MS22-P06

Molecular thermal smeared electrostatic potential

Christian Hubschle[1], Sander van Smaalen[1]

1. University of Bayreuth/Laboratory of Crystallography, Bayreuth, Germany

email: chuebsch@moliso.de

A method to compute the electrostatic potential (ESP) of dynamic-charge-density distributions[1] has been recently reported. Hirshfeld partitioning is a widely used and accepted technique to get individual properties of atoms or molecules in crystals[2]. It is a computationally easy fuzzy partitioning based on simple independent atom model (IAM). We present a way to partition thermal smeared dynamic electron densities. By combining both methods it is possible to get molecular thermal smeared electrostatic potential.

We will present the crystal ESP of dynamic charge densities of α-,γ-boron and boron carbide mapped on Hirshfeld surfaces and molecular ESP of nucleic acid bases. All methods can be easily and quickly applied within MoleCoolQt[3]. In that program it is also possible to export surfaces in file formats suitable for 3D printers.

Figure 1:

Left: Hirshfeld surfaces of Hoogsteen base pair Methyl-Adenine-Methyl-Thymine printed in PLA with magnets on the contact sites.

Right: Hirshfeld of the icosahedral substructure of γ-boron printed in PLA(lower) and mapped by the ESP of dynamic charge densities.(upper)

References:

[1] C. B. Hübschle. and S. van Smaalen. J. Appl. Cryst. (2017) 50.
[2] F. L. Hirshfeld, Theor. Chim. Acta (Berl.), 44, (1977), 129-138.
[3] C. B. Hübschle and B. Dittrich. J. Appl. Cryst. (2011). 44, 238-240.

Keywords: electrostatic potential, Hirshfeld surface, dynamic-charge-density

MS22-P07

Crystal and electronic structure of 3-(2'-tetrahydropyranyloxy)-4-methylthiazole-2(3H)-thione

Jozef Kozisek[1], Julia Koziskova [1], Lukáš Bučinský[1], Peter Herich[1], Jens Hartung[2], Mike Müller[2]

1. Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology in Bratislava , Bratislava, Slovakia
2. Fachbereich Chemie, Organische Chemie, Technische Universität Kaiserslautern, Kaiserslautern, Germany

email: jozef.kozisek@stuba.sk

The title compound is an O-ester structurally deriving from heterocyclic thiohydroxamic acid 3-hydroxy-4-methylthiazole-2(3H)-thione. When heated in the presence of organic peroxides or azo compounds as chemical initiators, the nitrogen-oxygen bonds in 3-alkoxy-4-methylthiazole-2(3H)-thiones breaks homolytically to yield oxygen-centered radicals in unprecedented specificity. Increasing steric demand at oxygen along the sequence primary, secondary, and tertiary alkyl surprisingly shortens the nitrogen oxygen bond in O-alkyl thiohydroxamates pointing to an unknown stabilizing electronic effect induced by steric demand. This responsivity is particularly significant for thiazole-2(3H)-thione-derived cyclic thiohydroxamic acids. In order to correlate N,O-bond lengths to changes in electron distribution the crystal and electronic structure of 3-(2'-tetrahydropyranyloxy)-4-methylthiazole-2(3H)-thione, $C_9H_{13}NO_2S_2$, has been determined and analyzed in terms of connectivity and packing patterns. The compound crystallizes in the monoclinic crystal system in the space group $P2_1/n$.

Data collection was performed on a Stoe STADIVARI diffractometer with a Dectris Pilatus 300K detector and with an Incoatec IµS Ag microfocus source (Ag-Kα, $\lambda = 0.56083$ Å) at 100 K using a nitrogen gas open-flow cooler Cobra from Oxford Cryosystems. Data reduction was processed using X-Area [1]. For numerical absorption corrections a crystal-shape model with 17 faces was employed. Resolution of 0.37 Å, an average redundancy of 14.29 gives R_{int} of 7.22%. Multipole refinement was performed on F^2 using XD suite of programs. The preliminary results shows that both N1 and O1 atoms are negatively charged and that the Laplacian has a small positive value. Comparison of experimental and theoretical results will be discussed.

References:

[1] STOE & Cie GmbH (2016). X-Area 1.76, software package for collecting single-crystal data on STOE area-detector diffractometers, for image processing, scaling reflection intensities and for outlier rejection; Darmstadt, Germany.
[2] Hübschle, C. B., Dittrich, B.; J. Appl. Crystallogr. 2011, 44, 238–240.

Keywords: quantum crystallography, IAM analysis, charge density