

s2.m1.p3 **Xylitol and Ribitol: Integrated properties of the charge density** A.Ø. Madsen and S. Larsen, *Centre for Crystallographic Studies, University of Copenhagen*.

Keywords: charge spin densities.

High-resolution x-ray data has been collected for the molecular crystals of *xylitol* and *ribitol*. The lowtemperature (122K) data collection was performed using MoK radiation. The diastereomeric compounds crystallizes in an acentric ($P2_12_12_1$) and centric ($P2_1/c$) spacegroup respectively.

These meso-pentitols have a non-planar conformation of the carbon chain, and their five hydroxo groups are engaged in a complex pattern of hydrogen bonds.

The data, extending to $(\sin \theta)/\lambda = 1.1 \text{ \AA}^{-1}$, (R_{int} equals 0.017 and 0.016 respectively), has been refined to a multipole model using the program *VALRAY*³, and different model approaches were employed in the description of the hydrogen atoms, since neutron-data are not available for the compounds.

The resulting charge density-models were investigated by performing a Bader-type analysis¹ – including a determination of the atomic basins defined by the zero-flux surfaces of the electron density,² and a subsequent determination of integrated properties².

As part of the analysis the following issues were addressed:

- Is it possible to obtain a sensible multipole-model of an acentric structure?
- Transferability of integrated properties between chemically equivalent atoms.
- The treatment of hydrogen atoms in the absence of positions from neutron-diffraction experiments.

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2 C. Flensburg and D. Madsen. Atoms in crystals - from experimental charge densities. *Acta Cryst.*, A(56):24-28, 2000.

3 R. F. Stewart, M. A. Spackman, and C. Flensburg. *VALRAY98 Users Manual*, July 1998.

s2.m1.p4 **High-resolution charge density studies of the amino acids DL-lysine·HCl, DL-serine and DL-valine.** R. Flaig^a, T. Koritsanszky^b, P. Luger^a, ^a*Institut für Chemie/Kristallographie, Freie Universität Berlin, Takustr. 6, 14195 Berlin, Germany*, ^b*Department of Chemistry, University of the Witwatersrand, WITS 2050, Johannesburg, South Africa*.

Keywords: charge density, topological analysis, amino acids.

The use of synchrotron primary radiation at a wavelength of $\lambda \approx 0.5 \text{ \AA}$ and CCD area detection at low temperatures ($T \leq 100 \text{ K}$) makes it possible to obtain diffraction data suitable for charge density work in a short acquisition time and thus allows comparative studies on an entire class of related compounds¹.

For the amino acids DL-lysine·HCl, DL-serine and DL-valine very high resolution diffraction data at 100 K have been measured up to 1.38, 1.54 and 1.54 \AA^{-1} , respectively. Multipole refinements based on the rigid pseudoatom formalism² were carried out using the program package XD³. With the obtained density distribution a topological analysis according to Baders theory of "atoms in molecules"⁴ was performed. All covalent bonds could be characterized and are compared to other experimental and theoretical results.

For similar bonds excellent agreement of bond-topological indices was found with an earlier comparative study on some amino acids⁵. In addition weak interactions were analysed in terms of the topology of the hydrogen bonds and the nonbonding valence shell charge concentrations. The latter and electrostatic potentials are discussed together with the results of high-level ab initio calculations.

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