*Supplementary data for:*

# Structural characterization, phase transition and switchable dielectric behaviors in a new zigzag chained organic-inorganic hybrid compound: $[C_3H_7NH_3]_2SbI_5$

*Chen-Yu Mao, Wei-Qiang Liao, Zhong-Xia Wang, Peng-Fei Li, Xing-Hui Lv,* Heng-Yun Ye* and *Yi Zhang**

Ordered Matter Science Research Center, College of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, PR China

*E-mail: hyye @seu.edu.cn

*E-mail: yizhang 1980@seu.edu.cn

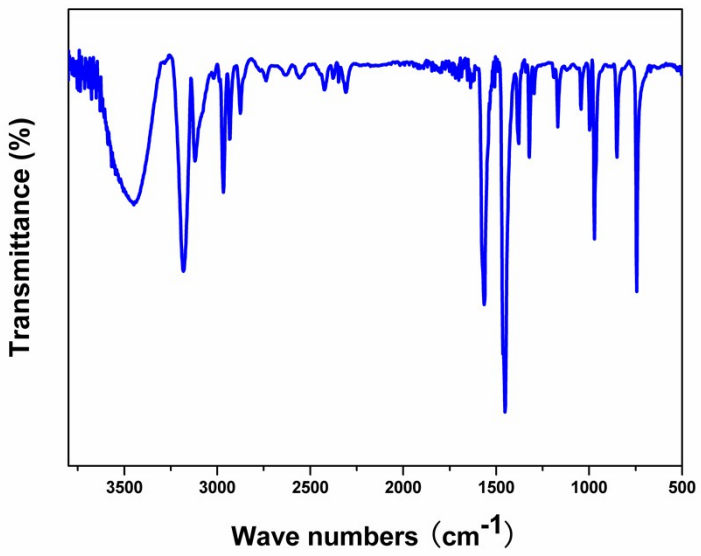


**Figure S1.** Infrared (IR) spectra of solid compound **1** in KBr pellet was recorded on a Shimadzu model IR-60 spectrometer at room temperature.

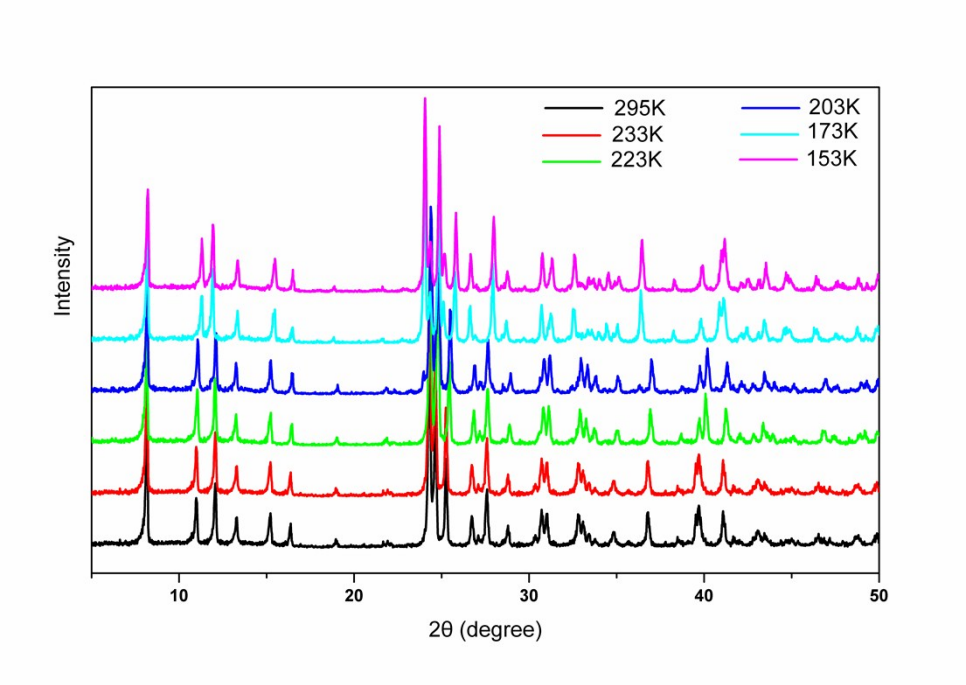


**Figure S2.** The variable-temperature X-ray powder diffraction (XRPD) patterns of **1** at different temperatures.

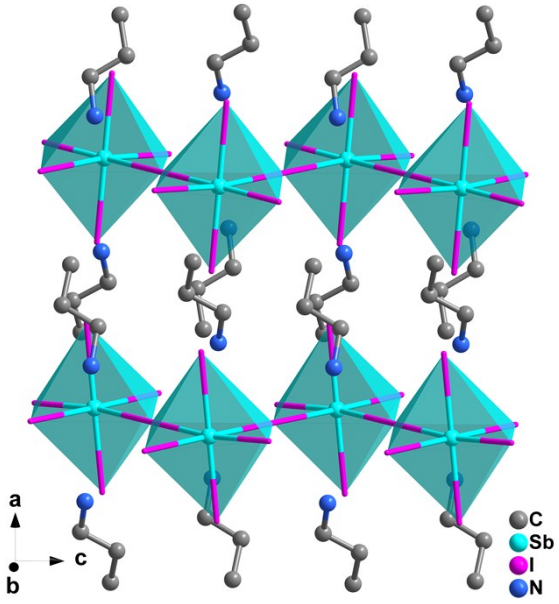


**Figure S3.** Packing diagram of **1** at 293 K, where $[C_3H_7NH_3]^+$ cations located in the cavies between the zigzag chains. All hydrogen atoms were omitted for clarity.

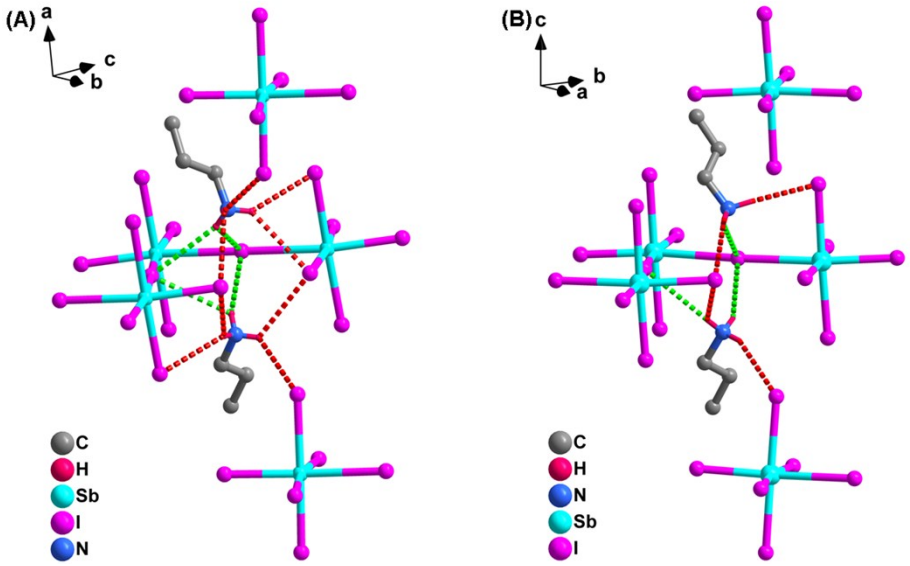


**Figure S4.** Hydrogen-bond geometry of the crystal structures of **1** at different temperatures (A) 293 K and (B) 203 K. The green and red dashed line representative the hydrogen bonds, whose accepter are bridging I atoms and terminal I atoms, respectively. All hydrogen atoms bonded to C atoms were omitted for clarity.

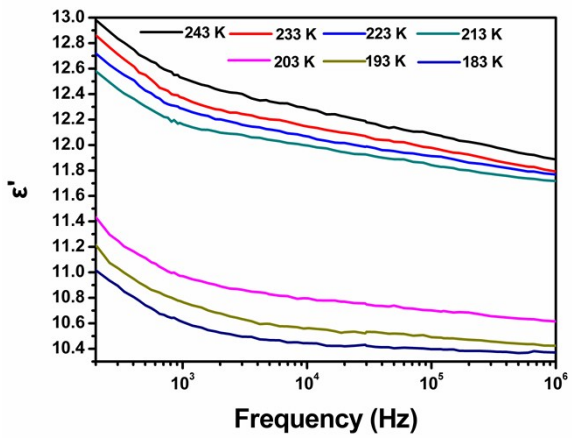


**Figure S5.** Frequency dependence of the real parts of the dielectric permittivities of **1** obtained at various temperatures.

**Table S1.** Hydrogen-Bond Geometry and length at 293 and 203 K in Compound **1**.

| | D–H···A | H···A (Å) | D···A (Å) | D–H···A (°) |
|---|---|---|---|---|
| 293 K | N1–H1C···I3$^{viii}$ | 3.14 | 3.971(10) | 157.1 |
| | N1–H1D···I1$^{i}$ | 3.16 | 3.90(1) | 141.6 |
| | N1–H1D···I2$^{ii}$ | 3.19 | 3.885(10) | 136.8 |
| | N1–H1E···I1$^{iii}$ | 3.08 | 3.701(9) | 128.3 |
| | N1–H1E···I2 | 3.21 | 3.769(9) | 122.7 |
| | N1–H1C···I3$^{i}$ | 3.33 | 3.849(9) | 119.8 |
| 203 K | N1–H1E···I3$^{iv}$ | 3.15 | 3.954(18) | 150.8 |
| | N1–H1D···I5$^{vi}$ | 2.89 | 3.701(17) | 152.9 |
| | N1–H1C···I1 | 2.95 | 3.767(18) | 153.5 |
| | N2–H2E···I5$^{vi}$ | 3.24 | 3.87(2) | 130.3 |

| | | | | |
|---|---|---|---|---|
| | N2–H2E···I1$^{vi}$ | 3.14 | 3.83(2) | 136.1 |
| | N2–H2D···I2$^{vii}$ | 2.93 | 3.75(3) | 154.6 |
| | N2–H2C···I1 | 2.90 | 3.73(3) | 156.2 |

Symmetry codes:

(i) *x, y, 1+z*; (ii) *1-x, y, 1.5-z*; (iii) *1.5-x, 0.5-y, 0.5+z*; (iv) *1.5-x, 0.5+y, z*; (v) *0.5+x, 0.5-y, 1-z*; (vi) *1.5-x, -0.5+y, z*; (vii) *0.5+x, y, 0.5-z*. (viii) *1-x, y, 0.5-z.*

**Table S2.** Selected Sb–I distances and length for Compound **1** at 293 and 203 K.

| | 293 K | | 203 K | |
|---|---|---|---|---|
| Bond lengths (Å) | Sb1–I1 | 3.0037(25) | Sb1–I1 | 3.3444(25) |
| | Sb1–I2 | 2.8454(21) | Sb1–I2 | 2.9957(29) |
| | Sb1–I3 | 3.3221(24) | Sb1–I3 | 2.9908(29) |
| | Sb1–I1$^{viii}$ | 3.0037(25) | Sb1–I4 | 2.8274(23) |
| | Sb1–I2$^{viii}$ | 2.8454(21) | Sb1–I5 | 2.8645(23) |
| | Sb1–I3$^{viii}$ | 3.3221(24) | Sb1–I1$^{vi}$ | 3.2870(24) |
| Bond angles (°) | I1–Sb1–I2 | 89.293(25) | I1–Sb1–I2 | 86.300(55) |
| | I1–Sb1–I3 | 87.676(21) | I1–Sb1–I3 | 93.623(54) |
| | I1–Sb1–I1$^{viii}$ | 177.705(26) | I1–Sb1–I4 | 169.302(61) |
| | I1–Sb1–I2$^{viii}$ | 89.222(25) | I1–Sb1–I5 | 90.709(50) |
| | I1–Sb1–I3$^{viii}$ | 94.101(21) | I1–Sb1–I1$^{vi}$ | 78.508(44) |
| | I2–Sb1–I3 | 169.116(27) | I2–Sb1–I3 | 178.263(77) |
| | I2–Sb1–I1$^{viii}$ | 89.222(25) | I2–Sb1–I4 | 90.327(60) |
| | I2–Sb1–I2$^{viii}$ | 99.360(26) | I2–Sb1–I5 | 89.039(60) |
| | I2–Sb1–I3$^{viii}$ | 91.051(25) | I2–Sb1–I1$^{vi}$ | 92.765(56) |
| | I3–Sb1–I1$^{viii}$ | 94.101(21) | I3–Sb1–I4 | 90.027(41) |
| | I3–Sb1–I2$^{viii}$ | 91.051(25) | I3–Sb1–I5 | 90.053(60) |
| | I3–Sb1–I3$^{viii}$ | 78.750(14) | I3–Sb1–I1$^{vi}$ | 88.919(54) |
| | I1$^{viii}$–Sb1–I2$^{viii}$ | 89.293(25) | I4–Sb1–I5 | 99.391(55) |
| | I1$^{viii}$–Sb1–I3$^{viii}$ | 87.676(21) | I4–Sb1–I1$^{vi}$ | 91.535(51) |
| | I2$^{viii}$–Sb1–I3$^{viii}$ | 169.116(27) | I5–Sb1–I1$^{vi}$ | 168.919(60) |

Symmetry codes:

(vi) *1.5-x, -0.5+y, z*; (vii) *0.5+x, y, 0.5-z*; (viii) *1-x, y, 0.5-z*.