

Supporting information for:

Crystal Structures, Phase Transitions, and Switchable Dielectric Behaviors: Comparison of a Series of N-heterocyclic Ammonium Perchlorates

Ping-Ping Shi, Qiong Ye*, Qiang Li, Hui-Ting Wang, Da-Wei Fu, Yi Zhang and Ren-Gen Xiong*

Ordered Matter Science Research Center, Southeast University, Nanjing 211189, P. R.

China

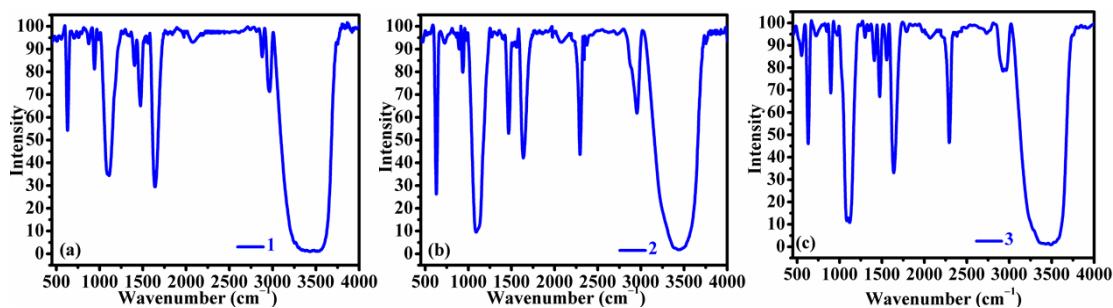


Figure S1. IR spectra of (a) [PMpip][ClO₄] (**1**), (b) [CMpip][ClO₄] (**2**), and (c) [CMmor][ClO₄] (**3**) obtained at room temperature. The intense peaks at approximately 3500 cm⁻¹ are due to the moisture of the KBr.

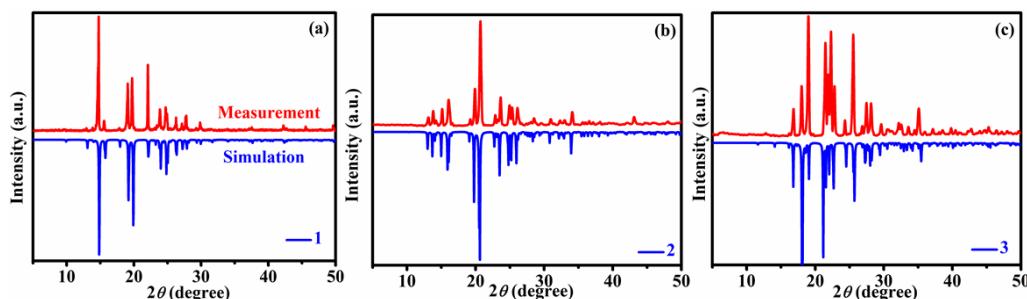


Figure S2. PXRD patterns of (a) [PMpip][ClO₄] (**1**), (b) [CMpip][ClO₄] (**2**), and (c)

[CMmor][ClO₄] (**3**) recorded at 298 K (red line), in good agreement with the simulated data based on the crystal structures (blue line).

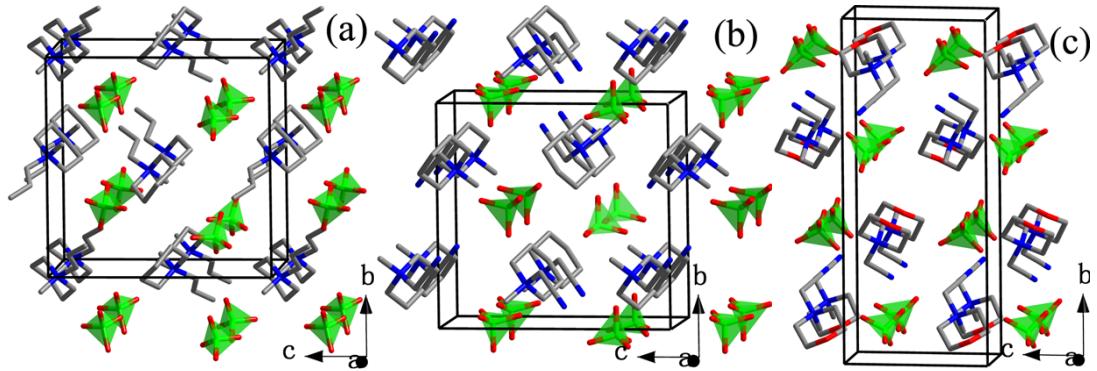


Figure S3. Packing diagrams of (a) [PMpip][ClO₄] (**1**), (b) [CMpip][ClO₄] (**2**) and (c) [CMmor][ClO₄] (**3**) viewed down the *a* axis.

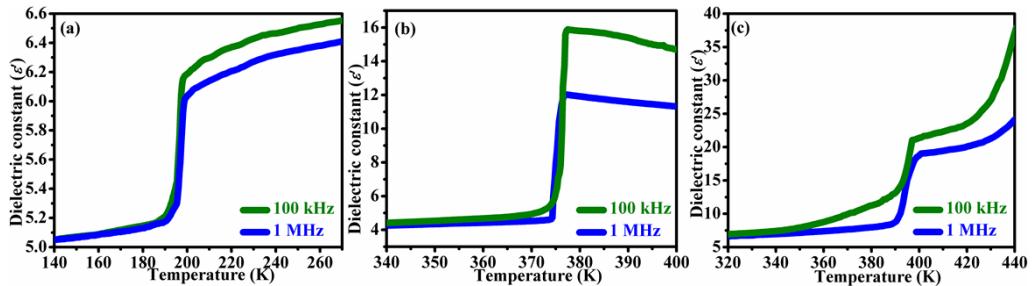


Figure S4. Temperature dependences of the real parts of dielectric constants (ϵ') for (a) [PMpip][ClO₄] (**1**), (b) [CMpip][ClO₄] (**2**) and (c) [CMmor][ClO₄] (**3**), measured in the cooling modes at 100 kHz and 1 MHz, respectively.

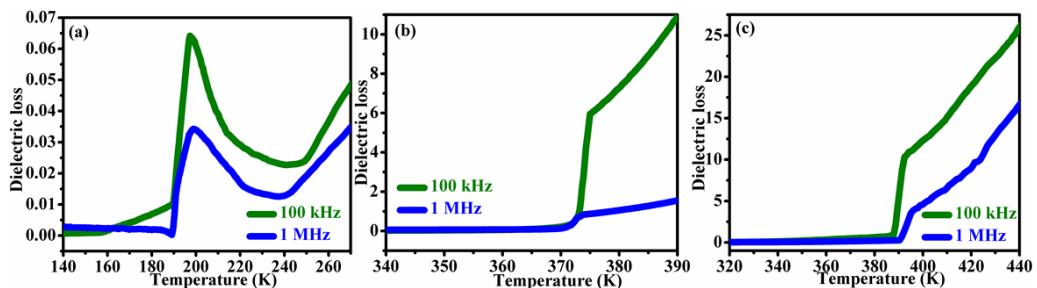


Figure S5. Temperature dependences of the dielectric losses for (a) [PMpip][ClO₄]

(1), (b) [CMpip][ClO₄] (2) and (c) [CMmor][ClO₄] (3), measured in the cooling modes at 100 kHz and 1 MHz, respectively.

Table S1. Equivalent isotropic displacement parameters (U_{iso}) for [PMpip][ClO₄]

(1), [CMpip][ClO₄] (2) and [CMmor][ClO₄] (3)

	1		2		3
Atom	U _{iso} (Å ²)	Atom	U _{iso} (Å ²)	Atom	U _{iso} (Å ²)
Cl1	0.0729(2)	Cl1	0.0481(4)	Cl1	0.0436(3)
O1	0.194(2)	O1	0.1027(14)	O1	0.1051(12)
O2	0.272(2)	O2	0.0902(12)	O2	0.0991(11)
O3	0.182(2)	O3	0.0951(13)	O3	0.0692(7)
O4	0.278(2)	O4	0.1038(14)	O4	0.0967(10)
N1	0.0849(10)	N1	0.0342(7)	N1	0.0309(4)
C1	0.1310(17)	N2	0.0705(11)	N2	0.0899(12)
C2	0.163(2)	C1	0.0402(8)	O5	0.0529(6)
C3	0.1404(19)	C2	0.0546(10)	C1	0.0398(6)
C4	0.1090(15)	C3	0.0548(10)	C2	0.0503(7)
C5	0.1076(16)	C4	0.0458(9)	C3	0.0509(7)
C6	0.1154(17)	C5	0.0601(11)	C4	0.0454(6)
C7	0.180(3)	C6	0.0435(8)	C5	0.0465(6)
C8	0.174(2)	C7	0.0488(9)	C6	0.0456(6)
C9	0.151(2)	C8	0.0600(11)	C7	0.0569(8)