

**MS27-1-4 It's been a long time coming - temperature dependent structure solution of Rb[SCN]  
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**Abstract**

K[SCN] was the first compound comprising the thiocyanate anion that was crystallographically determined just after the advent of single crystal X-ray diffraction, also introducing its own structure type [1]. The elucidation of the Na and Cs thiocyanates followed in the 1970s, where the Cs compound was found to show a phase transition at high temperature [2-3]. Surprisingly the structure of Li[SCN] was not published until 2014, even though its hydrate had already been commercially available for years [4].

The synthesis of Rb[SCN] had been established as well in the 1970s and its phase transition was discovered in the 1990s [5-6]. However, its low and high temperature structures were only assigned to the K[SCN] structure type and not further investigated.

Rb[SCN] crystallizes in the orthorhombic *Pbcm* space group type at temperatures below 432 K and in the tetragonal *I4/mcm* space group type at higher temperatures [7]. The structural details of the low and high temperature phases and their relations to other alkali-metal thiocyanates will be discussed.

**References**

- [1] H. P. Klug, *Z. Krist. – Cryst. Mater.*, **1933**, *85*, 214 – 222.
- [2] S. Manolatos, M. Tillinger, B. Post, *J. Solid State Chem.*, **1973**, *7*, 31–35.
- [3] P. H. van Rooyen, J. C. A. Boeyens, *Acta Crystallogr.*, **1975**, *B31*, 2933–2934.
- [4] O. Reckweg, A. Schulz, B. Blaschkowski, Th. Schleid, F. J. DiSalvo, *Z. Naturforsch. B Chem. Sci.*, **2014**, *69*, 17–24.
- [5] S. S. Ti, S. F. A. Kettle, Ø. Ra, *Spectrochim. Acta Mol. Spectrosc.*, **1976**, *32*, 1603–1613.
- [6] A. Fuith, *Phase Trans.*, **1997**, *62*, 1–93.
- [7] A. Shlyaykher, T. Pippinger, T. Schleid, O. Reckweg, F. Tambornino, *Z. Krist. - Cryst. Mater.*, **2022**, *237*, 69 – 75.