Charge Density of Phenoxymethylpenicillin (Penicillin V)

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Synchrotron radiation in combination with area detection allows fast and accurate single crystal data collection. Multipole refinements of the data makes a determination of the electronic charge distribution (EDD) of a molecule in a crystal possible. For penicillin V we have performed such a charge density study. Its structure was determined by Abrahammson, Hodgkin and Maslen in 1963 [1]. The evaluation of the EDD with the Atoms in Molecules-Formalism (AIM) of R.F.W. Bader [2] allows to obtain bond topological properties (the electron density ρ, the Laplacian $\nabla^2\rho$, the bond ellipticity ϵ at the bond critical point (bcp) and the distance d from the atom to the bcp), which is now routine work in this field. Recently also atomic properties like charge and volume, but also atomic dipole and multipole moments became accessible [3] via integration of the electron density, until now a computationally expensive process. We plan to compare bond topological and atomic properties from quantum chemical theoretical calculations with the experimental results. As two more penicillin derivatives have already been measured and evaluated with the procedure describes above these results will also be compared with penicillin V. To do that, successful multipole modelling of the X-ray reflexion data is needed. We are actually at a final stage of that process. The good figures of merit, the deformation as well as the residual density, shown here exemplarily in the plane containing the sulphur atom in figure 1, indicate, that atomic properties can now be calculated.

References

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Compound	Phenoxymethylpenicillin
formula	$C_{16}H_{18}N_2O_5S$
formula weight / $[\mathrm{g} \cdot \mathrm{mol}^{-1}]$	350.39
crystal system, space group, Z	monoclinic, C2, 4
beamline	F1
wavelength	0.5600
max. resolution (d)	0.42
sin θ/λ	1.20
max. 2θ [°]	84.2
temperature	100 K
number of collected reflections	50885
symmetry independent reflections	11219
reflections with $F_o > 2.5\ \sigma\ (F_o)$	9423
completeness [%]	93.8
redundancy after integration	4.4
$\mathrm{R}_{int}(F^2)$	0.037
$\mathrm{R}_w(F)$	0.021
$\mathrm{R}_1(F)$	0.021
$\mathrm{R}_{all}(F)$	0.028
Gof	1.09

Table 1: Experimental and crystal data, figures of merit

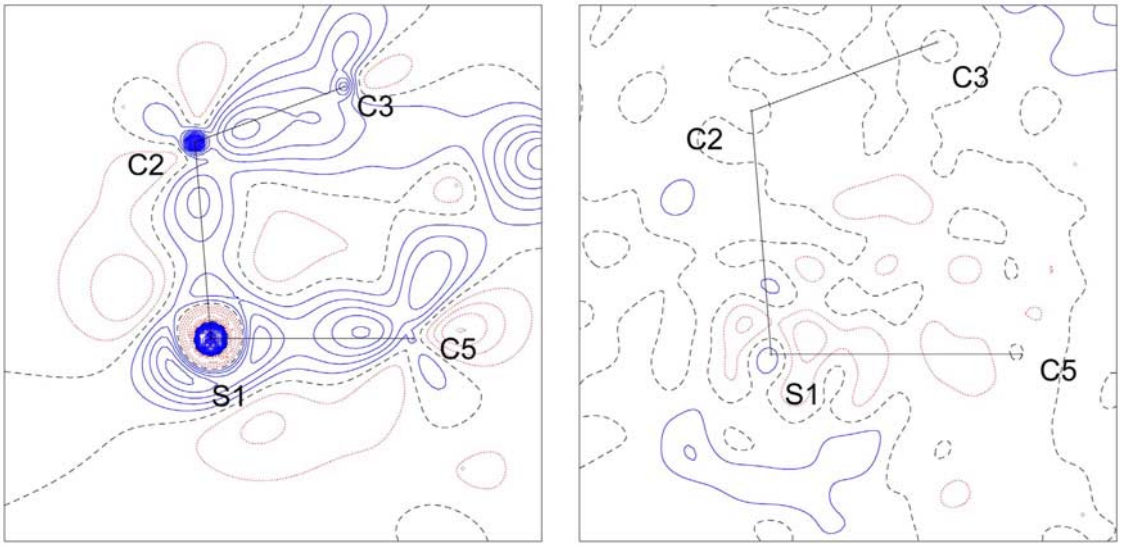

Figure 1: Deformation density (left) and residual density (right) in the plane containing the sulphur atom of phenoxymethylpenicillin (penicillin V); contour lines are 0.1 eÅ^{-3} (left) and 0.05 eÅ^{-3} (right)