Poster Presentations

[MS25-P26] Charge Densities of Three Polymorphs of Glycine

Aleksandra Pazio[a], Katarzyna Jarzembska[a], Anna Hoser[b], Matthias Gutmann, Paulina M. Dominiak[a], Krzysztof Woźniak[a*],

[a]*Department of Chemistry, Warsaw University, Warsaw, Poland*;
[b]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK* E-mail: apazio@chem.uw.edu.pl

The experimental charge densities of three polymorphs of glycine are presented. Two polymorphs crystallize in the monoclinic system: α-glycine in $P2_1/c$ and β-glycine in $P2_1$ space groups, whereas γ-glycine grows as merohedral twins composed of two trigonal lattices (space groups $P3_1$ and $P3_2$) combined by applying the [0 1 0 1 0 0 0 0 -1] twin matrix. The TAAM model of electron density (UBDB databank [1]) is used as a starting point in all refinements of experimental electron density. Different models of thermal motion were tested for all polymorphs (from the SHADE [2] server and theoretical calculations in Crystal09 [3]) and detailed results are discussed. The role of the anisotropic model of thermal motion of hydrogen atoms is emphasized.

References

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