A Challenge to Bonding Nature Study in Protein Crystallography

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Visualizing bonding electrons between atoms which construct a protein molecular, and precise positions of hydrogens in a protein leads us to the next stage of structural analysis of protein, such as precise chemistry and physics. The maximum entropy method is the most suitable tool to achieve this aim. This method enables us to visualize the least-biased electron distribution by refining the observed structure factors and phase by maximizing the information entropy of electron distribution which is not based on any chemical assumptions. As a result, the reliability factor of the obtained charge density becomes extremely low, for instance, R=2.4% for cytochrome *c*-553. Then, there are obvious differences between MEM charge density and the conventional Fourier map especially in the weak electron density region where the bonding electrons and the hydrogens exist. The obtained charge density clearly exhibits the characteristic anisotropy of the Fe-N coordinate bonds in the heme group and hydrogen charge density which can not be observed in the conventional method. Some other results for peroxidase, P450cam and P450nor will be also presented.

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