MS22-P04

Influence of chosen synthons on the polarizabilities of functional groups

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The correlation between the crystal structure and physical properties of a given material has long been a subject of many studies. One of the key features of designing efficient multifunctional materials is to use specific building blocks and/or synthons in order to increase a desired effect in the certain crystallographic direction. For example, to obtain efficient optical devices it is necessary to use highly polarizable functional groups which will promote high optical effect. It is thus crucial to get a precise information on how those group polarizabilities are influenced by common synthons used in crystal engineering.

Recently developed routine, PolaBer [1] allows to calculate atomic polarizabilities, and therefore group polarizabilities, based on the definition of atomic dipole moments given by Bader [2]. The routine uses the results of QTAIM partitioning of electron densities. According to QTAIM theory each atomic contribution can be expressed as a sum of *atomic polarization* and *charge translation* terms. The numerical derivatives of these quantities with respect to external electric field provide atomic and group polarizabilities. The advantage of using group polarizabilities rather than molecular ones, is the fact that we can extract separate information about the functional group and intermolecular contribution into linear susceptibility. This, on the other hand, enables to identify which group mostly contributes to the global dielectric constant, thus could be very helpful in reverse crystal engineering [3] purpose when designing new optically effective materials.

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MS22-P05

Deciphering the driving forces in crystal packings by analysis of electrostatic energies and contact enrichment ratios

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The decomposition of the crystal contact surface between pairs of interacting chemical species enables to derive an enrichment ratio [1,2,3]. This descriptor yields information on the propensity of chemical species to form intermolecular interactions with themselves and other species. The enrichment ratio is obtained by comparing the actual contacts in the crystal with those computed as if all types of contacts had the same probability to form.

The enrichments and contacts tendencies were analysed in several families of compounds, based on chemical composition and aromatic character. As expected, the polar contacts of type H···N, H···O and H···S, which are generally hydrogen bonds, show enrichment values larger than unity.

Hydrophobic contacts show different types of behaviour depending on the molecular content.

The electrostatic energy of short contacts was also computed using charge density models transfered from the ELMAM2 database.

The contact enrichment ratios were statistically compared with the electrostatic energy values.

The analysis suggests that strong attractive interactions are enriched and are a driving force in the crystal packing formation.

On the other hand repulsive interactions are generally avoided or under-represented.

The behaviour of weaker interactions is less contrasted and will be discussed.

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