

Crystal Structures and Dielectric Responses of Collective In-plane Molecular Rotator

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Interest in artificial solid-state molecular rotator systems is growing as they enable designing systems for achieving specific physical functions [1, 2, 3]. The phase transition behaviour of four halomesitylene crystals indicated dynamic in-plane molecular rotator characteristics in dibromiodomesitylene, tribromomesitylene, and dibromomesitylene crystals [2]. Such molecular rotation in diiodomesitylene crystals was suppressed by effective I•••I intermolecular interactions (Figure 1). The in-plane molecular rotation accompanied by a change in dipole moment resulted in dielectric phase transitions in polar dibromiodomesitylene and dibromomesitylene crystals. No dielectric anomaly was observed for the in-plane molecular rotation of tribromomesitylene in the absence of this dipole moment change. Typical antiferroelectric-paraelectric phase transitions were observed in the dibromomesitylene crystal, whereas the dielectric anomaly of dibromiodomesitylene crystals was associated with the collective in-plane molecular rotation of polar *n*-molecules in the *n*-stack. We found that the single-rope-like collective in-plane molecular rotator was dominated by intermolecular I•••I interactions along the *n*-stacking column of polar dibromiodomesitylene.

Phase transition from the antiferroelectric static ordered S3 phase to the paraelectric dynamic disordered M1 phase, accompanied by thermal hysteresis (Figure 2). Static disordered *n*-stacking columnar structure of polar molecule 1, where the orientation of iodine atoms was disordered, generating the macro dipole moment and dipole fluctuation. Phase transition from the static disordered S1 phase to the dynamic collective rotator phase M1 occurred at 380 K, and the static ordered S2 phase was formed from the M1 phase upon cooling.

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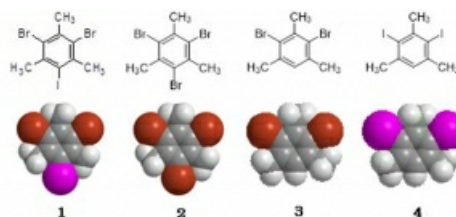


Figure 1 Molecular Structures of 1-4.

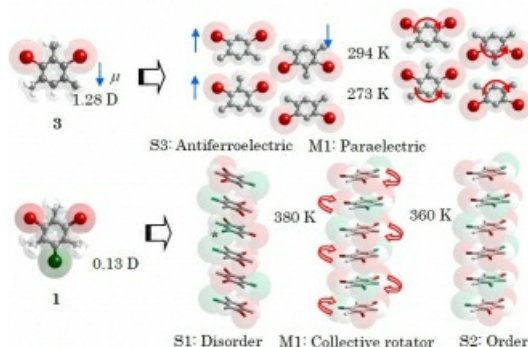


Figure 2 Schematic view of phase transitions of crystals 1 and 3.

Keywords: [Molecular Rotator](#), [Mesitylene](#), [Dielectric Property](#)