Topological Analysis of Bio-molecules

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Intra and intermolecular interactions of bio-molecules are investigated in terms of topological analyses. Ultra high resolution data helped us to determine the more accurate positions of atoms in protein and nucleic acid. We could find the hydrogen atoms in the difference Fourier maps. We also introduce the bio-molecule databank to the macromolecule and describe the more exact electron density of the structures. The electron density could be transferred to macromolecules as a multipole model which may be used to derive some physical properties including bond orders, electrostatic potential, hydrogen bond energies, bond paths, and atomic domains, atomic or fragment charges and their possible delocalization. When we build an adequate databank of the electron densities, it will useful to refine more accurately the lower resolution crystal structures. The electron densities are obtained both from X-ray diffraction data at low temperature and from a periodic density functional theory calculation. The features of the deformation densities, Laplacian distributions, bond pathes, and atomic domains are shown to describe the variety bonding. All the interactions are verified by the location of the bond critical point and its associated topological properties.

Keywords: charge density studies, multipole model, topological properties