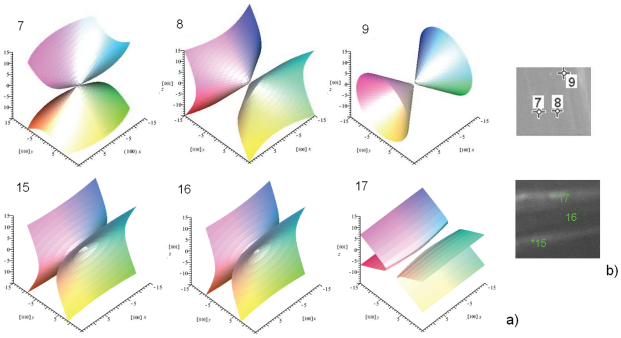

Figure 1. Characteristic surfaces of strain tensor (a), which corresponds to different local areas (labaled by numbers) of diamond crystal (b)

Keywords: EBSD, strain measurement, strain tensor, diamond crystals, weld joints

MS28. Charge density studies

Chairs: Anders Madsen, Simon Coles

MS28-P1 Lone electron pair dispersion - experimental charge density study of cubic arsenic(III) oxide

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The first experimental charge density study of arsenolite, cubic polymorph of arsenic(III) oxide, extended by periodic DFT calculations is reported. The presence of weak As···O interactions is confirmed and their topological characterization based on experimental electron density is provided utilizing both the Quantum Theory of Atoms in Molecules (QTAIM) and non-covalent interactions descriptor based on reduced density gradient (NCI-RDG). Spatial dispersion of arsenic lone electron pair (LEP) into three domains is observed in the Laplacian of electron density as well as in electron localization function (ELF) for the first time. The domains are located *trans* with respect to the primary As−O bonds as evidenced by the analysis of ELF. This could be related to the formation of these chemical bonds and/or to the tetrahedral clustering of arsenic atoms. Similar clustering has been observed in Sb(III) and Bi(III) oxysalts, suggesting LEPs may play significant role in this phenomenon. The dispersion of LEPs may be a more general effect for heavy elements and the issue should be investigated thoroughly to understand its origin and structural consequences.

Authors thank National Science Centre for financial support of this work (DEC2012/05/N/ST5/00283).

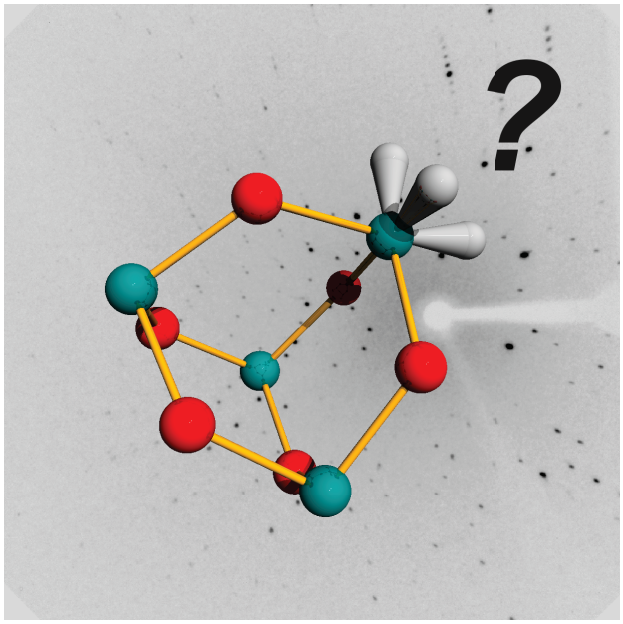

Figure 1. Dispersion of arsenic lone electron pair into three domains located *trans* with respect to the primary As–O bonds.

Keywords: charge density, arsenic(III) oxide, lone electron pair, stereoactivity

MS28-P2 Experimental charge density analysis for doxycycline

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Doxycycline is a well established wide-spectrum antibiotic, known for its antibacterial and anti-protozoal activity and included in the WHO Model List of Essential Medicines. The drug is commercially available in the hyclate (hydrochloride hemiethanolate hemihydrate) or monohydrate form. Since in the crystal structures of both doxycycline presents the same tautomeric form as that observed in the antibiotic-protein complexes, both crystal forms are interesting in terms of modeling antibiotic-protein interactions.

Presented here are the results of the experimental charge density analysis for both doxycycline monohydrate and doxycycline hydrochloride. The network of intra- and intermolecular interactions of the doxycycline in both crystal forms is analyzed and classified in terms of topological analysis, interaction energies and source function contributions. Interaction energies are also compared with the results of theoretical periodic calculations.

The additional proton bound to the O3 oxygen in the case of doxycycline hydrochloride does not change the global conformation of the antibiotic molecule, but it significantly influences the distribution of charges and the resulting electrostatic potential of the molecule. As the oxygen atom O3 is directly involved in the intermolecular interactions of doxycycline with the host proteins, availability of the electron density distribution for both protonated and deprotonated variant enables more exact prediction of the antibiotic-protein interactions at different host protein protonation states.

The conformation of the antibiotic in the crystal lattice of both forms is compared with the conformation known for the antibiotic-target protein complexes deposited in PDB. The major difference is the breaking of the intramolecular hydrogen bond network in order to form two protein-ligand contacts. The differences are also explored by means of Hirshfeld surface analysis of the doxycycline in the crystal network and doxycycline in the protein environment.

AM and KW acknowledge financial support within the Polish NCN MAESTRO grant, decision number DEC-2012/04/A/ST5/00609.