MS36 Software development in quantum mechanics-based methods of crystallography

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MATTS2021 data bank: application of cluster analysis to interpret electron density of atom types

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Abstract

An electron density model is necessary to interpret data from X-ray diffraction. In contrast to spherical Independent Atom Model (IAM), the Multipole Model (MM) uses aspherical approach to describe electron density, which includes the deformation of electron density arising from lone electron pairs and covalent bonds. The MATTS (Multipolar Atom Types from Theory and Statistical clustering) data bank gathers Multipole Model parameters specific for various atom types in proteins, nucleic acids, and organic molecules. However, the relations between and within atom types, how electron density of particular atoms responds to their surroundings, and which factors describe the electron density in molecules within the Multipole Model, were not yet investigated in details. By implementing data analysis methods such as clustering, we captured similarities in the spatial distribution of electron density for atom types and found out which of their features influence the multipole parameters of electron density the most. The resemblance between atom types gives potential for improving quality of the data bank by adding better parametrization, definitions, and local coordinate systems for atom types. The further development of the MATTS data bank and introducing atom types on various levels of generality and specificity, will lead to achieving the eventual goal of having a wider range of atom types necessary to construct the electron density of any molecule.

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References

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