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M Rousseau, J. Nouet, R. Almairac, B. Hennion. Soft phonon and central peak in RbCaf₃. Journal de Physique Lettres, 1976, 37 (2), pp.33-35. 10.1051/jphyslet:0197600370203300 . jpa-00231228

HAL Id: jpa-00231228

<https://hal.science/jpa-00231228>

Submitted on 1 Jan 1976

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Classification
 Physics Abstracts
 7.488

SOFT PHONON AND CENTRAL PEAK IN RbCaF_3

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(Reçu le 10 novembre 1975, accepté le 4 décembre 1975)

Résumé. — Nous présentons brièvement quelques résultats concernant les premières expériences de diffusion inélastique des neutrons qui ont permis de mettre en évidence un pic central et un *soft* phonon près de la transition structurale à 193 K dans RbCaF_3 .

Abstract. — We briefly present some results of preliminary neutron scattering experiments showing unambiguously the coexistence of a central peak and a soft phonon near the 193 K phase transition in RbCaF_3 .

1. Introduction. — In the fluoperovskite family into the general formula AMF_3 , up to now only KMnF_3 has been known for its structural phase transition due to MF_6 octahedra rotations [1]. Nevertheless ionic radius and force constants investigations allowed us to forecast the possibility of such rotations in the fluoperovskites containing M ions large enough to determine the dimensions of the cell and leave the A ions free to move with respect to the octahedra [2]. Indeed both X-ray diffraction and Raman scattering experiments have shown that RbCdF_3 , TlCdF_3 and RbCaF_3 undergo a transition from a cubic (O_h^1) to a tetragonal (D_{4h}^{18}) space group respectively at 124 K, 191 K and 193 K [2, 3, 4, 5]. These transitions are due to the condensation of a vibrational mode associated with the R point of the cubic Brillouin zone similar to the 105 K phase transition in SrTiO_3 and to the 186 K phase transition in KMnF_3 .

In the quadratic phase, the temperature dependence of the soft mode may be studied by Raman scattering experiments [2], [7, 8]. As this is no longer possible in the cubic phase, inelastic neutron scattering experiments are helpful to understand the behaviour of this mode [6]. Owing to the great absorption of neutrons by cadmium such experiments are impossible on RbCdF_3 and TlCdF_3 but may be carried out on RbCaF_3 . The first measurements performed at Oak Ridge [9] confirmed that the

transition arises from the condensation of an R_{25} zone boundary phonon. We briefly present in this paper some new results showing that as in e.g. SrTiO_3 , this phonon softening is accompanied by the appearance of a central peak in RbCaF_3 .

2. Experimental. — We have used a good single crystal (volume 2 cm^3 , mosaic spread less than $3'$ of arc) grown by the Bridgman-Stockbarger technique. Preliminary measurements were carried out on the EL 3 Saclay reactor, from which a rigid ion model was constructed and dynamical structure factors calculated.

Energy scans at the R point of the Brillouin zone were performed on the triple-axis spectrometer IN 2 at the I.L.L. High-Flux Reactor. The incident neutron energy was fixed at 4.9 meV from a pyrolytic graphite (002) monochromator. Higher-order contamination was reduced to a negligible level using a Ge (111) analyser combined with a cooled beryllium filter. The crystal was mounted in a liquid helium cryostat assuring a stability of temperature better than 0.03 K.

In order to perform the proper resolution corrections we have measured the curvatures of the dispersion surface in the vicinity of the R_{25} mode respectively in the R-X, R-M and R- Γ directions. The calculations are in progress and we just present here a summary of the most important rough data.

3. **Results.** — The critical temperature T_c was determined by monitoring the intensity of a $(\frac{3}{2} \frac{1}{2} \frac{1}{2})$ R point as a function of temperature. The results (Fig. 1) are consistent with our X-rays measurements giving $T_c = 193 \pm 1$ K.

FIG. 1. — Temperature dependence of the elastic scattering at the $(\frac{3}{2} \frac{1}{2} \frac{1}{2})$ R point.

Figure 2 shows high resolution constant- Q scans at the $(\frac{3}{2} \frac{1}{2} \frac{1}{2})$ R point performed successively for $T - T_c = 31, 22, 19$ and 8 K. This figure reveals two important features :

- the R_{25} soft phonon,
- a narrow central peak whose linewidth is that of the instrumental resolution. We may notice that this component already appears at 22 K above T_c .

Better statistic will be necessary in order to decide whether or not a quasi-elastic contribution is contained in the rather broad central component which lie at the bottom of the central peak (scans at 212 K and 215 K).

In order to measure the anisotropy of the correlation between octahedra we have done constant $\omega = 0$

FIG. 2. — High resolution constant Q scans at $(\frac{3}{2} \frac{1}{2} \frac{1}{2})$ for $T = 224$ K, 215 K, 212 K and 201 K.

FIG. 3. — Constant $\omega = 0$ scan along a line joining M and R points.

scans in the vicinity of the $(\frac{3}{2} \frac{1}{2} \frac{5}{2})$ R point respectively in the $(0 \ 0 \ \xi)$ and $(3 \ \xi \ \xi \ 0)$ directions. Contrary to NaNbO_3 recently studied by F. Denoyer *et al.* [10], for RbCaF_3 , even at 80 K above T_c , the elastic intensity is mainly restricted to the vicinity of the R point (Fig. 3). Further experiments near other R points are required to separate the T_5 and T_2 phonons contribution from the quasielastic critical scattering.

4. Conclusion. — From these first measurements, we conclude that RbCaF_3 with its well separated underdamped soft phonon and central peak shows

a behaviour very similar to SrTiO_3 . These results are very promising because RbCaF_3 seems to be the first fluoperovskite for which a full determination of the soft phonon and central component parameters as a function of temperature may be possible. Further experiments are planned in the near future and should provide a better understanding of these features.

Acknowledgments. — We thank J. Y. Gesland for the crystal growing, R. Currat and B. Dorner for their fruitful comments, P. Flores and B. Taffu for their opportune technical assistance.

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