CrystEngComm

CORRECTION

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Correction: High-pressure and low-temperature structural study of claudetite I, a monoclinic layered As2O3 polymorph

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Correction for 'High-pressure and low-temperature structural study of claudetite I, a monoclinic layered As2O3 polymorph' by Piotr A. Guńka et al., CrystEngComm, 2021, 23, 638–644, https://doi.org/10.1039/D0CE01401J.

Due to a calculation error, the authors would like to replace Fig. 5 in the original article with the revised version shown below:

This error does not affect the conclusions of the article; however, it does affect the discussion of the calculated bond valence vectors (BVVs) of arsenic lone electron pairs for claudetite.

Thus, in the Discussion, the following sentence of text on page 641:

"The magnitude of As resultant BVVs which represents the stereoactivity of the As LEP is fairly constant around 1.03 v. u. and is slightly smaller than the values observed for arsenolite."

should be replaced by

"The magnitude of As resultant BVVs which represents the stereoactivity of the As LEP is fairly constant around 1.22 v. u. and is larger than the values observed for arsenolite, but similar to the values observed for claudetite II."

And the following sentence on page 642:

"The fairly constant value of the LEP BVV of 1.03 v. u. for claudetite I and 1.05 v. u. for arsenolite corresponds to the LEP valence of 1.45 and 1.50 v. u., respectively, indicating that the LEPs are not fully stereoactive."

should be replaced by

"The fairly constant values of the LEP BVV of 1.22, 1.20 and 1.05 v. u. for claudetite I, claudetite II, and arsenolite, respectively, correspond to the LEP valence of 2.09, 2.00, and 1.50 v. u., respectively, indicating that the LEPs are fully stereoactive in the case of claudetite I and claudetite II, but not fully stereoactive in the case of arsenolite. This indicates that the stereoactivity of the As LEP is similar for layered As2O3 polymorphs and smaller for the molecular form, which results from stronger secondary As⋯O bonds in arsenolite revealed by the higher [1]VECN of As atoms in this polymorph."

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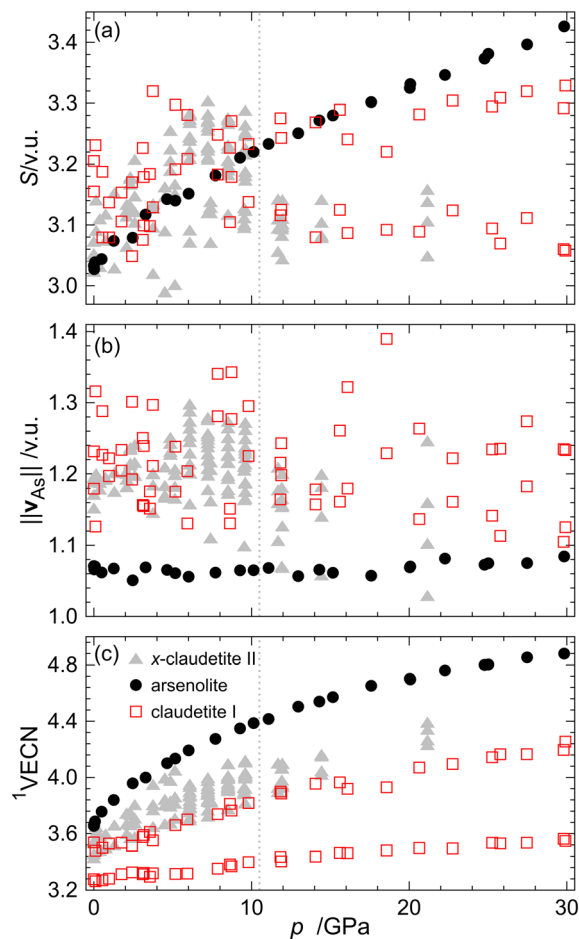
Fig. 5 (a) Bond valence sum, (b) magnitude of the resultant bond valence vector of As atoms and (c) first-order valence entropic coordination number of As atoms for various As_2O_3 polymorphs plotted as a function of pressure. Data for α-, α'-, α''- and β-claudetite II as well as arsenolite come from ref. 10. The grey dotted line indicates the pressure of the first-order phase transition from α''- to β-claudetite II.[2]

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.