

Supporting information

1,4-Diazabicyclo[2.2.2]octane-based disalts showing non-centrosymmetric structures and phase transition behaviors

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Table S1 Fractional coordinates (10^4) and equivalent temperature factors ($\text{\AA}^2 \cdot 10^3$) for ClO_4^- (233 K).

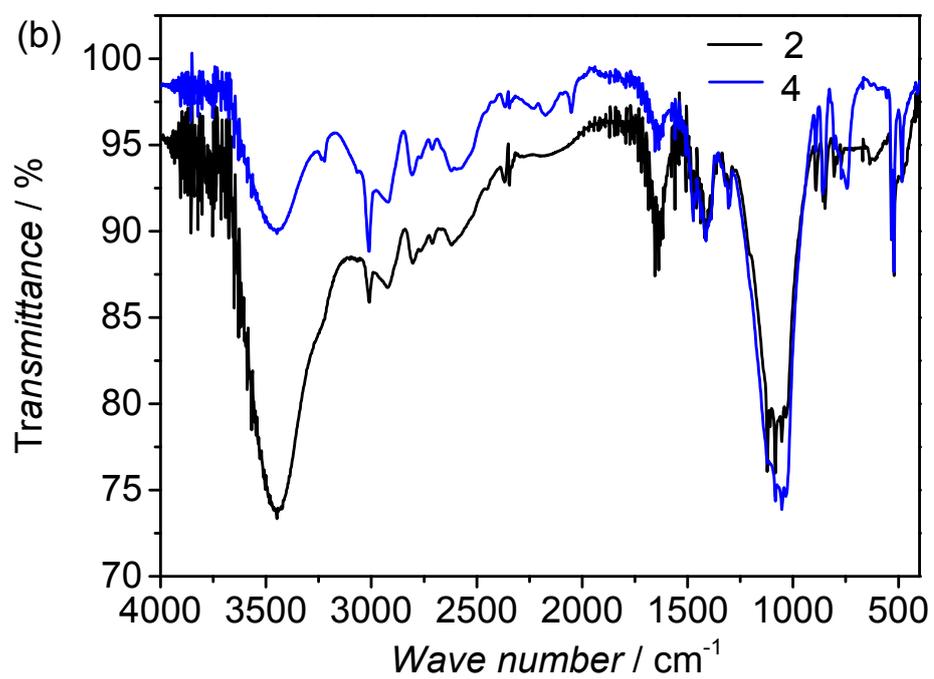
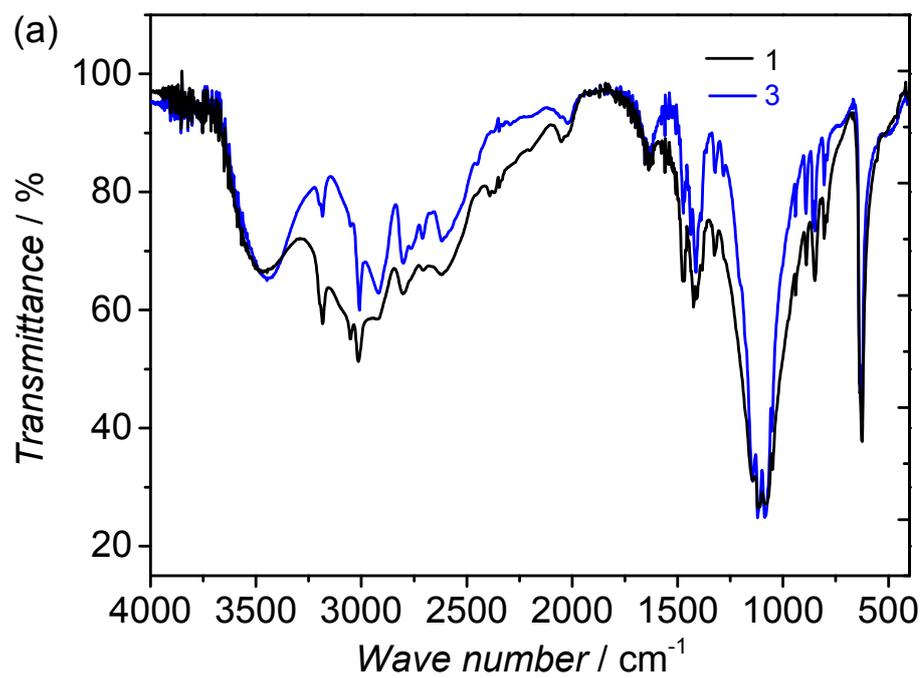


Figure S1 IR spectra of (a) **1** and **3** and (b) **2** and **4**.

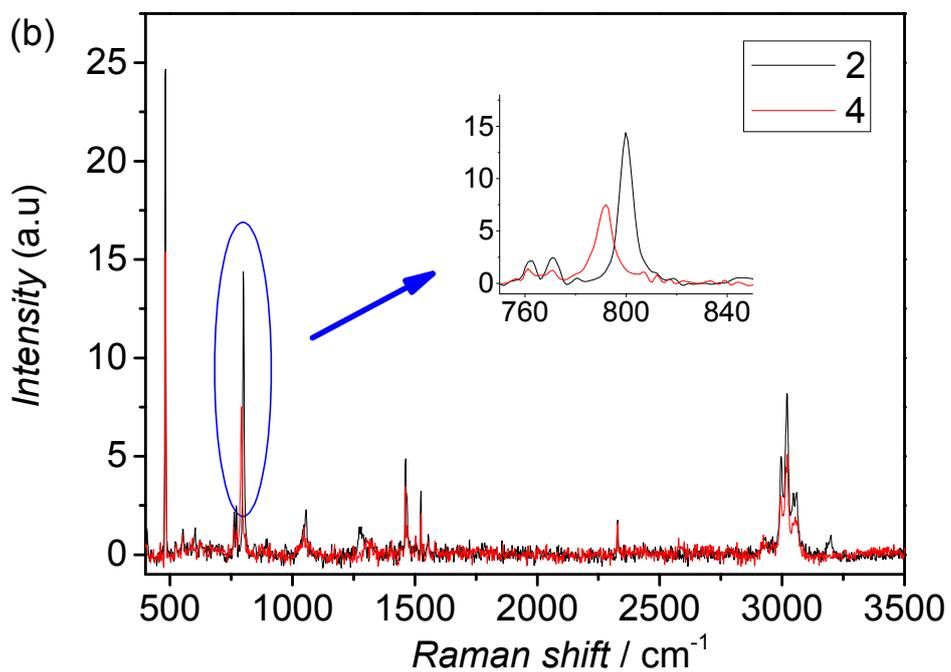
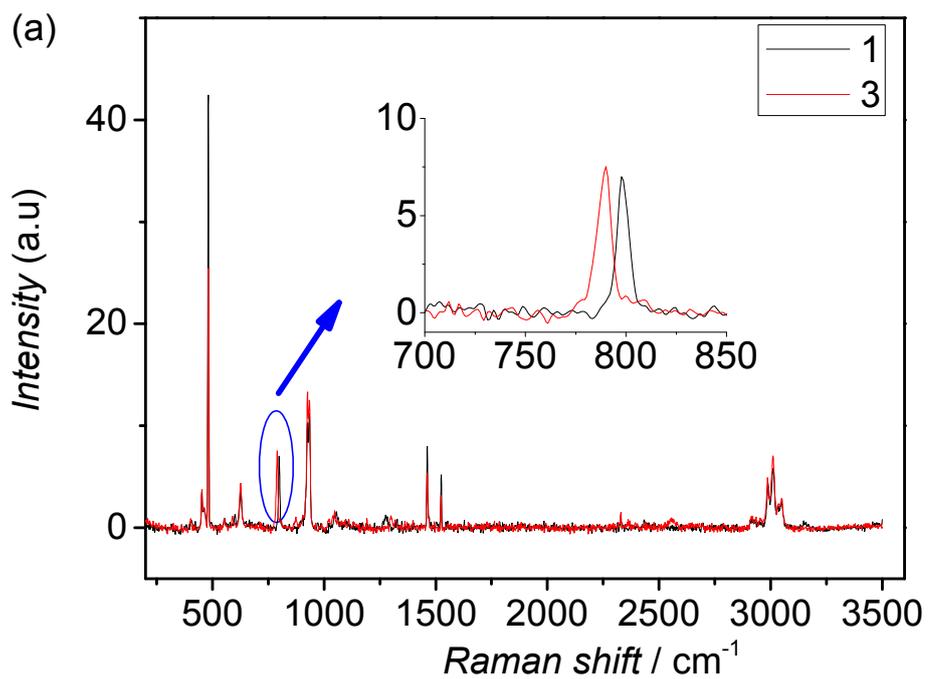


Figure S2 Raman spectra of (a) 1 and 3 and (b) 2 and 4.

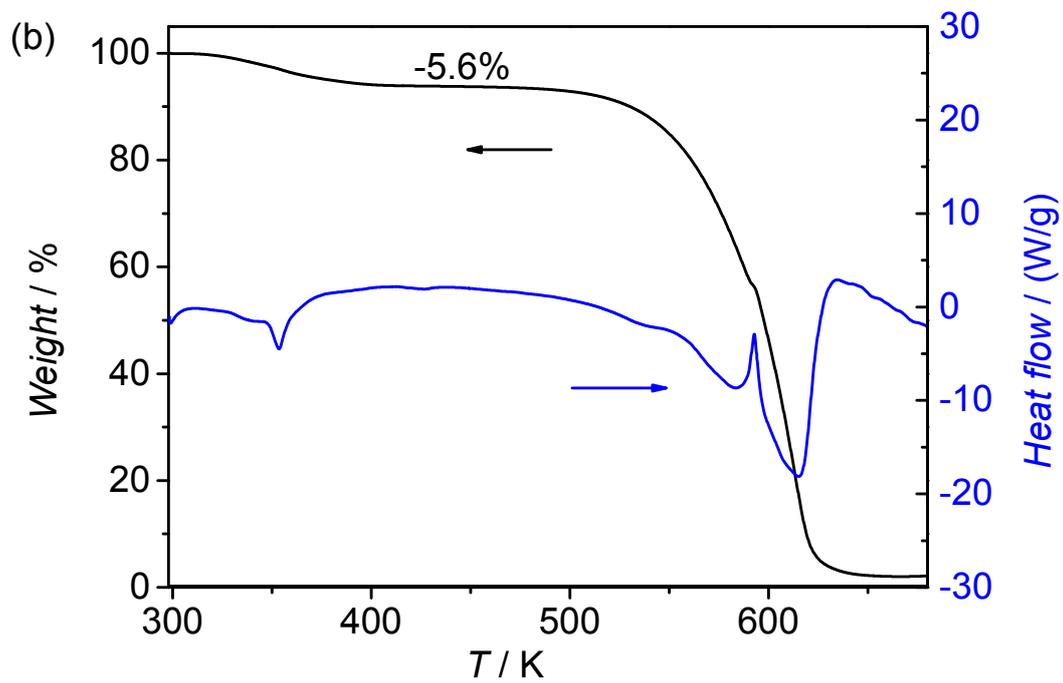
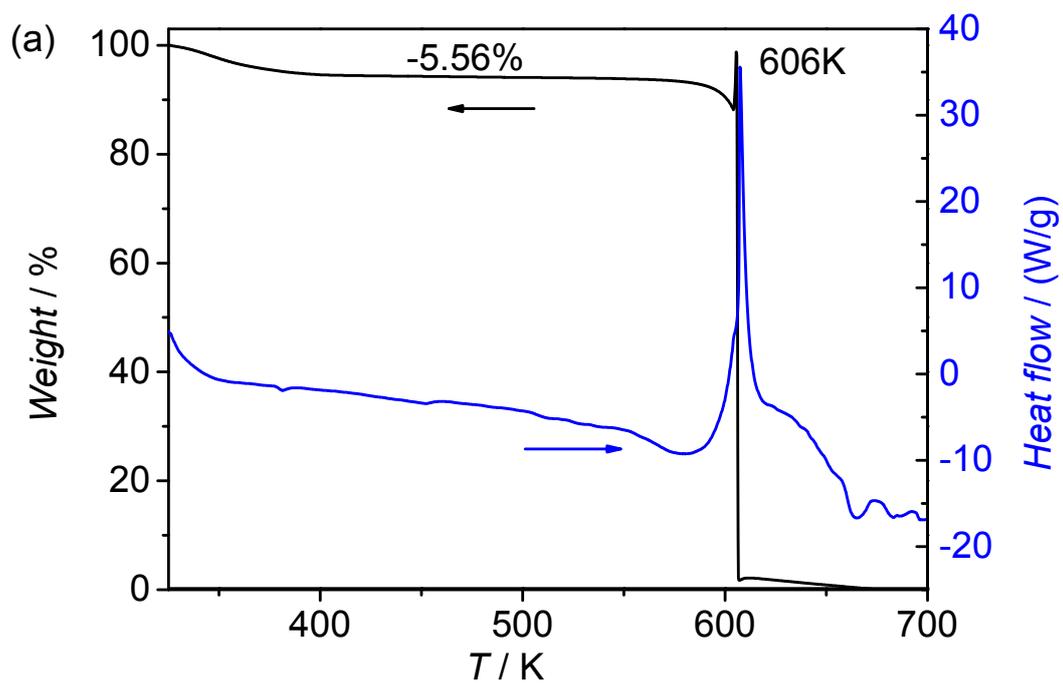
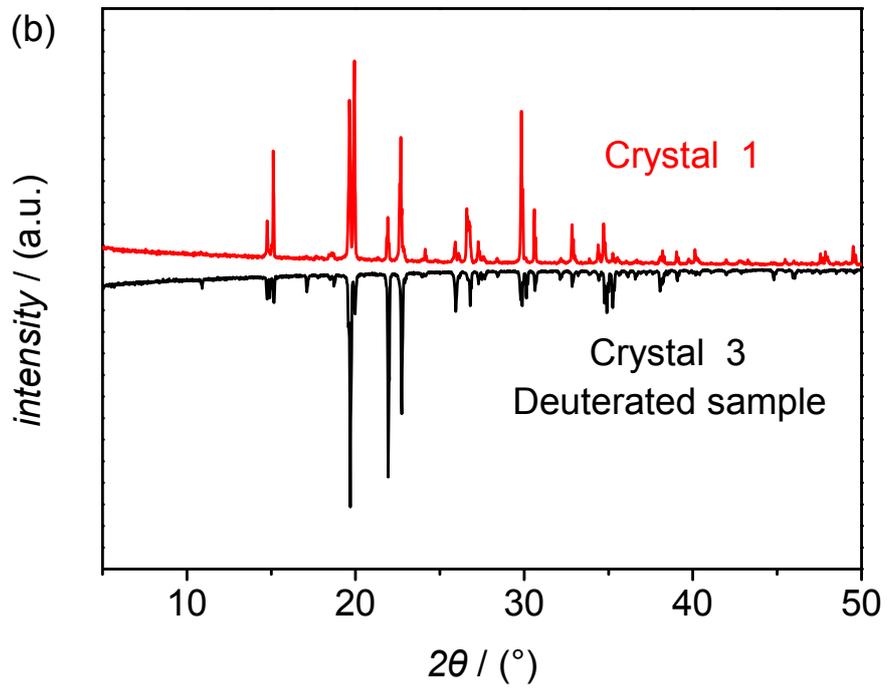
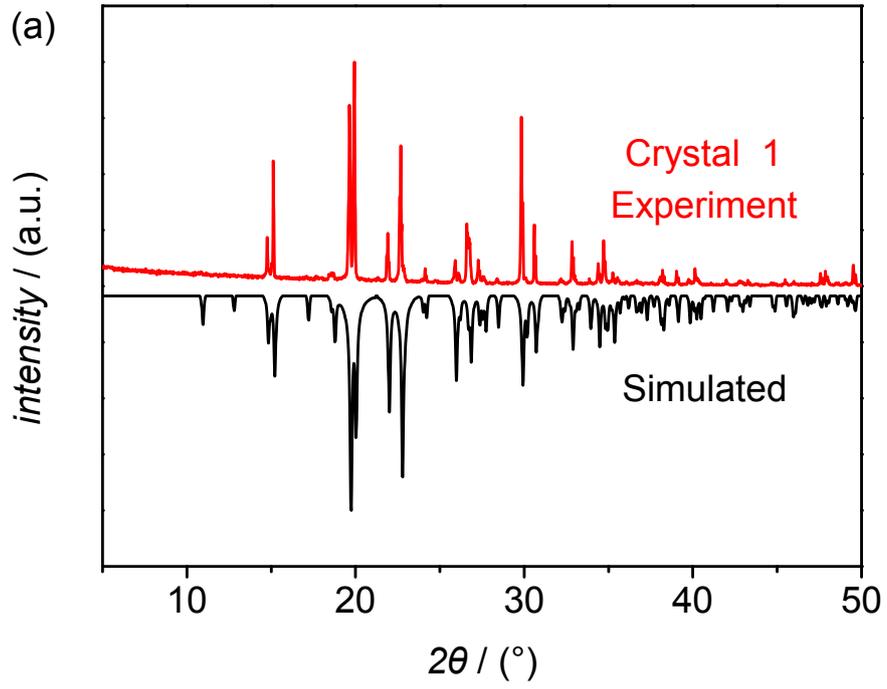


Figure S3 Thermogravimetric analysis for (a) 1 and (b) 2.



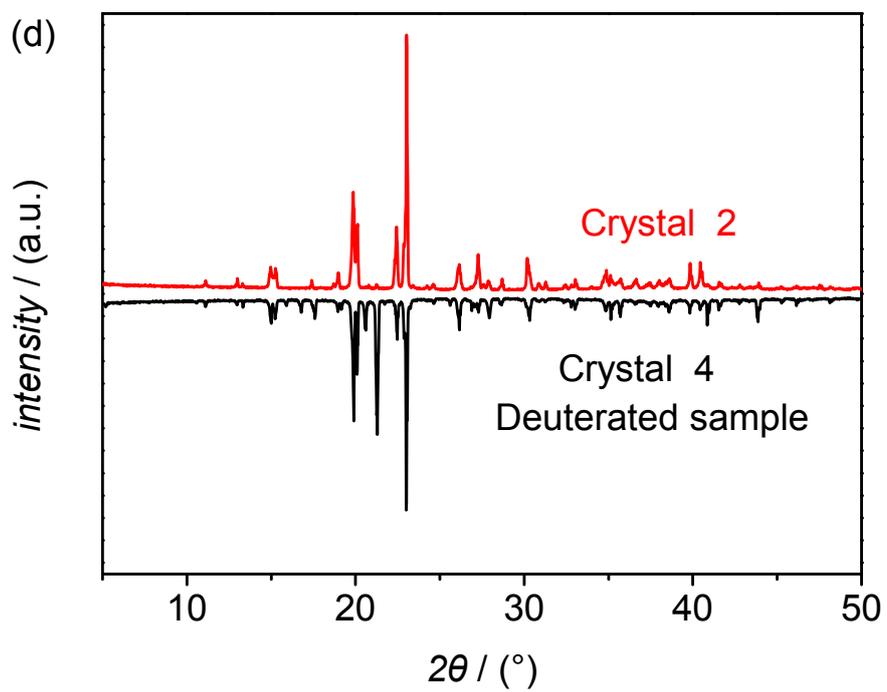
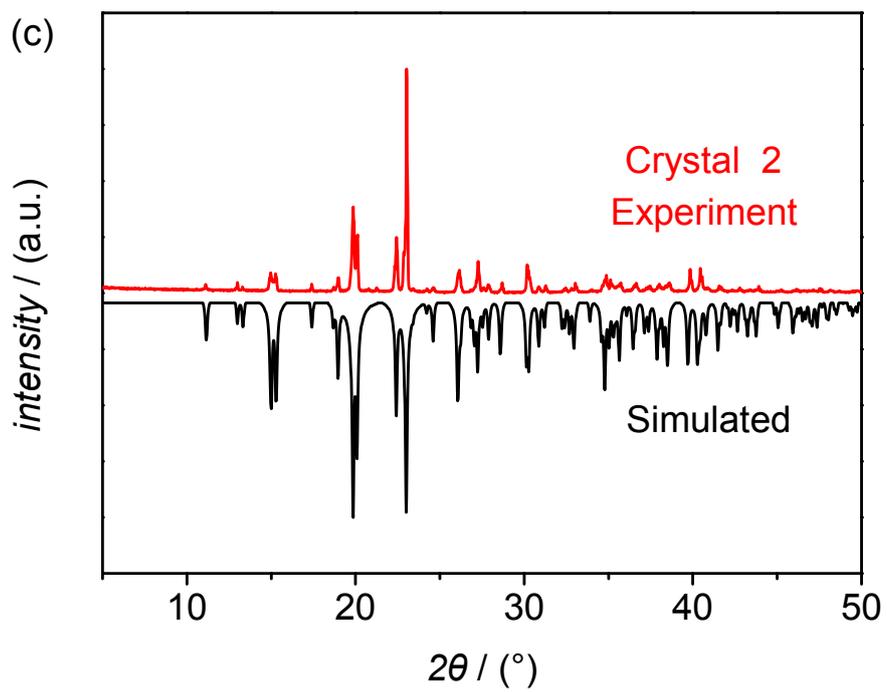
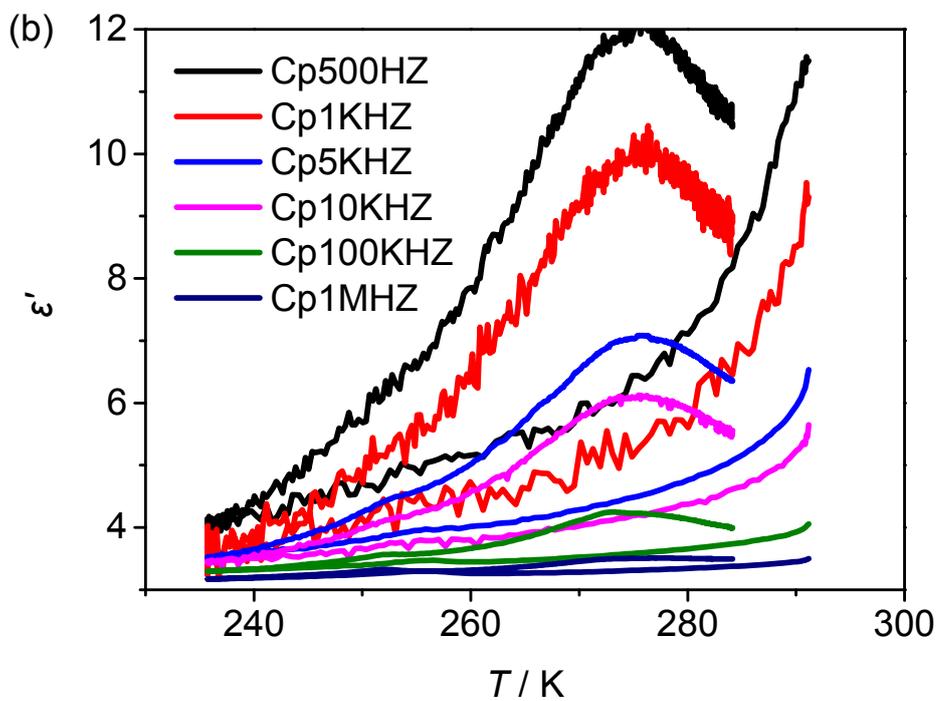
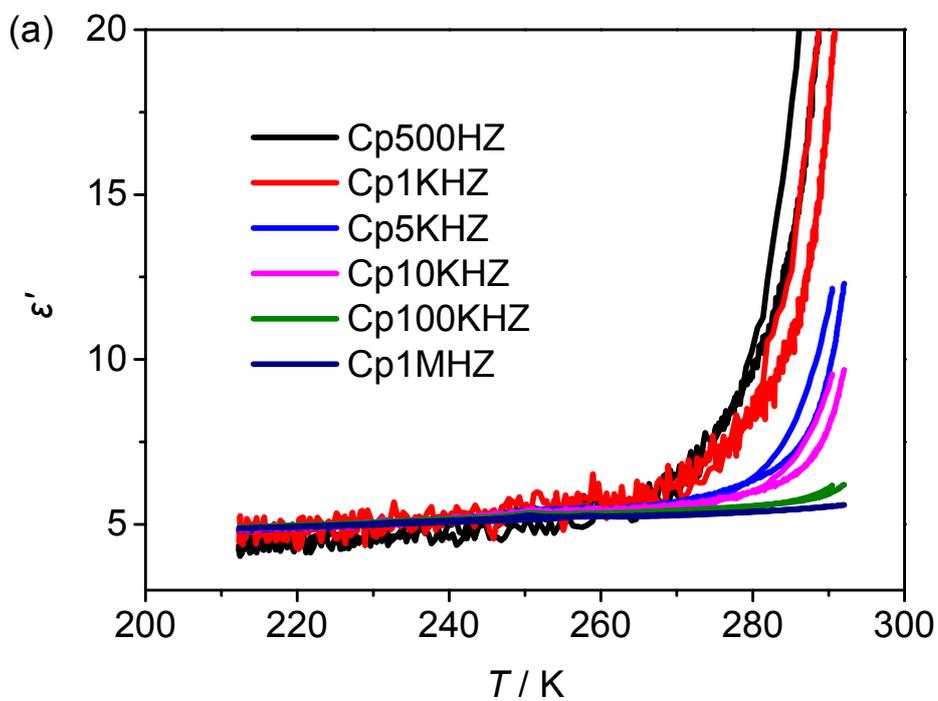


Figure S4 PXR D of 1–4.



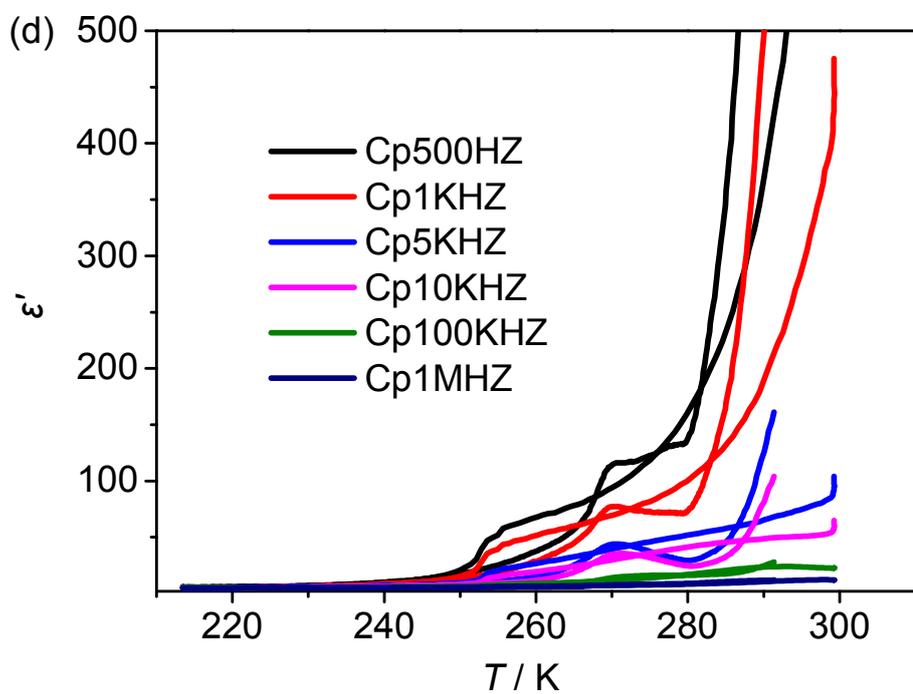
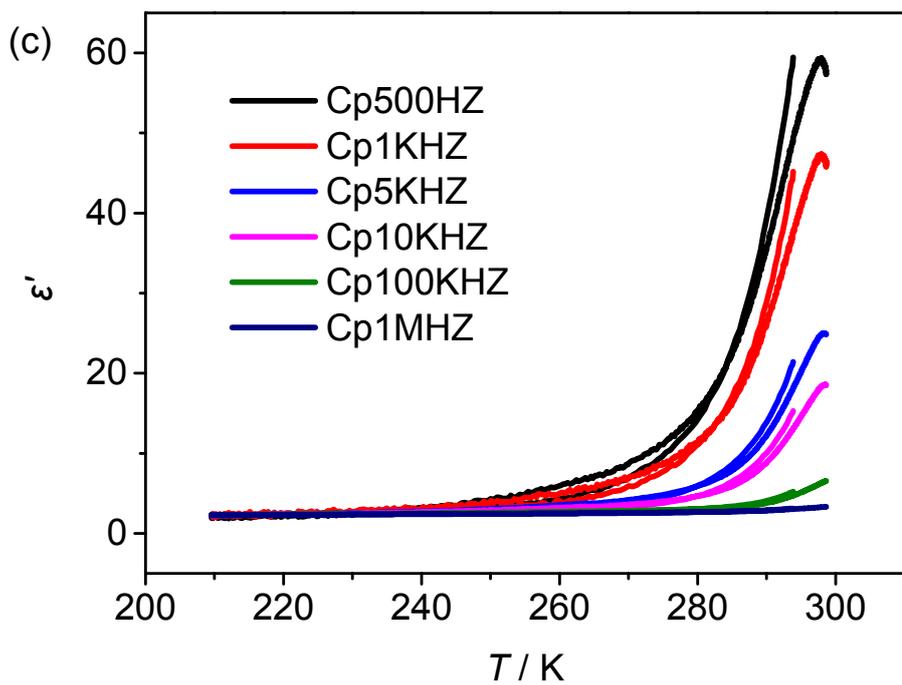


Figure S5 Dielectric spectra of 1–4.

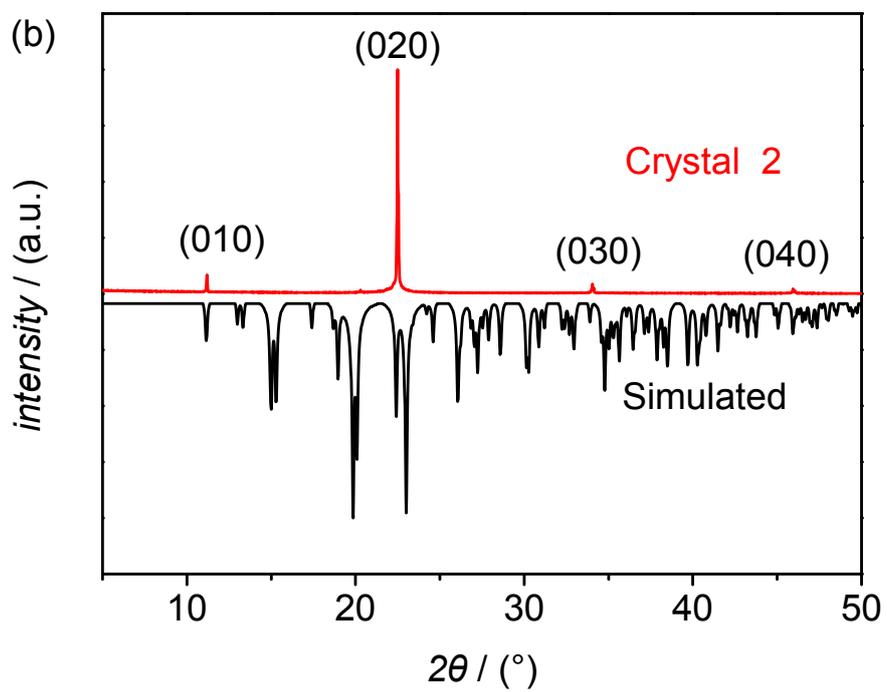
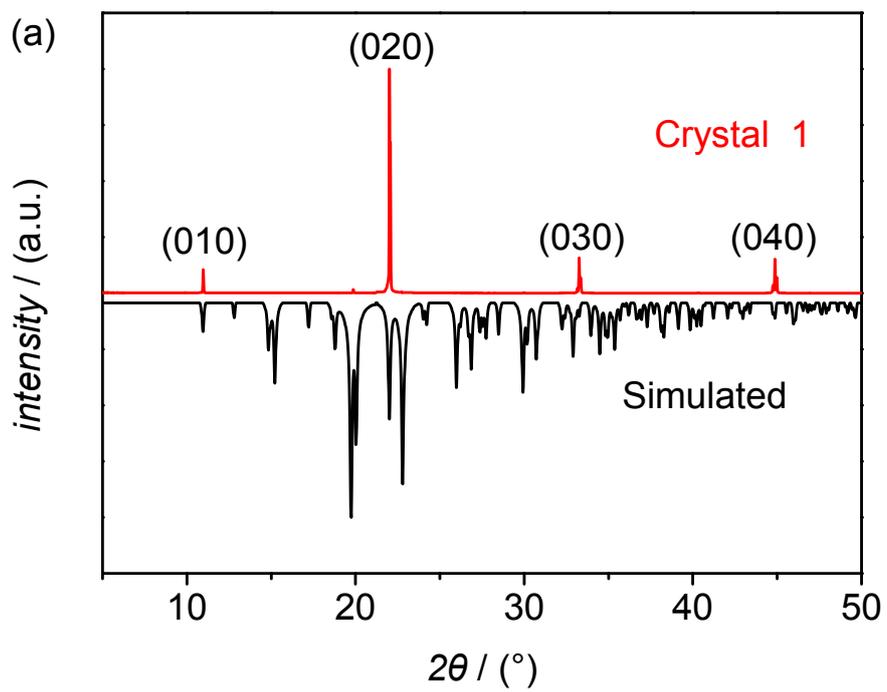
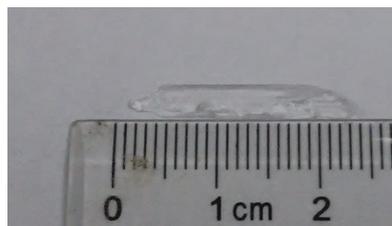


Figure S6 Crystal orientations of 1 and 2.



Crystal 1



Crystal 2

Figure S7 Crystal morphologies of **1** and **2**. The largest face of the crystals is the *b* face.

Table S1 Fractional coordinates (10^4) and equivalent temperature factors ($\text{\AA}^2 \cdot 10^3$) for ClO_4^- (233 K). U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

ATOM	X	Y	Z	U_{eq}
O1	8795(3)	1997(5)	3548(5)	49(1)
O2	7392(4)	3586(5)	4105(5)	61(1)
O3	7482(4)	2498(6)	2256(4)	51(1)
O4	7235(3)	728(5)	3812(4)	45(1)
O5	8655(5)	8633(7)	2244(4)	82(2)
O6	9042(4)	7885(6)	424(4)	51(1)
O7	8695(6)	5838(7)	1712(6)	90(2)
O8	10145(5)	7333(9)	1903(5)	85(2)