ESI

Two quasi-spherical molecules [1,4-diazabicyclo[3.2.2]nonane]X (X = ClO_4, ReO_4) exhibit switchable phase transition, dielectric and second harmonic generation properties

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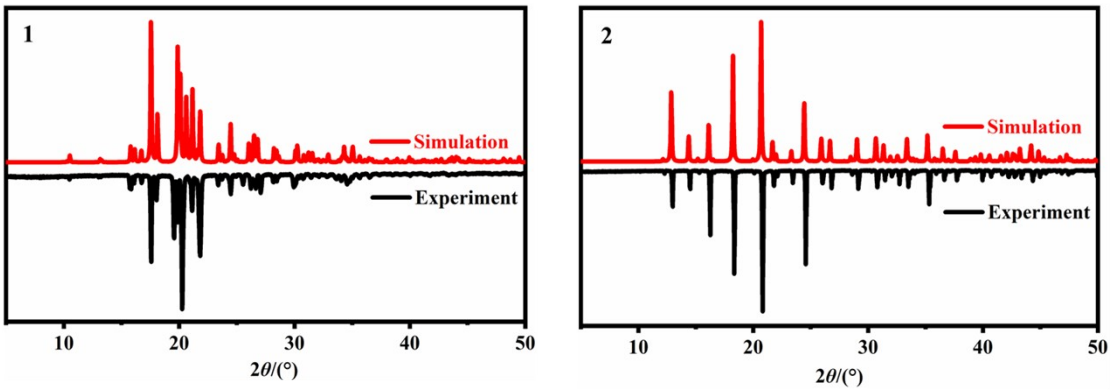

Fig. S1 The powder X-ray diffraction patterns of compounds **1** and **2** with the simulated one in red and the experimental one in black.

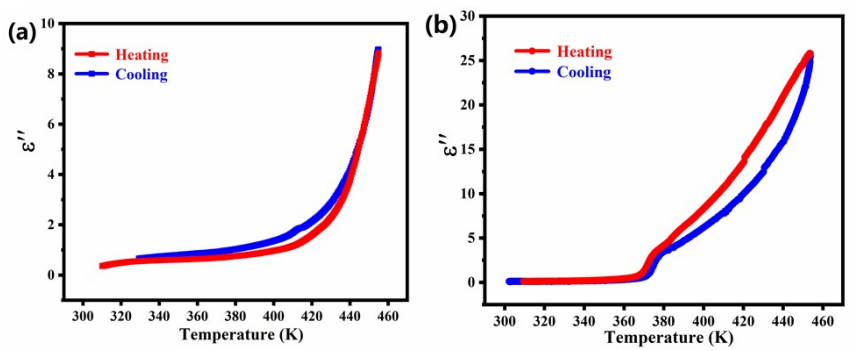

Fig. S2 Temperature dependences of the imaginary part of (ε'') of the dielectric permittivity of **1** at 1 MHz upon heating and cooling.

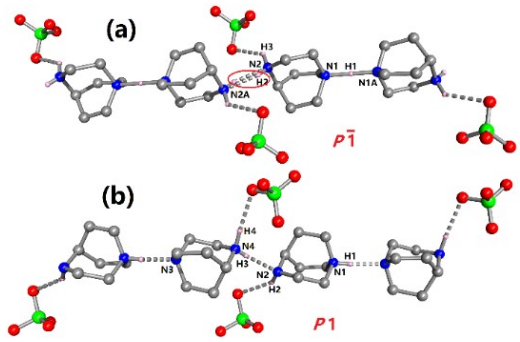

Fig. S3 The crystal structure of **1** solved in (a) $P\bar{1}$ and (b) *P*1 space groups at LTP.

Tab. S1. Crystal data and structure refinements for **1** at 298 K and 438 K.

Formula	$C_7H_{15}ClN_2O_4$	
Temperature	298 K	438 K
Formula Mass	226.66	778.6
Crystal system	triclinic	cubic
Space group	*P*1	$Pm\bar{3}m$
a (Å)	6.7331(3)	6.3959(10)
b (Å)	8.6522(3)	6.3959(10)

c (Å)	8.8761(3)	6.3959(10)
V (Å)^3	500.46(3)	261.64(12)
Z	2	1
D_{calc} (g·cm^{-3})	1.504	4.942
F (000)	240	388.9
θ_{max}	24.99	31.41
μ(Mo Ka,mm^{-1})	0.374	0.514
Flack parameter	0.27(13)	
Total no. of reflns.	5249	1524
No. of unique reflns.	2899[$R_{(int)}$ = 0.0218]	119[$R_{(int)}$ = 0.3041]
No. of variables	269	18
R_1, wR_2 (obsd data)	0.0630, 0.1656	0.2769, 0.5924
R_1, wR_2 (all data)	0.0718, 0.1756	0.4057, 0.6276
GOF, S	1.257	2.523
Max./min. peak (e. Å^{-3})	0.356, -0.276	1.78, -1.69

Tab. S2 Hydrogen bond lengths [Å] and angles [°] of **1** at 298 K.

D-H…A	D-H [Å]	H…A[Å]	D…A[Å]	D-H…A[°]
N1-H1…N3^1	0.91(2)	1.82(2)	2.726(3)	176.1(16)

N2-H2…O2	0.92(3)	2.60(4)	3.296(4)	133(3)
N2-H2…O3	0.92(3)	2.29(3)	3.059(3)	141(3)
N4-H4…O7[2]	0.997(17)	2.222(17)	3.217(5)	176.9(14)
N4-H4…O8[2]	0.997(17)	2.455(15)	3.101(3)	122.0(12)
N4-H3…N2[3]	0.69(3)	2.09(3)	2.772(3)	170(3)

For **1** at 298K: [1]*x*, *y*, 1+*z*; [2]-1+*x*, -1+*y*, *z*; [3]*x*, -1+*y*, *z*

Tab. S3. Crystal data and structure refinements for **2** at 297 K and 413 K.

Formula	$C_7H_{15}N_2O_4Re$	
Temperature	297 K	413 K
Crystal system	orthorhombic	tetragonal
Space group	*Pccn*	*P*-42*m*
a (Å)	10.9820(4)	6.8907(5)
b (Å)	13.7336(5)	6.8907(5)
c (Å)	13.7637(6)	5.8523(10)
V (Å)^3	2075.87(14)	277.88(6)
Z	8	1
D_{calc} (g·cm^{-3})	2.415	2.500
F (000)	1424	191
θ_{max}	31.74	31.46
μ(Mo Ka,mm^{-1})	11.7	10.937

Total no. of reflns.	13007	1960
No. of unique reflns.	1834 [$R_{(int)}$ = 0.0343]	449 [$R_{(int)}$ = 0.0234]
No. of variables	136	15
R_1, wR_2 (obsd data)	0.0191, 0.0599	0.0425, 0.1033
R_1, wR_2 (all data)	0.0270, 0.0652	0.0914, 0.1157
GOF, S	1.006	1.176
Max./min. peak (e. Å^{-3})	0.704, -0.466	0.368, -0.548

Tab. S4 Hydrogen bond lengths [Å] and angles [°] of **2** at 297 K.

D-H…A	D-H [Å]	H…A[Å]	D…A[Å]	D-H…A[°]
N2-H1…N1[1]	1.04(4)	1.80(4)	2.831(3)	178(5)
N2-H2…O1	0.92(4)	1.99(4)	2.876(4)	161(3)

For **2** at 297K: [1]-1/2+*x*, -*y*, 1/2-*z*.