

Structural Studies of Supramolecular Gyroscope-like Co-crystals

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The construction of small-sized devices has attracted great amount of research interest for decades. Among these researches, rational design and synthesis of molecular devices based on supramolecules are fascinating topics [1]. In our attempts to design and synthesis of supramolecular gyroscopes [2], co-crystals between decamethonium diiodide (i.e., $[(\text{CH}_3)_3\text{N}^+(\text{CH}_2)_{10}\text{N}^+(\text{CH}_3)_3][2\text{I}^-]$) and different *para*-dihalogen-substituted benzene moieties (i.e., $p\text{-C}_6\text{X}_2\text{Y}_4$, X = Br, I; Y = H, F) are obtained. Single-crystal X-ray diffraction (XRD) structures of three novel co-crystals exhibit supramolecular gyroscope-like structures constructed by halogen bonding of 1:1 stoichiometry of two components [3]. Variable-temperature ^{19}F NMR experiments are used to distinguish between dynamic and static disorder of rotor in selected product materials. The variable-temperature ^{19}F NMR spectra of co-crystals are insensitive to temperature, other than some very small shift changes (< 2 ppm over the full range of temperature). There are no discernible line width changes in this temperature range, which suggests that dynamic disorder of the rings is unlikely.

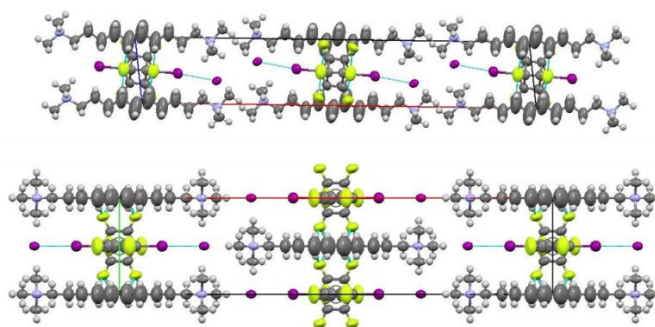


Figure 1: Crystal packing of decamethonium diiodide / I-(C₆F₄)-I adduct, viewed along *b* axis (top) and along *c* axis (bottom).

References

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