

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

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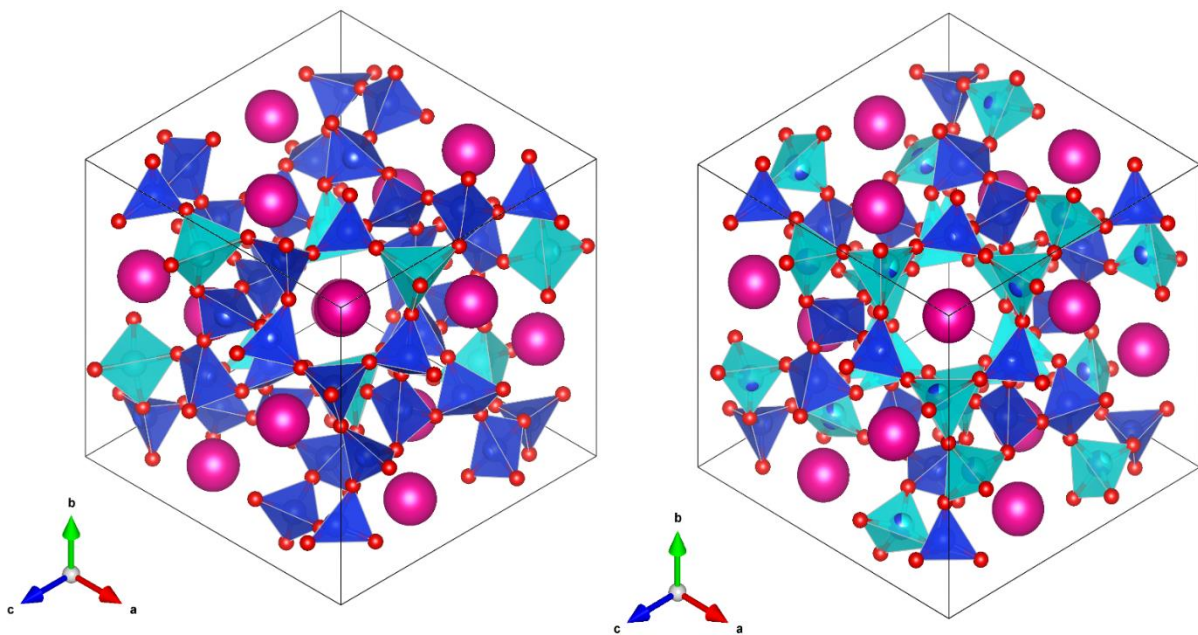
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Orthorhombic to cubic high temperature phase transition in synthetic $\text{Rb}_2\text{CoSi}_5\text{O}_{12}$ leucite analogue.

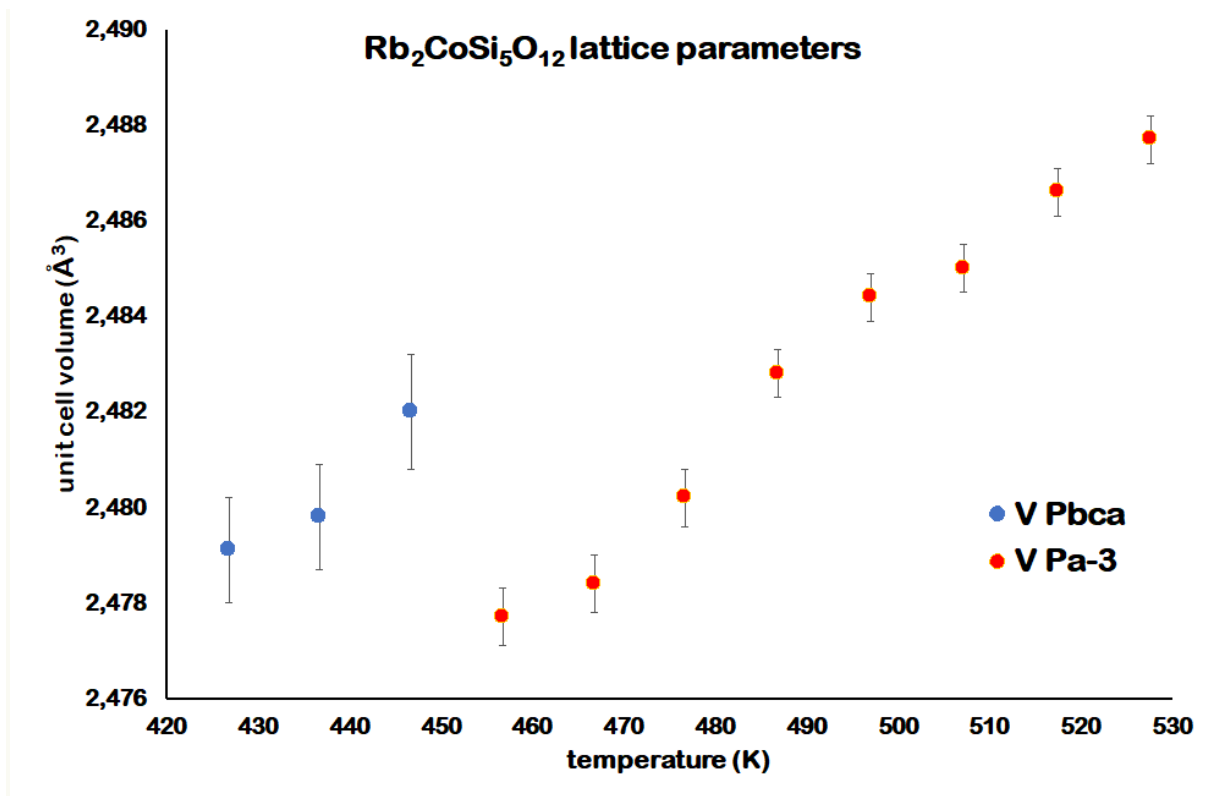
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The previously unknown crystal structure of the $\text{Rb}_2\text{CoSi}_5\text{O}_{12}$ leucite analogue has been determined to be $Pbca$ orthorhombic [1]. This is isostructural with the crystal structure of the $\text{Cs}_2\text{CdSi}_5\text{O}_{12}$ leucite analogue [2], which has ordered tetrahedrally coordinated sites (T-sites).

High temperature X-ray powder diffraction on $\text{Rb}_2\text{CoSi}_5\text{O}_{12}$ 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 $\text{Cs}_2\text{ZnSi}_5\text{O}_{12}$ leucite analogue [3]. In the $Pbca$ leucite structure for $\text{Rb}_2\text{CoSi}_5\text{O}_{12}$ 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.