

04-Crystallography of Biological Small Molecules

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OPS-04.03.09 VITAMIN C AT 118°K: EXPERIMENTAL AND THEORETICAL STUDY OF THE CHARGE DENSITY

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Vitamin C is an extremely interesting molecule, not only for its important biological properties, but also for its structure in which the formation of several hydrogen bonds plays an important role. Its crystal structure was determined at room temperature, both by X-ray and by neutron diffraction, by Hvolslef [Acta Cryst., B24, 23 and 1431 (1968)]. We have now collected low temperature X-ray diffraction data at -155°C up to $\sin\theta/\lambda \approx 1$ on a Siemens four circle diffractometer, using monochromated MoK α radiation. The crystals do not undergo any phase transformation and the space group remains P2₁ with two independent molecules in the asymmetric unit. The low temperature unit cell parameters are: $a=6.390(1)$, $b=6.262(1)$, $17.127(4)\text{\AA}$, $\beta=99.36(2)^\circ$, with a decrease in the volume of 12.4\AA^3 . At the end of the standard crystallographic least-squares refinement, the final difference Fourier map showed significant residual maxima, midway all bonds between non-hydrogen atoms, with the highest maxima located on the double bonds. Bonding non-spherical electron density is therefore clearly indicated.

Bond distances and angles do not show relevant variations. The network of intermolecular hydrogen bonds is retained at low temperature, but the O---O distances are shorter with significant variations of the O-H---O angles.

A study by means of a multipole expansion of the electron density is now in progress; the experimental electrostatic potential obtained in this way may then be compared with that computed by ab-initio calculations on the isolated molecule, in order to attain a better understanding of the effects of crystal packing on the charge distribution. Other one-electron properties, such as the dipole moment, may be evaluated and compared. In addition a comparison of the topology of experimental and theoretical electron densities is derived also to judge the reliability of the multipole model.

We also intend to compute the electrostatic potential by means of a crystal-orbital approach using the program CRYSTAL [R. Dovesi, M. Causá, R. Orlando, C. Roetti and V.R. Saunders, J. Chem. Phys, 92, 7402 (1990)].