Topological properties of the electron density distribution in amino-acid phosphates. W. Maniukiewicz (1), E. Molins (2) and R.H. Blessing (3-6)

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The protein phosphorylation involves condensation of phosphate with the side-chain hydroxyl group of serine, threonine or tyrosine residues. This produces important changes in various physicochemical properties of the protein molecule. The Hansen-Coppens [1] multipole model of charge density has been fitted to low temperature high-resolution X-ray diffraction data for the racemic and the nonracemic crystals of serine and threonine or tyrosine residues. This produces important changes in various physicochemical properties of the protein molecule. The Hansen-Coppens [1] multipole model of charge density has been fitted to low temperature high-resolution X-ray diffraction data for the racemic and the nonracemic crystals of serine and threonine phosphates. A comparative analysis of resulting model parameters is performed in terms of Bader's topological theory [2]. The critical points of the electron density have been located in order to characterize the covalent bonds and intermolecular interactions. The results show that chemically similar bonds in different molecules are topologically equivalent.

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Reference: