

Supporting Information

A ferroelastic molecular rotator [(Me₂N(CH₂)₂NH₃)(18-crown-6)]triflate with dual dielectric switches

Meng-Meng Lun,^a Tie Zhang,^a Chang-Yuan Su,^a Jie Li,^a Zhi-Xu Zhang,^{*a} Da-Wei Fu,^{*a} Hai-Feng Lu^{*b}

^a Ordered Matter Science Research Center, Jiangsu Key Laboratory for Science and Applications of Molecular Ferroelectrics, Southeast University, Nanjing, 211189, P. R. China. (E-mail: dawei@seu.edu.cn, zhixu@seu.edu.cn)

^b Institute for Science and Applications of Molecular Ferroelectrics, Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Zhejiang Normal University, Jinhua, 321004, P.R. China. (E-mail: luhaifeng@zjnu.edu.cn)

EXPERIMENTAL MEASUREMENT METHODS

Single-crystal X-ray Diffraction (SXRD). The crystallographic structures of compounds were identified by using a Rigaku single-crystal X-ray diffractometer with Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). The structures of samples were determined by direct methods and refined by the full matrix method through the SHELXTL software package. All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms which were generated geometrically possessed isotropic displacement parameters. The crystallographic information and structure refinement of compounds are summarized in Table S2. The selected bond lengths and angles, hydrogen bonds of compounds are displayed in Table S3 and S4. Moreover, the crystallographic structures of compounds have been deposited at the Cambridge Crystallographic Data Center (CCDC) (deposition numbers: 2143582-2143585 and 2153009) and can be obtained free of charge from the CCDC *via* www.ccdc.cam.ac.uk/getstructures.

Powder X-ray Diffraction (PXRD). The powder X-ray diffraction patterns of microcrystalline compounds were characterized by using a Rigaku D-MAX diffraction

system using Cu- α radiation in the 2θ range from 5° to 50° with a step size of 0.02° at 298 K. Simulated powder patterns of samples were calculated by Mercury software package using the crystallographic information file from the single-crystal X-ray experiment.

Infrared (IR) Spectrometry. The IR spectra of compounds were performed at room temperature using a Shimadzu IR-60 spectrometer in the range from 4000 to 400 cm^{-1} .

Dielectric. For dielectric characterization, these crystals were ground to become powders, and then pressed into a plate with 0.5 mm thickness. Both plate surfaces were coated with silver paste and dried in an oven at 333 K for 5 h. The plate was then used as an electrode to record the curve of temperature-dependent dielectric permittivity ε by a Tonghui TH2828A Precision LCR meter with an AC voltage of 1 V.

The complex dielectric permittivity ε ($\varepsilon = \varepsilon' - \varepsilon''$), where ε' is the real part, and ε'' is

the imaginary part, dielectric loss $\tan\delta = \frac{\varepsilon''}{\varepsilon'}$.

Differential Scanning Calorimetry (DSC). DSC measurements of compounds were characterized using a NETZSCH-214 instrument, and microcrystalline compounds were heated and cooled in an aluminum crucible with the rate of 10 K/min.

Thermogravimetry (TG). TG curves of compounds were characterized by a NETZSCH STA 449F5 instrument, and microcrystalline compounds were heated and cooled in an aluminum crucible with the rate of 10 K/min under an atmosphere of dry N_2 flowing at $20\text{ cm}^3/\text{min}$ in the temperature range of 293-1073 K.

Ferroelastic Measurement. For the observation of ferroelastic domain, the crystals of compound **3** were dissolved in the mixed solvent containing methanol and water with a 2:1 ratio to form a precursor solution with 50 mg/mL. The thin film was obtained by using the drop-coating method. Specifically, 20 μL of precursor solution was spread on a clean ITO (indium tin oxide) glass which underwent the surface treatment by an

ozone instrument, and then annealed at 323 K for 30 min. The domain structures were observed by an Olympus BX51TRF polarizing microscope with a variable temperature system, in which the equipped temperature control is INSTEC HCC602.

Hirshfeld Surfaces Analysis. Hirshfeld surfaces and the associated 2D fingerprint plots were calculated by the CrystalExplorer program by inputting the crystallographic structure file of the compound generated by SXR. Hirshfeld surfaces of three compounds were obtained using a standard (high) surface resolution, which can provide the information about intermolecular interactions in the crystal. The 2D fingerprint plot is a combination of d_e and d_i that provides the summary of intermolecular contacts in the crystal and is in complement to the Hirshfeld surfaces, where d_i is the distance to the nearest atom center interior to the surface, and d_e exterior to the surface. The normalized contact distance d_{norm} is based on d_e , d_i and the van der Waals (vdW) radii of the two atoms external (r_e^{vdW}) and internal (r_i^{vdW}) to the surface:

$$d_{norm} = \frac{d_i - r_i^{vdW}}{r_i^{vdW}} + \frac{d_e - r_e^{vdW}}{r_e^{vdW}}$$

d_{norm} surface is used for the identification of close intermolecular interactions. The value d_{norm} is negative or positive when intermolecular contacts are shorter or longer than r^{vdW} , respectively. Hirshfeld surface with d_{norm} values display a red-blue-white color scheme: where red regions correspond to closer contacts and negative d_{norm} value; the blue regions correspond to longer contacts and positive d_{norm} value; and the white regions correspond to the distance of contacts is exactly the van der Waals separation and with a d_{norm} value of zero.

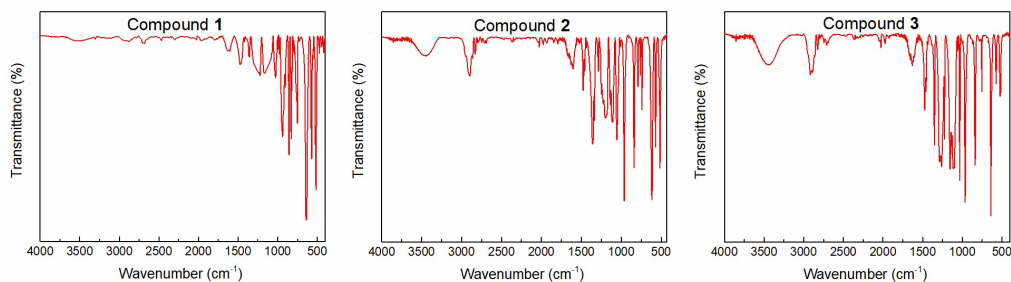


Fig. S1 IR spectra of compounds measured at room temperature. The peaks in the range of 1360-1200 cm^{-1} are assigned to the characteristic absorption of crown ether molecules; the peaks in the range of 1730-1550 and 3600-3100 cm^{-1} correspond the vibrational absorption of NH_3^+ and -OH in H_2O , respectively; the characteristic peaks of sulfone and C-F bond are located in the vicinity of 1630 and 1030 cm^{-1} , respectively.

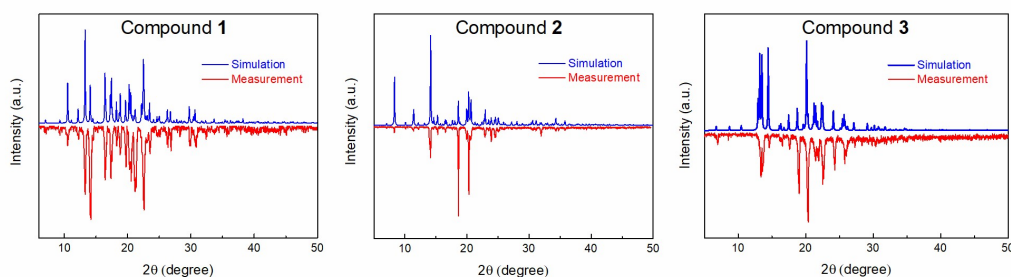


Fig. S2 The measured and simulated PXRD patterns of compounds at room temperature.

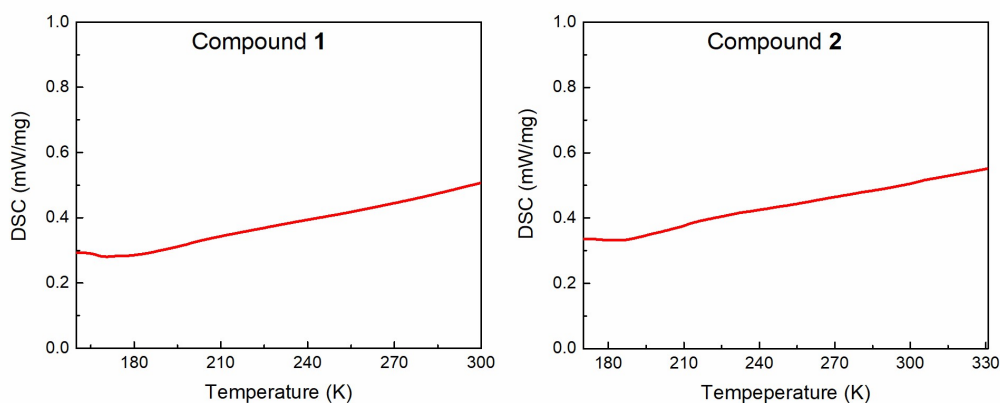


Figure S3. DSC curves of compound 1 and 2 in heating run.

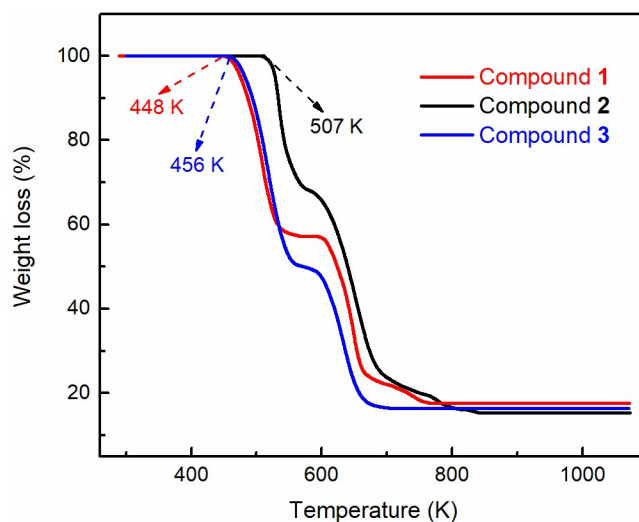


Fig. S4 TG curves of compounds in the temperature range of 293 to 1073 K.

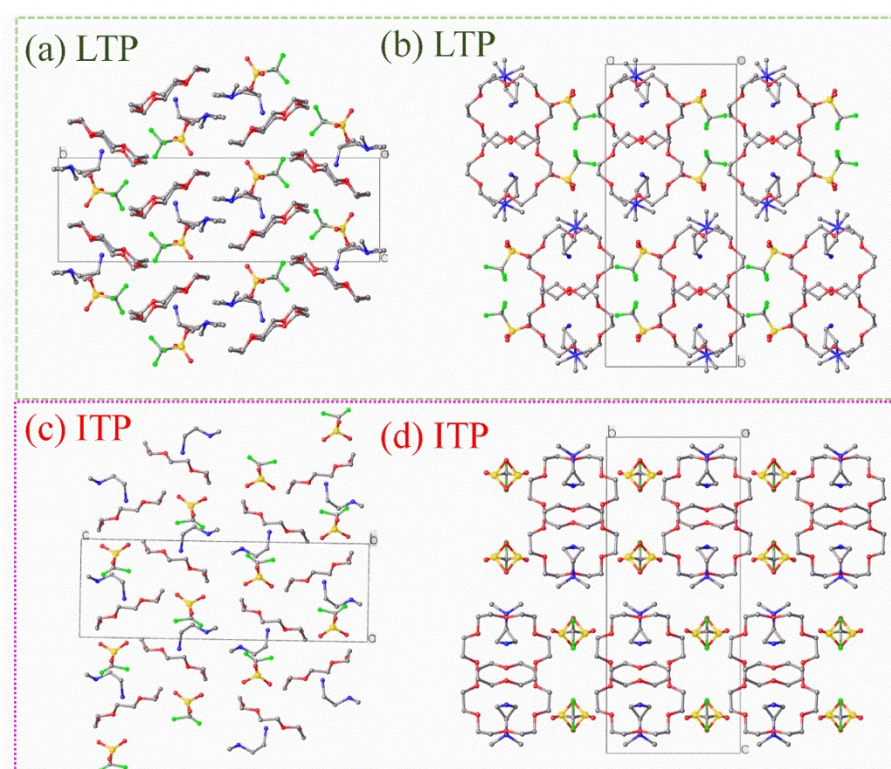


Fig. S5 Packing views of compound 3 in the LTP (a, b) and HTP (b, c). Hydrogen atoms are omitted for clarity.

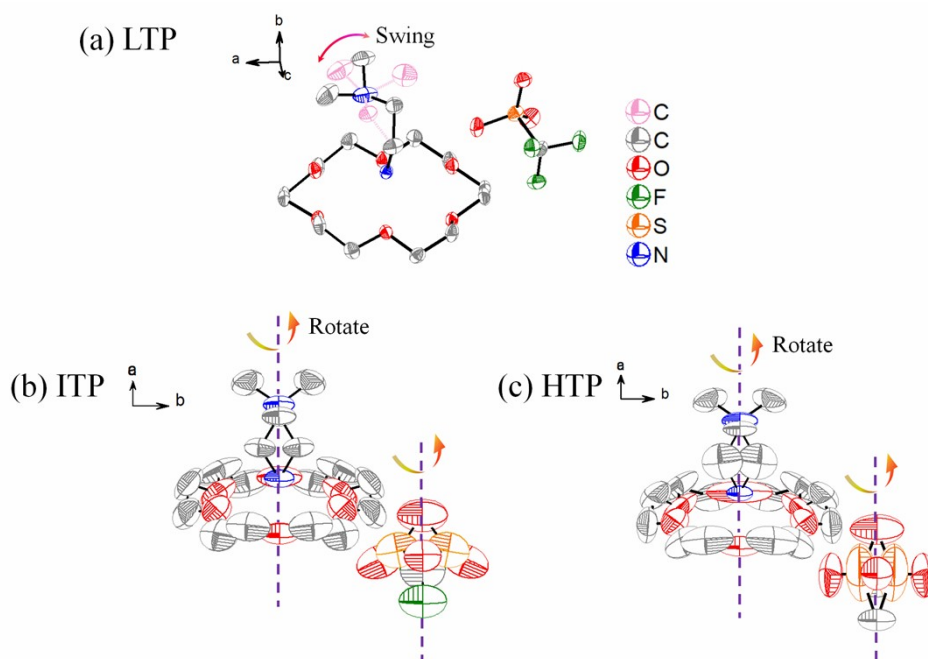


Fig. S6 Displacement ellipsoids of compound **3** at different temperatures were drawn at the 30% probability level. Hydrogen atoms were omitted for clarity.

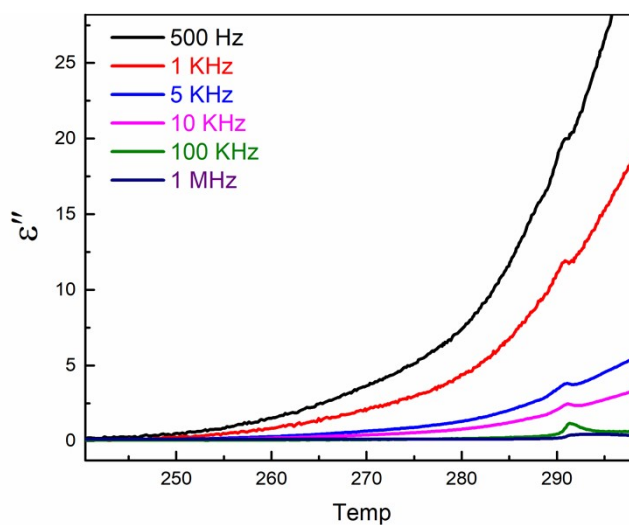


Fig. S7 The dielectric loss as a function of temperature for compound **3** measured at different frequencies on cooling.

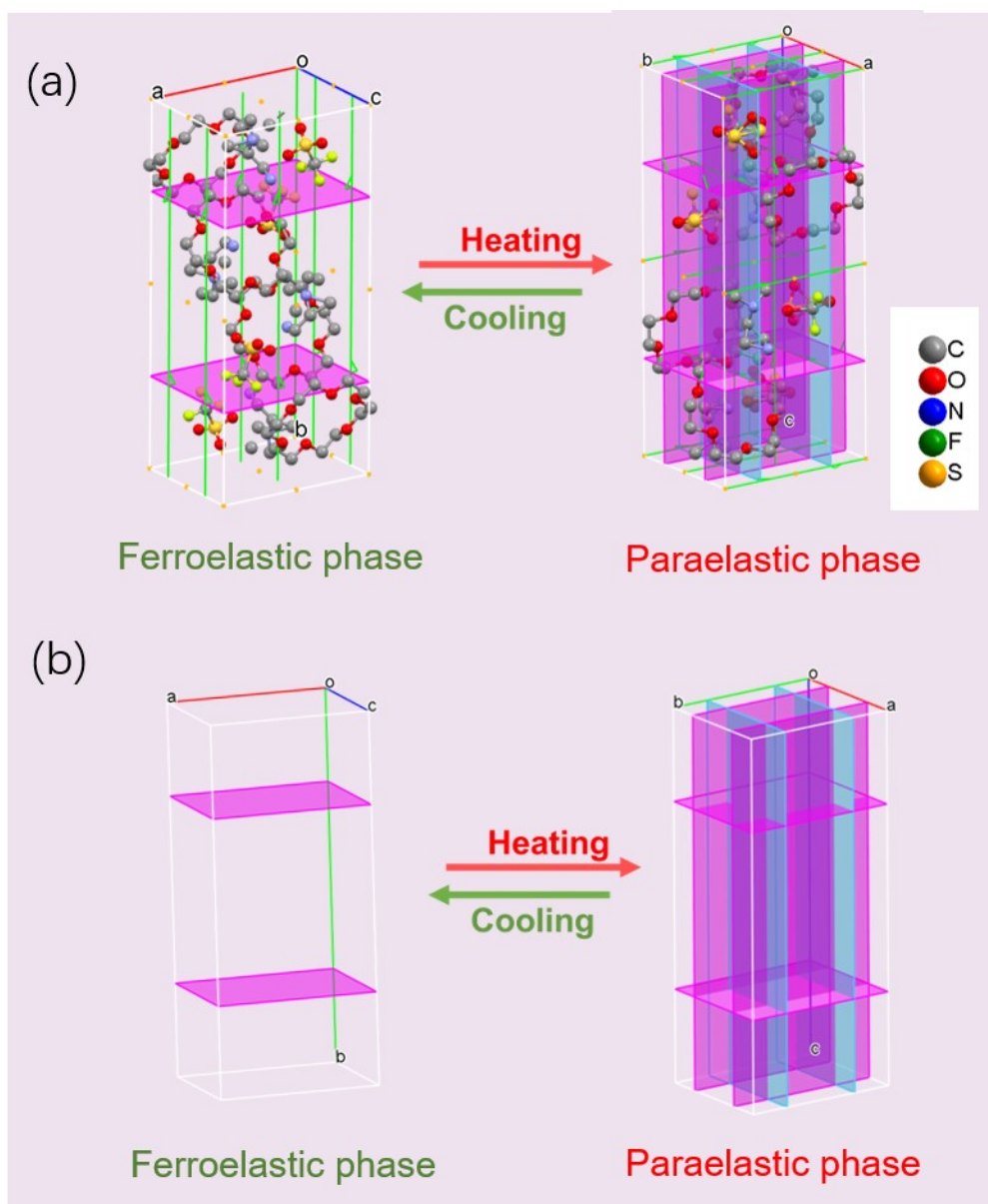


Fig. S8 (a) All symmetry operations of compound **3** in ferroelastic and prototypical unit cells. (b) Partial symmetry operations showed for clarity, and the same symmetrical elements E , C_2 , i , σ_h as well as all atoms in the unit cells were omitted.

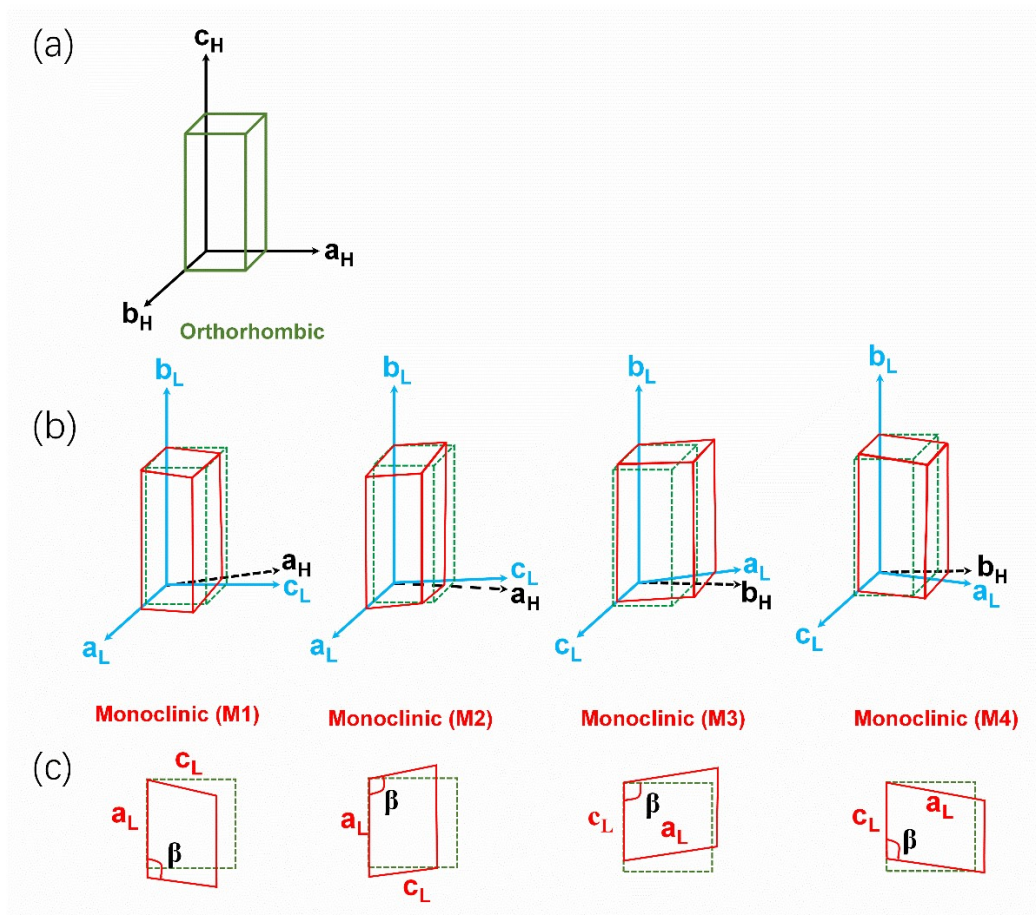


Fig. S9 (a) The crystal lattice of compound **3** crystallized as paraelastic phase. (b) The comparison of the crystal lattices of compound **3** between the paraelastic (green dot line) and ferroelastic (red line) phase. (c) The associated projection of the (010) plane for the ferroelastic phase.

Table S1. Selected known crown ether-based ferroelastics in molecular motor crystals.

Structure	Chemical name	Ferroelastic phase	Paraelastic phase	T_c (K)	Aizu notation	References
	$[(H_3O)(18\text{-Crown-}6)]PF_6$	$P2_1/c$ (No.14)	$Pnma$ (No.62)	287.2	$mmmF2/m$	1
	$[(4\text{-ethylanilinium})(18\text{-crown-}6)]BF_4$	$P2_1/c$ (No.14)	$Pnma$ (No.62)	180	$mmmF2/m$	2
	$[(\text{cyclopentylamine})(18\text{-crown-}6)]ClO_4$	$C2/c$ (No.15)	$Pbcn$ (No.60)	187.4	$mmmF2/m$	3



[(4-fluorobenzylammonium)(18-crown-6)]ClO₄

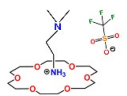
*P*2₁ (No.4)

*Cmc*2₁
(No.36)

208

*mm*2F2

4



[(Me₂N(CH₂)₂NH₃)(18-crown-6)]triflate

*P*2₁/*c* (No.14)

Pnma
(No.62)

295

*mmm*F2/*m*

This work

Table S2. Crystal data and structure refinement for compounds

Compound	Compound 1	Compound 2	Compound 3		
Empirical formula	C ₁₅ H ₃₃ F ₃ N ₂ O ₈ S	C ₁₈ H ₃₇ F ₆ N ₃ O ₁₀ S ₂		C ₁₇ H ₃₇ F ₃ N ₂ O ₉ S	
Formula weight	458.49	633.62		502.55	
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic
Space group	<i>P2₁/c</i> (No.14)	<i>P2₁/n</i> (No.14)	<i>P2₁/c</i> (No.14)	<i>Pnma</i> (No.62)	<i>Pnma</i> (No.62)
Temperature	223 K	293 K	243 K	299 K	308 K
a (Å)	9.1334(3)	9.0270(3)	11.2767(7)	8.9025(5)	8.9299(6)
b (Å)	24.9176(9)	15.4322(6)	26.0498(18)	11.0151(7)	10.9955(10)
c (Å)	10.5204(4)	21.430(1)	8.4301(6)	26.0682(16)	26.179(3)
α	90°	90°	90°	90°	90°
β	105.358(1) °	99.370(4)°	93.060(6)°	90°	90°
γ	90°	90°	90°	90°	90°
V (Å ³)	2308.76(14)	2945.5(2)	2472.9(3)	2556.3(3)	2570.4(4)
Z	4	4	4	4	4
Radiation	Mo-K _α	Mo-K _α	Mo-K _α	Mo-K _α	Mo-K _α
Calculated density (g/cm ³)	1.319	1.429	1.350	1.160	1.127
Absorption coefficient (mm ⁻¹)	0.204	0.270	0.20	0.18	0.17
F (000)	976	1328	1072	888	873
Data collection range	2.2-25.0°	1.9-26.0°	1.8-25.0°	2.0-25.0°	2.0-25.0°
R (int)	0.091	0.025	0.039	0.018	0.037
Completeness to θ	1	1	1	99.8%	99.7%
Data, restraints, parameters	4066, 245, 281	5781, 7, 376	4336, 331, 330	2379, 160, 169	2386, 60, 163
Goodness-of-fit on F ²	1.040	1.036	1.001	1.005	1.035
R ₁ , wR ₂ [I > 2σ(I)]	0.094, 0.195	0.053, 0.175	0.131, 0.334	0.233, 0.299	0.183, 0.294
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.90, -0.64	0.42, -0.31	1.09, -0.63	0.49, -0.44	0.49, -0.38

Table S3. The selected bond lengths and angles for compounds

Bond lengths (Å) and bond angles (°)					
Compound 1 at 223 K					
C1—C2	1.478 (4)	C7—O4	1.430 (4)	C13—N2	1.385 (5)
C1—O1	1.406 (4)	C8—O5	1.399 (4)	C14—N2	1.435 (5)
C2—O2	1.424 (3)	C9—C10	1.502 (2)	C15—F1	1.231 (4)
C3—C4	1.488 (4)	C9—O5	1.330 (3)	C15—F2	1.323 (5)
C3—O2	1.430 (3)	C10—O1	1.405 (4)	C15—F3	1.318 (5)
C4—O3	1.420 (4)	C11—C12	1.540 (8)	C15—S1	1.793 (3)
C5—C6	1.493 (5)	C11—C12'	1.423 (7)	O6—S1	1.403 (2)
C5—O3	1.415 (3)	C11—N1	1.461 (3)	O7—S1	1.426 (3)
C6—O4	1.416 (4)	C12—N2	1.406 (8)	O8—S1	1.381 (3)
C7—C8	1.497 (4)	N1—C11—C12	113.9 (3)	O1—C1—C2	108.1 (2)
O2—C2—C1	111.8 (2)	N2—C12—C11	112.1 (4)	C13—N2—C12	92.6 (4)
O2—C3—C4	108.0 (2)	F1—C15—F2	109.4 (4)	O8—S1—O7	116.2 (2)
O3—C4—C3	108.5 (2)	F1—C15—F3	109.9 (4)	C13—N2—C14	105.1 (4)
O3—C5—C6	108.0 (2)	F1—C15—S1	112.6 (3)	C10—O1—C1	105.7 (2)
O4—C6—C5	108.5 (3)	F2—C15—S1	111.1 (3)	C2—O2—C3	113.7 (2)
O4—C7—C8	112.3 (3)	F3—C15—F2	102.4 (3)	C5—O3—C4	113.0 (2)
O5—C8—C7	107.9 (3)	F3—C15—S1	110.9 (3)	C6—O4—C7	113.3 (2)
O5—C9—C10	115.9 (2)	C12—N2—C14	131.8 (4)	C9—O5—C8	114.4 (2)
O1—C10—C9	114.3 (2)	O8—S1—C15	105.07 (16)	O6—S1—C15	104.16 (18)
O8—S1—O6	116.22 (19)				
Compound 2 at 293 K					
C1—C2	1.494 (5)	C9—O6	1.408 (4)	C17—F2	1.328 (4)
C1—O2	1.401 (4)	C10—O1	1.431 (4)	C17—F3	1.318 (4)
C2—O3	1.413 (4)	C11—C12	1.489 (5)	C17—S1	1.806 (3)
C3—C4	1.487 (5)	C11—O1	1.405 (4)	C18—F4	1.321 (3)
C3—O3	1.401 (4)	C12—O2	1.421 (4)	C18—F5	1.312 (4)
C4—O4	1.417 (4)	C13—C14	1.443 (7)	C18—F6	1.296 (4)
C5—C6	1.486 (5)	C13—C14'	1.337 (8)	C18—S2	1.816 (3)
C5—O4	1.396 (4)	C13—N1	1.474 (4)	N3—S1	1.569 (3)
C6—O5	1.420 (4)	C14—N2	1.434 (6)	N3—S2	1.557 (2)
C7—C8	1.483 (5)	C14'—N2	1.509 (7)	O7—S1	1.422 (2)
C7—O5	1.402 (4)	C15—N2	1.416 (5)	O8—S1	1.397 (2)
C8—O6	1.425 (4)	C16—N2	1.422 (5)	O9—S2	1.416 (3)
C9—C10	1.480 (5)	C17—F1	1.315 (4)	O10—S2	1.424 (2)
O2—C1—C2	109.7 (3)	F1—C17—F3	108.3 (3)	C11—O1—C10	112.5 (2)

O3—C2—C1	109.5 (3)	F1—C17—S1	111.6 (2)	C1—O2—C12	112.3 (2)
O3—C3—C4	109.2 (3)	F2—C17—S1	109.7 (2)	C3—O3—C2	113.3 (3)
O4—C4—C3	109.2 (3)	F3—C17—F2	108.0 (3)	C5—O4—C4	112.4 (3)
O4—C5—C6	109.5 (3)	F3—C17—S1	111.2 (2)	C7—O5—C6	113.2 (2)
O5—C6—C5	109.9 (3)	F4—C18—S2	110.0 (2)	C9—O6—C8	113.2 (2)
O5—C7—C8	108.0 (3)	F5—C18—F4	107.4 (3)	N3—S1—C17	100.27 (15)
O6—C8—C7	109.2 (3)	F5—C18—S2	111.1 (2)	O7—S1—C17	103.87 (17)
O6—C9—C10	109.3 (3)	F6—C18—F4	106.8 (2)	O7—S1—N3	109.92 (15)
O1—C10—C9	109.2 (3)	F6—C18—F5	109.3 (3)	O8—S1—C17	105.14 (17)
O1—C11—C12	109.6 (2)	F6—C18—S2	112.1 (2)	O8—S1—N3	117.21 (15)
O2—C12—C11	110.5 (2)	C15—N2—C14	92.7 (5)	O8—S1—O7	117.75 (17)
C14—C13—N1	118.1 (4)	C15—N2—C14'	129.0 (5)	N3—S2—C18	102.10 (14)
C14'—C13—N1	117.3 (4)	C15—N2—C16	107.4 (4)	O9—S2—C18	102.14 (16)
N2—C14—C13	114.5 (5)	C16—N2—C14	131.3 (5)	O9—S2—N3	109.52 (16)
C13—C14'—N2	116.3 (5)	C16—N2—C14'	91.6 (5)	O9—S2—O10	119.15 (19)
F1—C17—F2	107.8 (3)	S2—N3—S1	127.27 (16)	O10—S2—C18	104.96 (15)
O10—S2—N3	116.26 (15)				

Compound **3** at 243 K

C1—C2	1.476 (9)	C8—O5	1.458 (6)	O7—S1	1.462 (4)
C1—O1	1.449 (6)	C9—C10	1.483 (8)	O8—S1	1.400 (5)
C2—O2	1.443 (6)	C9—O5	1.418 (7)	O9—S1	1.410 (5)
C17—C4	1.526 (8)	C10—O6	1.420 (7)	N1—C13	1.472 (7)
C17—O2	1.412 (7)	C11—C12	1.489 (8)	C13—C3	1.467 (14)
C4—O3	1.397 (7)	C11—O6	1.397 (7)	N2—C3	1.319 (14)
C5—C6	1.509 (9)	C12—O1	1.439 (7)	N2—C14	1.366 (15)
C5—O3	1.411 (7)	C18—F1	1.321 (7)	N2—C3A	1.332 (15)
C6—O4	1.407 (7)	C18—F2	1.297 (7)	N2—C15	1.672 (18)
C7—C8	1.472 (9)	C18—F3	1.382 (6)	N2—C14A	1.60 (2)
C7—O4	1.447 (7)	C18—S1	1.840 (6)	N2—C15A	1.28 (3)
O1—C1—C2	109.5 (4)	O6—C11—C12	110.2 (5)	O8—S1—O7	113.2 (3)
O2—C2—C1	108.5 (5)	O1—C12—C11	108.8 (5)	O8—S1—O9	120.3 (3)
O2—C17—C4	107.4 (5)	C12—O1—C1	112.7 (4)	O9—S1—C18	102.4 (3)
F1—C18—S1	111.8 (4)	C17—O2—C2	110.0 (4)	O9—S1—O7	113.8 (3)
F2—C18—F1	111.9 (5)	C4—O3—C5	112.1 (4)	C3—C13—N1	112.6 (7)
F2—C18—F3	106.8 (4)	C6—O4—C7	110.9 (4)	C3—N2—C14	139.2 (10)
O3—C4—C17	108.3 (5)	C9—O5—C8	112.0 (4)	C3—N2—C15	62.9 (8)
O3—C5—C6	107.5 (5)	C11—O6—C10	114.2 (4)	C14—N2—C15	98.7 (10)
O4—C6—C5	108.1 (5)	F1—C18—F3	106.1 (4)	C3A—N2—C14A	58.1 (11)

O4—C7—C8	108.5 (4)	F2—C18—S1	111.1 (4)	C15A—N2—C3A	151.0 (15)
O5—C8—C7	107.2 (5)	F3—C18—S1	108.9 (4)	C15A—N2— C14A	107.0 (16)
O5—C9—C10	107.6 (5)	O7—S1—C18	100.4 (3)	N2—C3—C13	117.7 (10)
O6—C10—C9	110.0 (5)	O8—S1—C18	103.1 (3)		

Compound **3** at 299 K

C1—C2	1.557 (9)	C5—O3	1.407 (7)	C10—F1	1.422 (11)
C1—O1	1.461 (6)	C6—O4	1.470 (8)	C10—F2	1.101 (10)
C2—O2	1.375 (7)	C7—C8	1.421 (8)	C10—S1	1.624 (8)
C3—C4	1.512 (11)	C7—N1	1.682 (7)	O5—S1	1.705 (7)
C3—O2	1.470 (8)	C8—N2	1.441 (6)	O6—S1	1.103 (9)
C4—O3	1.465 (7)	C9—N2	1.491 (6)	O7—S1	1.677 (5)
C5—C6	1.356 (10)	O1—C1—C2	102.3 (4)	O2—C2—C1	109.4 (5)
O2—C3—C4	105.8 (6)	F2—C10—F1	132.6 (9)	C10—S1—O5	83.1 (4)
O3—C4—C3	103.4 (5)	F2—C10—S1	124.1 (6)	C10—S1—O7	96.5 (4)
C6—C5—O3	105.0 (5)	C5—O3—C4	110.0 (5)	O6—S1—C10	75.2 (6)
C5—C6—O4	110.4 (5)	C8—C7—N1	106.4 (5)	O6—S1—O5	119.7 (5)
C2—O2—C3	112.4 (5)	C7—C8—N2	114.3 (5)	O6—S1—O7	149.1 (5)
F1—C10—S1	92.5 (5)	C8—N2—C9	111.2 (3)	O7—S1—O5	88.0 (3)

Compound **3** at 308 K

C1—C2	1.18 (4)	C5—C6	1.52 (3)	C11—S1	1.795 (19)
C2—O2	1.37 (3)	C5—O3	1.41 (3)	O5—S1	1.117 (9)
C3—C4	1.68 (6)	C8—N2	1.406 (13)	O6—S1	1.83 (2)
C3—O2	1.25 (4)	C9—N2	1.517 (10)	S1—O8	1.73 (2)
C4—O3	1.41 (3)	C10—S1	1.86 (2)	O2—C2—C1	136 (4)
O2—C3—C4	102 (3)	C5—O3—C4	104 (2)	O6—S1—O5	112.8 (16)
O3—C4—C3	106 (3)	C11—S1—C10	89.8 (14)	O8—S1—C10	91.5 (11)
O3—C5—C6	100 (2)	O5—S1—C10	103.0 (15)	O8—S1—C11	139.6 (8)
N2—C8—C7	115.7 (11)	O5—S1—C11	112.8 (16)	O8—S1—O5	106.2 (16)
C9—N2—C8	107.4 (8)	O6—S1—C10	143.8 (6)	O8—S1—O6	74.6 (13)
C3—O2—C2	125 (4)	O6—S1—C11	80.8 (9)		

Table S4. Hydrogen bonds for compounds [\AA and $^\circ$]

D-H...A	d (D-H)	d (H...A)	d (D...A)	<DHA
---------	---------	-----------	-----------	------

Compound **1** at 223 K

N1-H1C...O8	0.980	2.013	2.860	156.12
N1-H1D... O1	0.900	2.174	3.041	161.52
N1-H1D...O2	0.900	2.337	2.852	116.24
N1-H1E...O3	0.900	2.621	3.071	111.81
N1-H1E...O4	0.900	1.973	2.870	173.86
<hr/>				
Compound 2 at 293 K				
N1-H1C...O1	0.890	2.202	2.962	142.94
N1-H1C...O2	0.890	2.197	2.905	136.15
N1-H1D...O3	0.890	2.293	3.025	139.51
N1-H1D...O4	0.890	2.340	2.949	125.68
N1-H1E...O5	0.890	2.118	2.966	159.12
N1-H1E...O6	0.890	2.370	2.933	121.39
<hr/>				
Compound 3 at 243 K				
N1-H1C...O5	0.890	2.387	3.047	131.10
N1-H1C...O6	0.890	2.177	2.932	142.32
N1-H1D...O1	0.890	2.443	2.934	115.18
N1-H1D...O2	0.890	2.000	2.867	164.25
N1-H1E...O3	0.890	2.495	2.997	116.21
N1-H1E...O4	0.890	2.181	2.975	148.34
<hr/>				

References

1. Y.-Z. Tang, Z.-F. Gu, C.-S. Yang, B. Wang, Y.-H. Tan and H.-R. Wen, Unusual Two-step Switchable Dielectric Behaviors and Ferroelastic Phase Transition in a Simple 18-Crown-6 Clathrate, *ChemistrySelect*, 2016, **1**, 6772-6776.
2. D.-H. Wu, L. Jin and Y. Zhang, Temperature-triggered Reversible Ferroelastic Phase Transition in an 1:1 Inclusion Complex of 18-crown-6 with 4-Ethylanilinium Tetrafluoroborate, *Inorg. Chem. Commun.*, 2012, **23**, 117-122.
3. Y.-Z. Tang, Z.-F. Gu, J.-B. Xiong, J.-X. Gao, Y. Liu, B. Wang, Y.-H. Tan and Q. Xu, Unusual Sequential Reversible Phase Transitions Containing Switchable

Dielectric Behaviors in Cyclopentyl Ammonium 18-Crown-6 Perchlorate, *Chem. Mater.*, 2016, **28**, 4476-4482.

4. F. Jiang, C.-F. Wang, Y.-X. Wu, H.-H. Li, C. Shi, H.-Y. Ye and Y. Zhang, Nonlinear Optical and Photoluminescence Bistable Responses Accompanied by Tunable Dielectric Behaviors in Crown Inclusions, *J. Phys. Chem. C*, 2020, **124**, 5796-5801.