## Sheffield Hallam University

## Orthorhombic to cubic high temperature phase transition in synthetic Rb2CoSi5O12 leucite analogue

BELL, Anthony <http://orcid.org/0000-0001-5038-5621>

Available from Sheffield Hallam University Research Archive (SHURA) at:

https://shura.shu.ac.uk/32987/

This document is the Accepted Version [AM]

## Citation:

BELL, Anthony (2023). Orthorhombic to cubic high temperature phase transition in synthetic Rb2CoSi5O12 leucite analogue. In: British Crystallographic Association Spring Meeting, Sheffield, UK, 04-06 Apr 2023. British Crystallographic Associaton. (Unpublished) [Conference or Workshop Item]

## Copyright and re-use policy

See http://shura.shu.ac.uk/information.html

Orthorhombic to cubic high temperature phase transition in synthetic Rb<sub>2</sub>CoSi<sub>5</sub>O<sub>12</sub> leucite analogue.

A.M.T.Bell (Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, S1 1WB, UK).

The previously unknown crystal structure of the  $Rb_2CoSi_5O_{12}$  leucite analogue has been determined to be *Pbca* orthorhombic [1]. This is isostructural with the crystal structure of the  $Cs_2CdSi_5O_{12}$  leucite analogue [2], which has ordered tetrahedrally coordinated sites (T-sites).

High temperature X-ray powder diffraction on Rb<sub>2</sub>CoSi<sub>5</sub>O<sub>12</sub> shows a phase transition [1] from *Pbca* orthorhombic to *Pa*-3 cubic at 457 K. This is a similar phase transition to that observed at 566 K in Cs<sub>2</sub>ZnSi<sub>5</sub>O<sub>12</sub> leucite analogue [3]. In the *Pbca* leucite structure for Rb<sub>2</sub>CoSi<sub>5</sub>O<sub>12</sub> there are 6 T-sites, 5 fully occupied by Si and 1 fully occupied by Co. However, in the corresponding *Pa*-3 structure there are only 2 T-sites, 1 fully occupied by Si and 1 partially ordered by Si (2/3 occupancy) and Co (1/3 occupancy). The central channel of the *Pbca* leucite structure is more distorted than for the *Pa*-3 structure. The decrease in distortion of this central channel means that there is a unit cell *decrease* on passing through the transition!



Left Pbca 447 K - Right Pa-3 457 K.



[1] Bell, A.M.T. *Minerals* **13**, (2023) 210.

[2] Bell, A.M.T. et al. Acta Cryst. B50, (1994) 560-566.

[3] Bell, A.M.T. & Henderson, C.M.B. Mineralogical Magazine, 76, (2012) 1257-1280.