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

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Orthorhombic to cubic high temperature phase transition in synthetic $Rb_2CoSi_5O_{12}$ leucite analogue.

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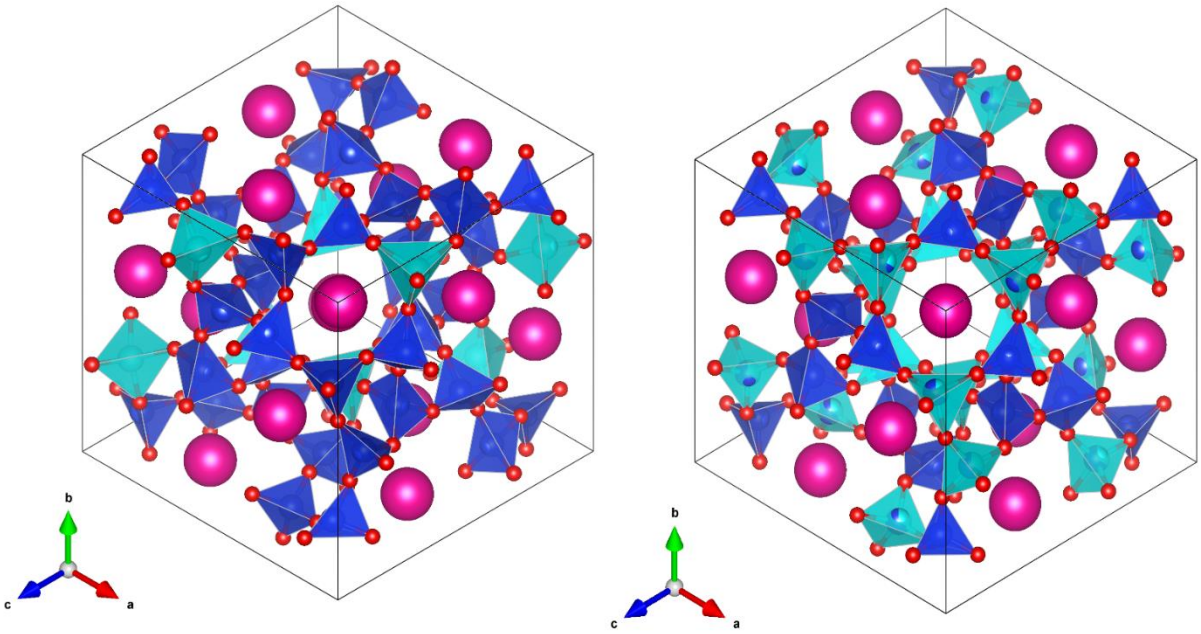
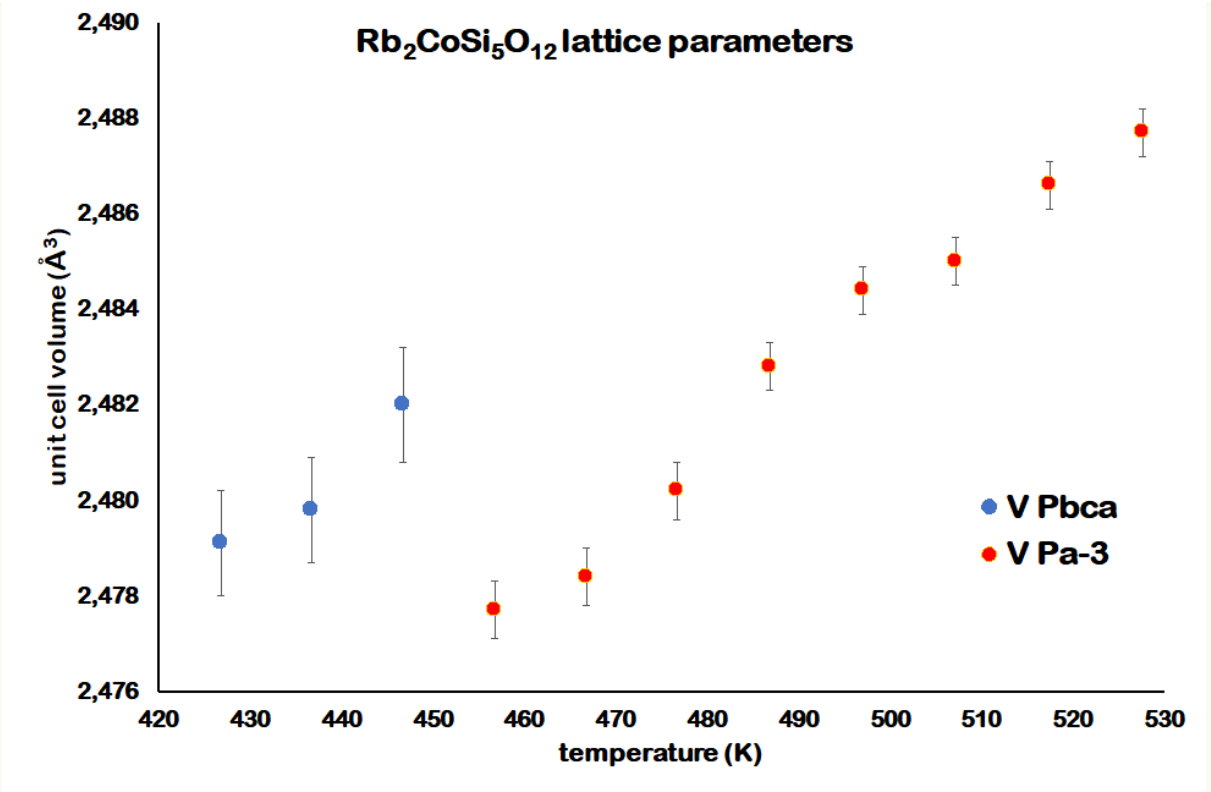
The previously unknown crystal structure of the $Rb_2CoSi_5O_{12}$ leucite analogue has been determined to be *Pbca* orthorhombic [1]. This is isostructural with the crystal structure of the $Cs_2CdSi_5O_{12}$ leucite analogue [2], which has ordered tetrahedrally coordinated sites (T-sites).

High temperature X-ray powder diffraction on $Rb_2CoSi_5O_{12}$ 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 $Cs_2ZnSi_5O_{12}$ leucite analogue [3]. In the *Pbca* leucite structure for $Rb_2CoSi_5O_{12}$ 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.