

# Polar Molecule-Based Material with Optic–Electric Switching Constructed by Polar Anions

*Xue-Mei Zhao, Dong Li, Hai-Xia Zhao\*, Yan-Ping Ren, La-Sheng Long\*, Lan-Sun Zheng*

Collaborative Innovation Center of Chemistry for Energy Materials, State Key Laboratory of Physical Chemistry of Solid Surfaces and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China.

\*Correspondence and requests for materials should be addressed to H.-X. Zhao and L.-S.Long (E-mail: [hxzao@xmu.edu.cn](mailto:hxzao@xmu.edu.cn), [lslong@xmu.edu.cn](mailto:lslong@xmu.edu.cn)).

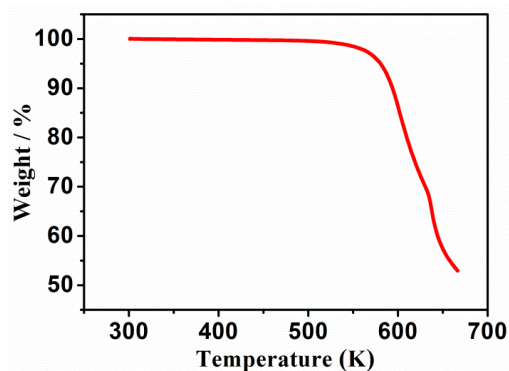


Figure S1. TGA data of compound **1** from 300 K to 670 K.

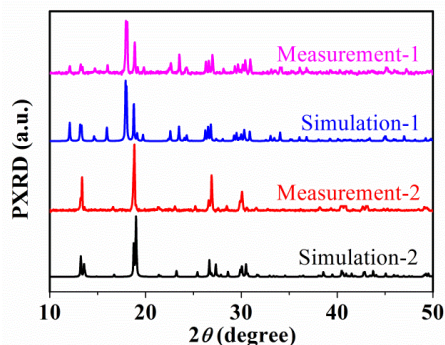


Figure S2. Simulation and experimental PXRD patterns of compound **1** and **2**.

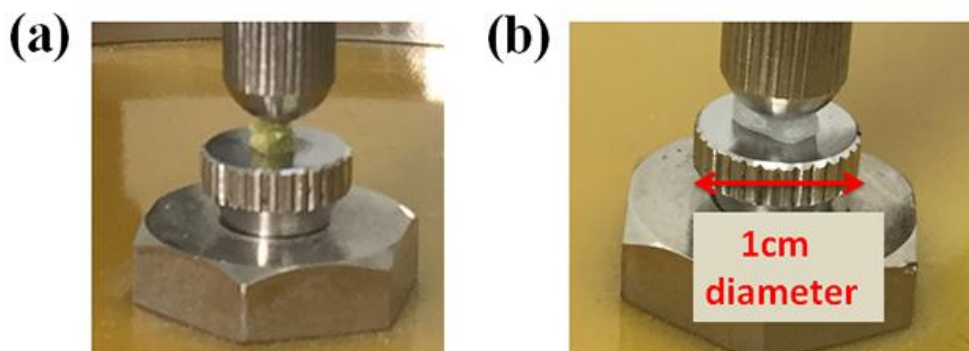


Figure S3. (a) Crystal size of compound **1** and (b) Crystal size of compound **2** for the piezoelectric measurement.

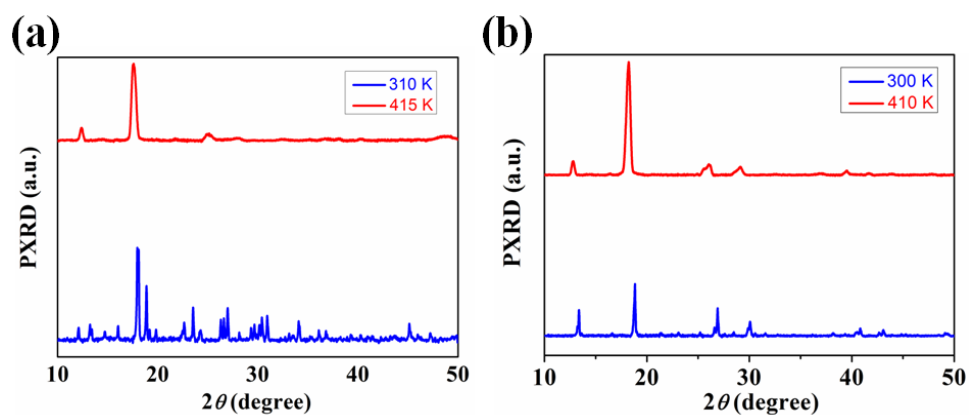


Figure S4. (a) Experimental PXRD patterns of compound **1** at RTP (310 K) and HTP (415 K), (b) Experimental PXRD patterns of compound **2** at RTP (300 K) and HTP (410 K).

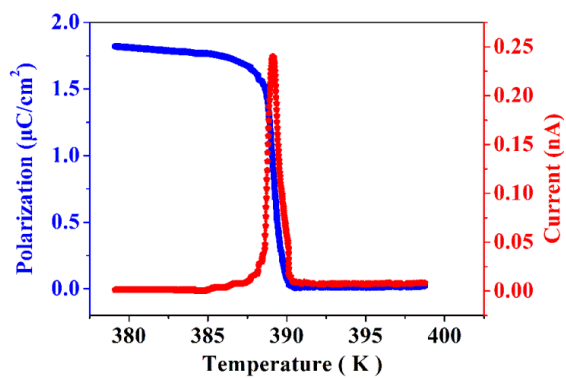


Figure S5. Polarization determined by integration of the pyroelectric current.

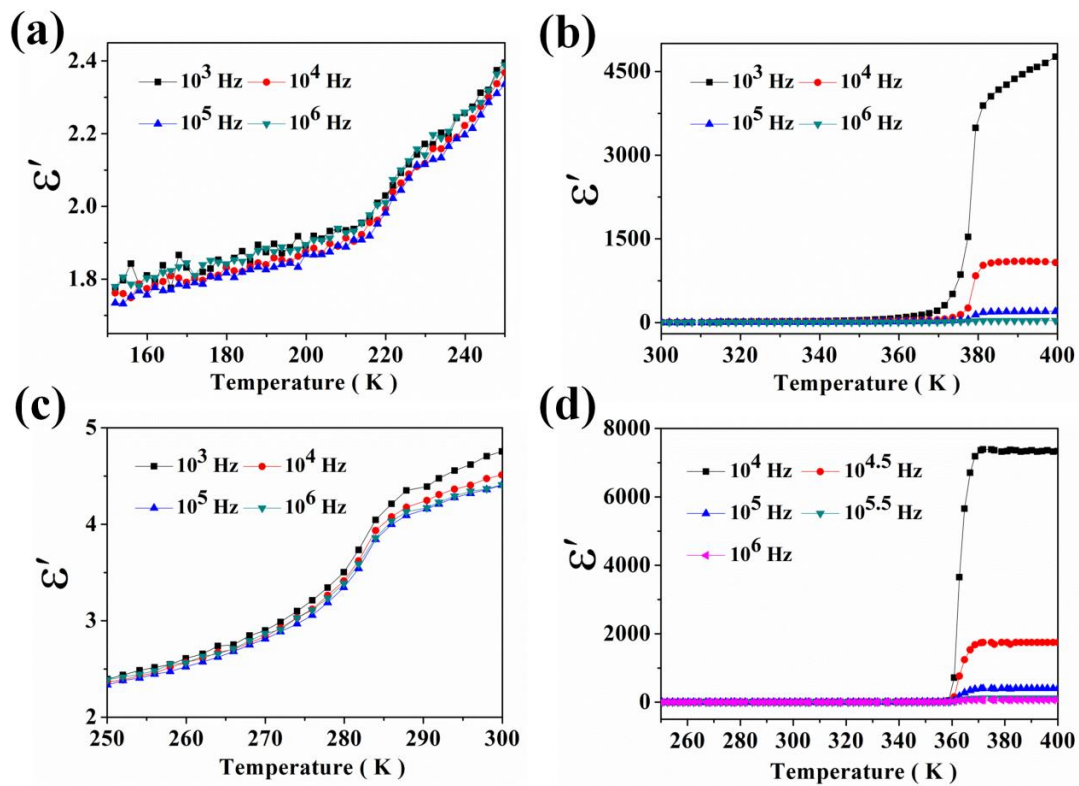


Figure S6. (a, b, c) Temperature dependence of the dielectric constants for compound 1 at selected frequencies, (d) Temperature dependence of the dielectric constants for compound 2 at selected frequencies.

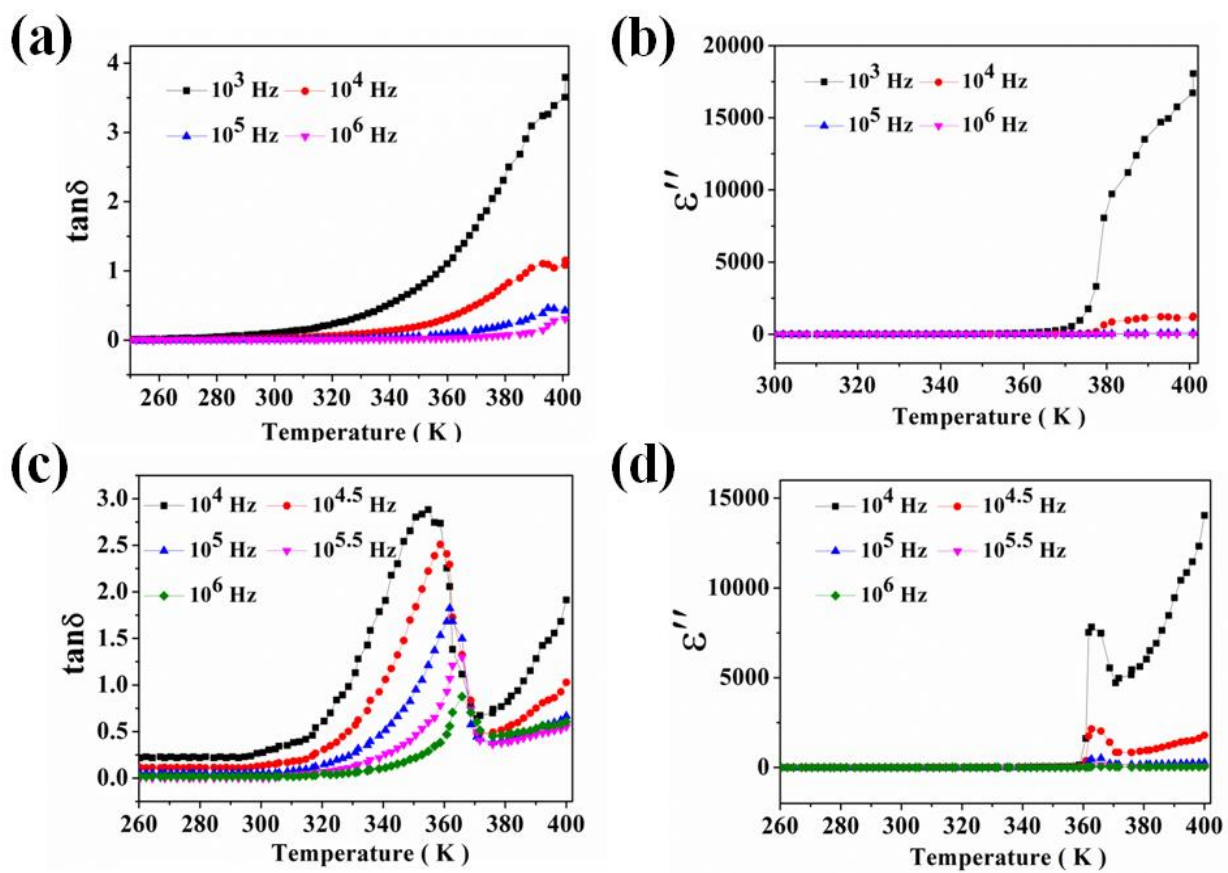


Figure S7. (a, b) Temperature dependence of the dielectric loss and imaginary part of the dielectric constant of compound **1** at selected frequencies, (c, d) Temperature dependence of the dielectric loss and imaginary part of the dielectric constant of compound **2** at selected frequencies.



Figure S8. Piezoelectric  $d_{33}$  data of compound **2**.

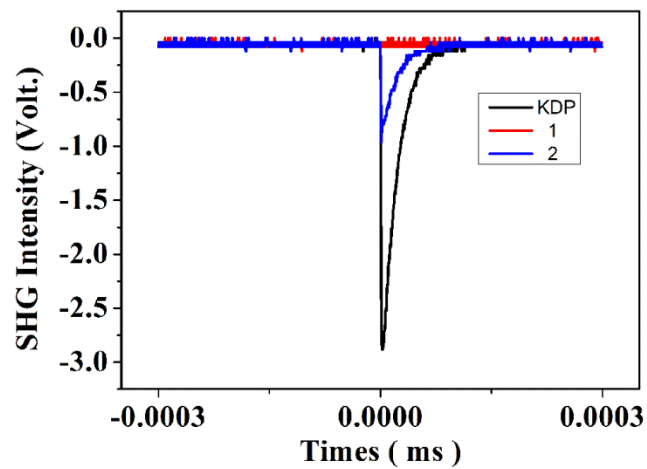


Figure S9. Oscilloscope traces of the second harmonic generated signals KDP, compound 1 and 2.