

been assigned (Ryan & Swanson, 1976) as $P4/nmc$, derives from a $\text{Cr}(\text{CN})_6^{3-}$ rotary mode condensing out at the zone boundary (X point). Furthermore, the tetragonal diffraction exhibited by $\text{Cs}_2\text{LiCr}(\text{CN})_6$ at room temperature is a result of twinning which is clearly evident in the optical properties.

C. Cs^+ ion translation

The space group reported by Chowdhury (1976) does not allow translational degrees of freedom for the Cs^+ ion. This is inconsistent with the observation that the second phase change (310 K) is second order involving a soft mode (Raman) which can only be assigned to Cs^+ translational motion (Ryan & Swanson, 1976). Moreover, the X-ray intensities of a class of reflections in $P2_1/n$, which are attributable primarily to Cs^+ displacement, can be traced from below 310 K to zero intensity.

Finally, replacement of the Li atom in the related $\text{Cs}_2\text{LiFe}(\text{CN})_6$ by Na or K results in room-temperature-stable phases in $P2_1/n$ (Fletcher & Gibb, 1977). The replacement of Li by its larger congeners is roughly equivalent to lowering the temperature of the $\text{Cs}_2\text{LiFe}(\text{CN})_6$ crystal (Rafalko, Swanson & Beall, 1977). Raman scattering and optical-microscope studies of $\text{Cs}_2\text{LiFe}(\text{CN})_6$ (Swanson, Lucas & Ryan, 1978) show that this material undergoes two phase transformations below room temperature ($T_c^1 = 221$ K and $T_c^2 = 170$ K). We believe that the temperature-dependent structure of $\text{Cs}_2\text{LiCr}(\text{CN})_6$ is important in that it is one of a limited set of crystals which exhibit a true second-order

structural phase change; heat capacity data for $\text{Cs}_2\text{LiCr}(\text{CN})_6$ exhibit a small anomaly at 310 K characteristic of a second- or higher-order displacive phase change (McCormack, private communication). It is likely that the lattice instabilities exhibited by $\text{Cs}_2\text{LiCr}(\text{CN})_6$ are common to several members of the large class of salts possessing the elpasolite structure.

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References

- CHOWDHURY, M. R. (1976). *Acta Cryst.* **B32**, 2728–2729.
 CHOWDHURY, M. R., WEDGWOOD, F. A., CHADWICK, B. M. & WILDE, H. J. (1977). *Acta Cryst.* **B33**, 46–52.
 FLETCHER, S. R. & GIBB, T. C. (1977). *J. Chem. Soc. Dalton Trans.* pp. 309–316.
 RAFALCO, J. J., SWANSON, B. I. & BEALL, G. W. (1977). *J. Solid State Chem.* **21**, 195–201.
 RYAN, R. R. & SWANSON, B. I. (1974). *Inorg. Chem.* **13**, 1681–1684.
 RYAN, R. R. & SWANSON, B. I. (1976). *Phys. Rev. B*, **13**, 5320–5329.
 SWANSON, B. I. & JONES, L. H. (1974). *Inorg. Chem.* **13**, 313–316.
 SWANSON, B. I., LUCAS, B. C. & RYAN, R. R. (1978). *J. Chem. Phys.* In the press.

Acta Cryst. (1978). **B34**, 1399

The room-temperature structure of $\text{Cs}_2\text{LiCr}(\text{CN})_6$. By M. R. CHOWDHURY, *Materials Physics Division, AERE Harwell, Oxfordshire OX11 0RA, England*

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In a previous paper the results were reported of a profile analysis of neutron powder diffraction data on the room-temperature structure of $\text{Cs}_2\text{LiCr}(\text{CN})_6$ (Chowdhury, Wedgwood, Chadwick & Wilde, 1977). The structure was shown to be consistent with the space group $P4/nmc$. Because of twinning problems it has not been possible to carry out a sufficiently reliable single-crystal analysis of the room-temperature structure of the compound (Ryan & Swanson, 1974); hence the special significance of the powder profile results. According to Ryan & Swanson (1978), the room-temperature structure is $P2_1/n$, there being an intermediate phase transformation between the high temperature ($T > 350$ K) $Fm3m$ and the room-temperature structure. Their arguments are based largely on

the evidence of optical spectroscopic data. In the light of this evidence, the powder data of Chowdhury *et al.* (1977) need to be re-examined; it will then be possible to say whether a better agreement is obtained with the space group $P2_1/n$, proposed by Ryan & Swanson (1978).

References

- CHOWDHURY, M. R., WEDGWOOD, F. A., CHADWICK, B. M. & WILDE, H. J. (1977). *Acta Cryst.* **B33**, 46–52.
 RYAN, R. R. & SWANSON, B. I. (1974). *Inorg. Chem.* **13**, 1681–1684.
 RYAN, R. R. & SWANSON, B. I. (1978). *Acta Cryst.* **B34**, 1398–1399.