Poster Presentation

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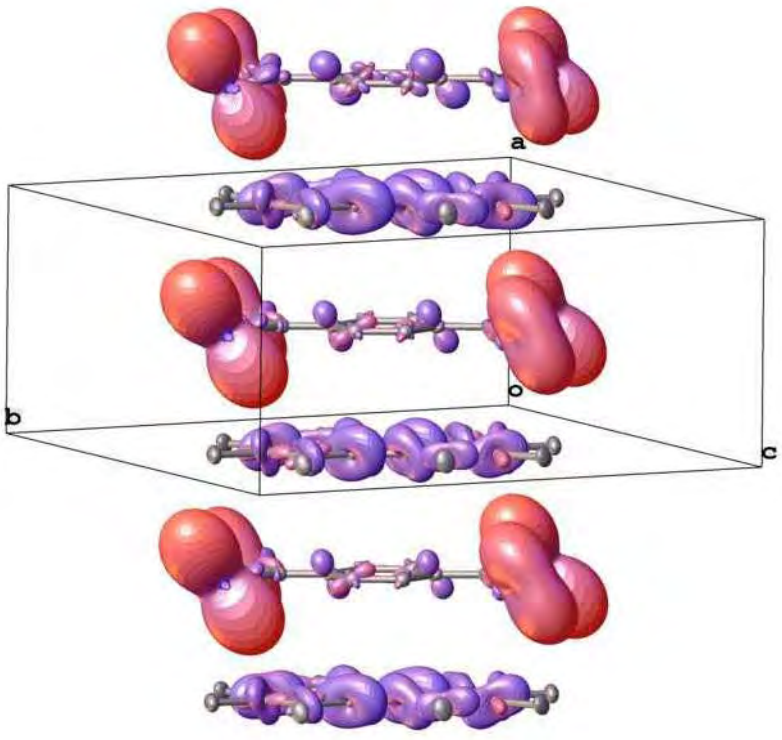
Electronic interactions in 1D-π-assemblies from TLS analysis of thermal motion

S. Lindeman[1], M. Talipov[1], S. Wadumethrige[1], O. Dolomanov[2], R. Rathore[1]

[1]*Marquette University, Chemistry Department, Milwaukee, USA,* [2]*Durham University, Chemistry Department, Durham, UK*

Advanced features of TLS analysis within Olex2 program package allow for a detailed analysis of electronic redistribution in supramolecular systems. Particularly, the possibility of calculating TLS tensors in user-defined coordinate systems along with qualitative graphical representation of difference thermal motion are especially useful for analysis of atomic asphericity and intra- and inter-molecular electron redistribution. In addition, these features allow for a directional dynamic analysis of intermolecular motions from variable-temperature experiments. We explored the exciting new possibilities analyzing supramolecular assemblies closely resembling modern electronic materials for a series of electron donor-acceptor complexes and ion-radical salts based on aromatic octamethyl-anthracene and anti-aromatic octamethyl-biphenylene substrates. The difference TLS analysis revealed intimate details of chemical bond polarization and electronic shell expansion for acceptor components along with electronic shell contraction for donor components of the complexes indicative of intra- and intermolecular charge transfer. Also, the variable-temperature analysis of relative thermal motion of the complex components in the crystals revealed some widening of the potential-energy minima in direction of the electronic overlap as a result of intermolecular pi-orbital coupling both in charge-transfer and charge-resonance supramolecular assemblies. A theoretical interpretation of the observed peculiarities was undertaken supported by respective spectroscopic data.



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