

Oral Contributions

[MS13-03] Revealing noncovalent interactions in quantum crystallography

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Understanding non-covalent interactions (NCIs) is of paramount importance due to their ubiquity and versatility. These so-called “weak interactions” constitute the foundation of many fields of modern science and technology, for example, crystal engineering, molecular recognition, and self-assembly.[1–4]

The recently proposed NCI index of reduced density gradient (RDG) of Johnson and Yang [9–11] relates the NCI to a density and its derivatives. A three-dimensional (3D) isosurface plot of the RDG is used to provide qualitative information about individual NCI.

We have adapted this method to visualize the non-covalent interactions from experimentally refined charge densities using a quantum crystallographic ansatz.[12] The appearance of additional nonzero RDG isosurfaces around the peripheral of the molecule is observed during the refinement procedure, due to the presence of intermolecular NCI in the crystal structure.

Furthermore, the existing NCIs (e.g., intramolecular) are enhanced during the refinement procedure. The original NCIPLOT was proposed for studying theoretical charge densities, and this study has demonstrated that it is equally applicable to study experimentally refined charge densities using quantum crystallography. This should open new possibilities for directly comparing experimental and theoretical charge density distributions.

Interestingly, the RDG isosurface has also been studied using the popular multipole model[13].

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