

Poster Presentations

[MS13-P05] **Charge Density Studies of Arsenic(III) Oxide.** Piotr A. Guńka¹, Radosław Kamiński², Janusz Zachara¹

¹ Faculty of Chemistry, Warsaw University of Technology

² Chemistry Department, University at Buffalo, The State University of New York.

E-mail: piogun@ch.pw.edu.pl

Stereoactive lone electron pairs (LEPs) situated on arsenic atomic cores in arsenic(III) compounds are responsible for a number of their interesting structural features. Thanks to their presence, arsenic may be involved in weak interactions such as As...O and As...X (X stands for halogen).[1] It is the directional As...O interactions that cause the sphere-like As₄O₆ molecules to pack in a diamondoid network in the cubic polymorph of As₂O₃, arsenolite, rather than in the closest-packed-sphere-type structure as P₄O₆ molecules do in phosphorus(III) oxide. [2] Recently, Gibbs and co-workers have determined the charge density distribution (CDD) in As₂O₃ polymorphs by means of *ab initio* calculations and have analysed its topological features. [3] Matsumoto et al. investigated the role of LEPs in As, Sb and Bi sesquioxides.[4] We have carried out a very precise high-angle diffraction experiment on arsenolite single crystal using laboratory X-ray source. The obtained charge density distribution (CDD) has been refined in the multipolar model [5] and analysed within the QTAIM (Quantum Theory of Atoms in Molecules) framework. [6] The localisation of stereoactive LEP was used to validate the predictions of the bond valence vector model.[7] The results have been compared with benchmark calculations performed within the Wien2k program suite utilizing the linearized augmented plane wave method. The computations performed by Gibbs et al. are critically evaluated by comparison with the experimental results extended by our own calculations in Gaussian

basis sets.

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

- [1] Pertlik, F. (1979). *Monatshefte Für Chem. Chem. Mon.* **110**, 387–392. Pertlik, F. (1988). *Monatshefte Für Chem. Chem. Mon.* **119**, 451–456. Jiang, X.-M., Xu, Z.-N., Zhao, Z.-Y., Guo, S.-P., Guo, G.-C., & Huang, J.-S. (2011). *Eur. J. Inorg. Chem.* **2011**, 4069–4076.
- [2] Gibbs, G. V., Wallace, A. F., Zallen, R., Downs, R. T., Ross, N. L., Cox, D. F., & Rosso, K. M. (2011). *J Phys Chem.* **114**, 6550–6557.
- [3] Gibbs, G. V., Wallace, A. F., Cox, D. F., Dove, P. M., Downs, R. T., Ross, N. L., & Rosso, K. M. (2009). *J. Phys. Chem. A.* **113**, 736–749.
- [4] Matsumoto, A., Koyama, Y., Togo, A., Choi, M., & Tanaka, I. (2011). *Phys. Rev. B.* **83**, 214110.
- [5] Hansen, N. K. & Coppens, P. (1978). *Acta Crystallogr. Sect.* **A34**, 909–921.
- [6] Bader, R. F. (1994). *Atoms in molecules: a quantum theory*, Oxford University Press Inc.
- [7] Zachara, J. (2007). *Inorg. Chem.* **46**, 9760–9767.

Keywords: arsenic compounds; charge density studies; weak interactions