Poster Presentation

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Dispersed Lone Electron Pairs in Cubic Polymorph of Arsenic(III) Oxide

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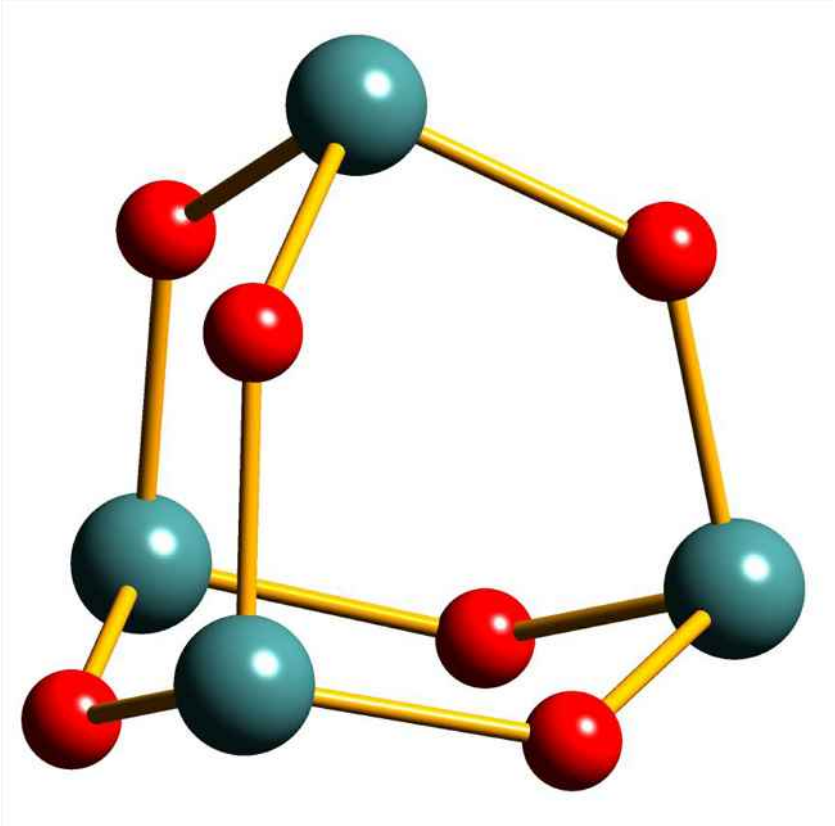
Stereoactive lone electron pairs (LEPs) situated on arsenic atomic cores in arsenic(III) compounds are responsible for a number of their interesting structural features. Thanks to their presence, arsenic may be involved in weak interactions such as As···O and As···X (X stands for halogen). It is the directional As···O interactions that cause the sphere-like As_4O_6 molecules to pack in a diamondoid network in the cubic polymorph of As_2O_3, arsenolite, rather than in the closest-packed-sphere-type structure as P_4O_6 molecules do in phosphorus(III) oxide. Recently, Gibbs and co-workers have determined the charge density distribution (CDD) in As_2O_3 polymorphs by means of periodic *ab initio* calculations and have analysed its topological features.[1] Matsumoto et al. investigated the role of LEPs in As, Sb and Bi sesquioxides.[2] We have carried out a very precise high-angle diffraction experiments on arsenolite single crystals using both laboratory X-ray source and synchrotron X-ray radiation. The obtained diffraction data have been analysed utilising the Hansen-Coppens multipolar model and X-ray constrained wavefunction refinement. CDD resulting from both models has been analysed within the QTAIM (Quantum Theory of Atoms in Molecules) framework. The structural activity and localisation of LEPs has been compared with the predictions of bond valence vector model.[3] 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. The obtained results suggest arsenic LEPs are dispersed into three distinct regions in arsenic atomic core vicinity.

[1] *G. V. Gibbs, A. F. Wallace, D. F. Cox, P. M. Dove, R. T. Downs, N. L. Ross, K. M. Rosso, J. Phys. Chem. A., 2009 113, 736–749.,* ***[2]*** *A. Matsumoto, Y. Koyama, A. Togo, M. Choi, I. Tanaka, Phys. Rev. B., 2011, 83, 214110.,* ***[3]*** *J. Zachara, Inorg. Chem., 2007, 46, 9760–9767.*



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