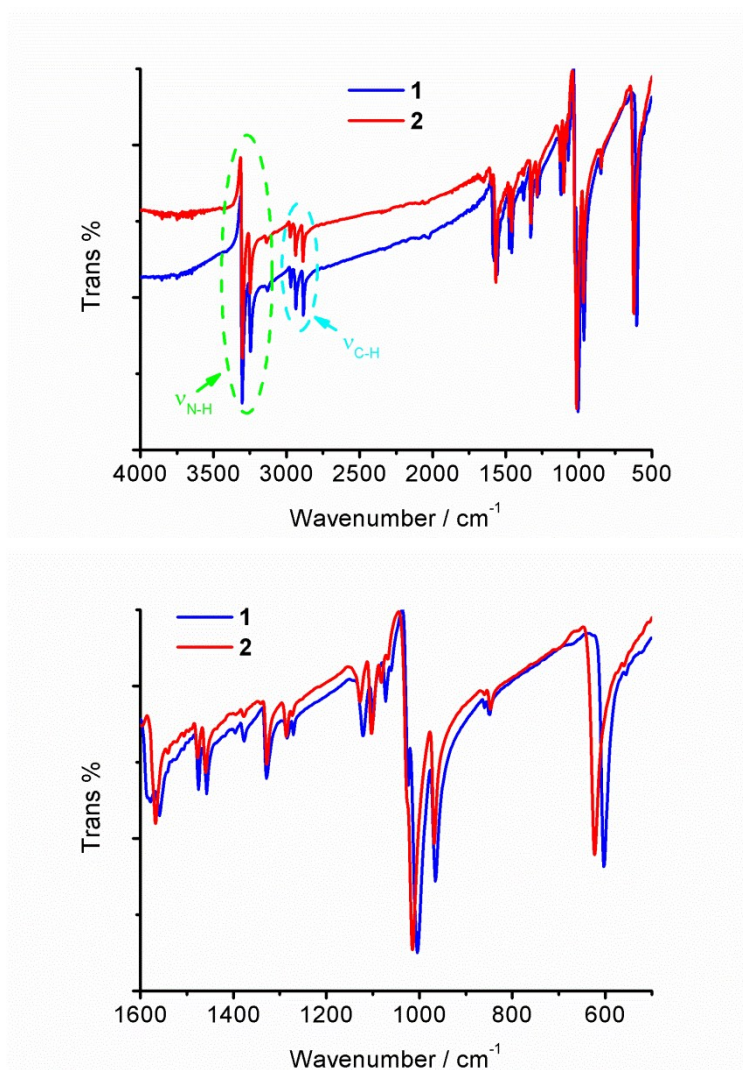


Fig. S4 IR spectra of **1** and **2**.