

## **Interactions in Selected Dicarboxylic Acids Derived from Electron Charge Density**

Mateusz Pitak, Katarzyna Stadnicka, *Faculty of Chemistry, Jagiellonian University, Kraków, Poland.* E-mail: pitak@chemia.uj.edu.pl

High-resolution X-ray diffraction data were collected for tartaric acid, malic acid and its adduct with urea at 80 K to obtain accurate crystal data and experimental electron density. The measurements were performed on Nonius KappaCCD diffractometer equipped with Oxford Cryosystems 700 Series Cryostream Cooler. The quality of tartaric acid data was compared with that of the data obtained using a point detector at 105 K.

Data was interpreted using the multipole formalism [1] to derive the electron density and related properties such as the electrostatic potential and atomic moments. The electron density and its Laplacian extracted from the data were analyzed in terms of the topological properties of covalent bonds and non-bonded interactions [2].

Charge density and topological properties for the studied crystal structures were carried out to explore the character and role of both inter- and intra-molecular hydrogen bonds.

The interesting features related to the differences of electron density distribution were found for the same functional groups (hydroxyl and/or carboxyl). The differences caused by molecular interactions have influence on the molecular symmetry. The results are compared to those obtained for analogous molecules.

[1] Hansen N. K., Coppens P., *Acta Cryst.*, 1978, **A34**, 909. [2] Bader R. F. W., *Atoms in Molecules: A Quantum Theory*, Oxford, Calderon Press, 1995.

**Keywords:** electron charge density, dicarboxylic acids, interactions