A Ferroelectric Inorganic-Organic Hybrid Based On NLO-phore Stilbazolium

Gang Xu, Yan Li, Wei-Wei Zhou, Guo-Jian Wang, Xi-Fa Long, Li-Zhen Cai, Ming-Sheng Wang, Guo-Cong Guo,* and Jin-Shun Huang

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fischou, Fujian 350002, P. R. China

Grazyna Bator, Ryszard Jakubas

Faculty of Chemistry, University of Wroclaw, Joliot-Curie 14, 50-383 Wroclaw, Poland

Synthesis and \(^1\)HNMR spectra of (DAMS)PTS (PTS = p-Toluenesulfonate)

\[
\begin{align*}
\text{CH}_3\text{N} + \text{CH}_3\text{I} & \xrightarrow{\text{EtOH, reflux}} \text{CH}_3\text{N}^+\text{CH}_3^- \quad (1) \\
\text{CH}_3\text{SO}_3\text{H} & \xrightarrow{\text{Ag}_2\text{O, heat}} \text{CH}_3\text{SO}_3\text{Ag} \quad (2) \\
(1) + (2) & \xrightarrow{\text{H}_2\text{O, heat}} \text{CH}_3\text{N}^+\text{CH}_3^-\text{SO}_3^- \quad (3)
\end{align*}
\]

\[
\begin{align*}
\text{CHO-CH} = \text{CH-CH=CH-N}^+\text{CH}_3^- + (3) & \xrightarrow{\text{piperidine, reflux}} \text{H}_3\text{C-CH=CH-CH=CH-N}^+\text{CH}_3^- \quad (\text{DAMS})\text{PTS}
\end{align*}
\]
Figure S1. The LC-ESI-MS$^n$ spectrum for 1.

Figure S2. The PXRD patterns for 1.
Figure S3. The one dimensional chain of bismuth chloride in 1 with 40% thermal ellipsoids.

Figure S4. Representation of the packing diagram for [TAMS]^{2+} viewed along the c axis. The head-tail arrangement of the pyridinium head and trimethylammonium tail with the centroid to centroid distance of adjacent organic molecules being 4.015 Å.
Figure S5. TG –DTA and DSC curves for 1.
Figure S6. The electric hysteresis loops of a pellet obtained from a powdered sample of 1, the chubby $P(E)$ loop at 473 K clarify the presence of huge conductivity of 1.

**Crystal structure analysis**

The intensity data set for 1 was collected on a Rigaku Mercury CCD diffractometer equipped with a graphite monochromated MoKα radiation ($\lambda = 0.71073 \text{ Å}$) using $\omega$ scan technique at 293(2) K. The data set was reduced by CrystalClear program. The structure was solved by direct methods using the Siemens SHELXTL™ Version 5 package of crystallographic software. The difference Fourier maps based on these atomic positions yield the other non-hydrogen atoms. The structure was refined using full-matrix least-squares refinement on $F^2$. The hydrogen atoms were allowed to ride on their respective parent atoms and included in the structure factor calculations with assigned isotropic thermal parameters. Especially, the methyl H atoms at C1 were generated using the AFIX 137 command, H atoms at C15, C16 and C17 were generated using the AFIX 33 command, and H atoms at other C atom were generated using the AFIX 43 command and that their orientation may not be totally reliable.

---

1. Rigaku. CrystalClear, version 1.35; Rigaku Corp.: Tokyo, Japan, 2002