Comments

Comment on "Structure of $NaBi_3V_2O_{10}$ and Implications for Ionic Conductivity"

The recent publication in this journal by Sleight's group[1] describing the structure and ionic conductivity prompts us to comment on their observations in light of our earlier published work.[2] Our publication clearly brought out the existence of two polymorphic modifications of $NaBi_3V_2O_{10}$ and we were the first to establish the structure of the α form from the ab initio powder X-ray diffraction technique. It may be pointed out that the work published by Sinclair's group[3,4] was ambiguous as the structure reported in ref 4 (*β*-form) was entirely different from the one reported in ref 3 for which the conductivity data were provided.

This report[1] is misleading in this context since there is no reference to the polymorphic forms of $NaBi_3V_2O_{10}$ to start with and the concluding remarks give an impression to the reader that the structure assigned by us is incorrect. It is elementary knowledge that when structure determination is made via X-ray powder diffraction the oxygen positions are inaccurate and it is obvious that a "re-determination" of the structure using single-crystal and neutron data provide more accurate positions. Also, Sleight's group seems not to refine oxygen occupancies either with single-crystal data or neutron data, which could have provided better insights into implications for ionic conductivity. It must be noted that the vanadium site in the BIMEVOX series is known to display a dynamic disorder[5] and our conclusion was based on this general observation.

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