

Molecular Ferroelastic Induced by Mono-/double-protonating Strategy

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April 07, 2024

Abstract

Molecular ferroelastic with the natural features of mechanical flexibility and switchable spontaneous strain have attracted widespread attention in the scientific community due to their potential applications in tunable gratings, flexible memorizers, strain sensors, and intelligent actuators. However, most designs of molecular ferroelastics remain in the stage of blind exploration, posing a challenge to achieve a functional ferroelastic more effectively. Herein, we have successfully obtained a molecular ferroelastic, $[\text{Me}_2\text{NH}(\text{CH}_2)_2\text{NH}_3](\text{ReO}_4)_2$ ($\text{Me}_2\text{NH}(\text{CH}_2)_2\text{NH}_3 = \text{N,N-dimethylethylenediammonium}$), under the guidance of the mono-/double-protonating strategy. The double-protonated $[\text{Me}_2\text{NH}(\text{CH}_2)_2\text{NH}_3](\text{ReO}_4)_2$ undergoes a paraelastic-ferroelastic phase transition with the Aizu notation of $2/mF-1$ at 322 K. Meanwhile, the theoretical calculation and experimental measurement simultaneously show that $[\text{Me}_2\text{NH}(\text{CH}_2)_2\text{NH}_3](\text{ReO}_4)_2$ possesses good mechanical flexibility, because its elastic modulus (E) of 8.26 GPa and hardness (H) of 0.45 GPa is smaller than the average value of organic crystals (E of 12.05 GPa and H of 0.5 GPa), which makes it promising to apply in wearable pressure sensors, implantable medical sensors, high-precision tuners, etc. This work further enriches the molecular ferroelastic family and demonstrates that mono-/double-protonation is one of the effective molecular modification strategies for designing ferroelastics.

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