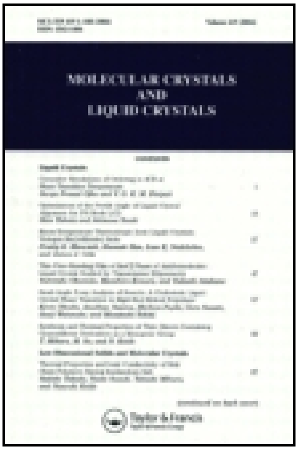

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Neutron and X Ray Studies of The Quasi One Dimensional Conductor $K_{0\,3}MoO_3$

J. P. Pouget [a], C. Escribe-filippini [b], B. Hennion [c], R. Currat [d], A. H. Moudden [a], R. Moret [a], J. Marcus [b] & C. Schlenker [c]

[a] Laboratoire de Physique des Solides, F91905, Orsay
[b] L.E.P.E.S., C.N.R.S., BP 166, F38042, Grenoble
[c] L.L.B., C.E.N., Saclay, F91191 Gif sur, Yvette
[d] I.L.L., Avenue des Martyrs, 156 X, F 38042, Grenoble

Version of record first published: 20 Apr 2011.

To cite this article: J. P. Pouget, C. Escribe-filippini, B. Hennion, R. Currat, A. H. Moudden, R. Moret, J. Marcus & C. Schlenker (1985): Neutron and X Ray Studies of The Quasi One Dimensional Conductor $K_{0\,3}MoO_3$, Molecular Crystals and Liquid Crystals, 121:1-4, 111-115

To link to this article: http://dx.doi.org/10.1080/00268948508074842

Mol. Cryst. Liq. Cryst. 1985, Vol. 121, pp. 111-115
0026-8941/85/1214-0111/$10.00/0

NEUTRON AND X RAY STUDIES OF THE QUASI ONE DIMENSIONAL CONDUCTOR $K_{0.3}MoO_3$

J. P. POUGET[(a)], C. ESCRIBE-FILIPPINI[(b)], B. HENNION[(c)]
R. CURRAT[(d)], A. H. MOUDDEN[(a)], R. MORET[(a)],
J. MARCUS[(b)], and C. SCHLENKER[(b)]

(a) Laboratoire de Physique des Solides, F91905 Orsay
(b) L.E.P.E.S., C.N.R.S., BP 166, F38042 Grenoble
(c) L.L.B., C.E.N. Saclay, F91191 Gif sur Yvette
(d) I.L.L., Avenue des Martyrs, 156 X, F 38042 Grenoble

Abstract A detailed study of the temperature dependence of the Kohn anomaly and of the wave vector of the incommensurate modulation of $K_{0.3}MoO_3$ is given.

INTRODUCTION

The quasi 1D metal $K_{0.3}MoO_3$ shows at T_c(~180K) a metal to semiconductor Peierls transition toward a charge density wave (C.D.W.) modulated structure characterized by the wave vector $\vec{q}_o = (0,q_b,0.5)$, where the in chain component, q_b, is incommensurate and temperature dependent[1]. Furthermore, nonlinear conductivity attributed to the sliding of C.D.W. has been observed below T_c[2].

II NEUTRON EVIDENCE OF A KOHN ANOMALY

After the X ray observation of quasi 1D structural fluctuations above T_c[1], Sato et al[3] show evidences of the formation of a Kohn anomaly in the phonon spectrum without identifying clearly in which branch it takes place. Subsequent measurements[4], summarized in Fig. 1, show that it primarily belongs to an optic branch which couples with the acoustic branch polarized along the monoclinic b (chain) direction.

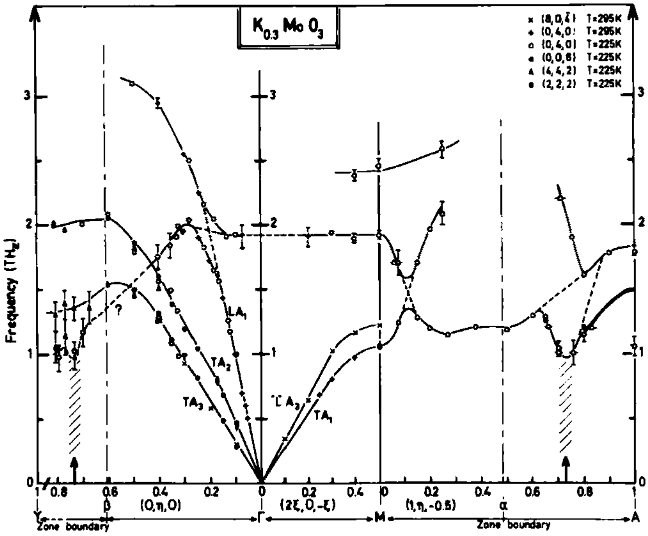

FIGURE 1 Low lying phonon branches of $K_{0.3}MoO_3$. Arrows point toward the position of the Kohn anomaly. (only the largest error bars are given)

III DYNAMICS OF THE KOHN ANOMALY

The softening of the Kohn anomaly and the growth of a central peak, as one approaches T_c from above are best illustrated by the scans shown in Fig. 2. Thus the scattering cross section can be parameterized by the sum of a damped harmonic oscillator and of a (resolution limited) central peak:

$$S(Q,\omega) = \frac{N}{\pi} \frac{\omega}{\left(1-\exp\frac{-\hbar\omega}{kT}\right)} \frac{\Gamma_q}{\left(\omega^2-\omega_q^2\right)^2 + \omega^2\Gamma_q^2} + N_o\delta(\omega) \quad (1)$$

Because of the sharpness of the Kohn anomaly, reliable values of the quasi harmonic frequency ω_o, and of the damping constant Γ_o, at the critical wave vector, $\vec{q}_o$, can be obtained only after deconvolution of the experimental data with the experimental

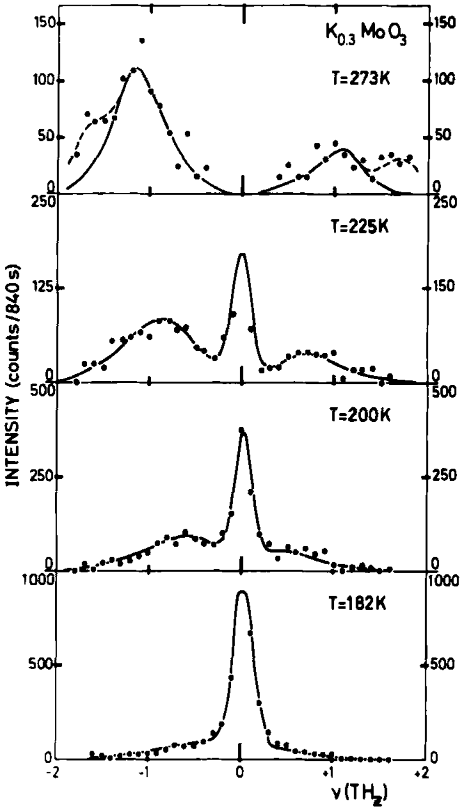

FIGURE 2 Energy scans at $\vec{Q}=(1,3.27,-0.5)$. (The background has been substracted)

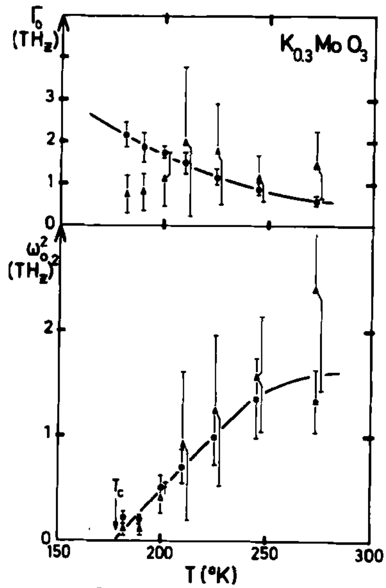

FIGURE 3 Temperature dependence of Γo and ω_o^2. Full dots and empty triangles correspond respectively to N constant and free to vary in the fitting procedure of eq. (1).

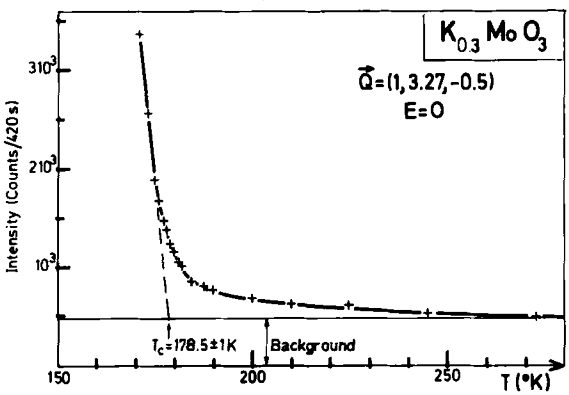

FIGURE 4 Temperature dependence of the elastic scattering at $\vec{Q}=(1,3.27,-0.5)$.

resolution. The procedure, given in ref. (4), leads to the results shown in Fig. 3. When T_c is approached from above, the quasi harmonic frequency has a mean field temperature dependence $\left[\omega_o^2 \sim (T-T_c)\right]$, with perhaps a slight saturation at about 0.4 TH_z near T_c, when the central peak begins to grow sharply (Fig. 4). The temperature dependence of the damping constant Γo is more difficult to obtain. However with the approximation usually done, N = constant in (1), Γo (dots in Fig. 3) appears to increase for T decreasing. This increase is expected in the case of a Peierls instability.

IV TEMPERATURE DEPENDENCE OF THE WAVE VECTOR

After an almost linear increase, from 0.71 ± 0.01 at room temperature, the $2k_F$ wave vector $(1-q_b)$ saturates below about 100K at a value: $1-q_b = 0.7495 \pm 0.0005$ for the X ray data of

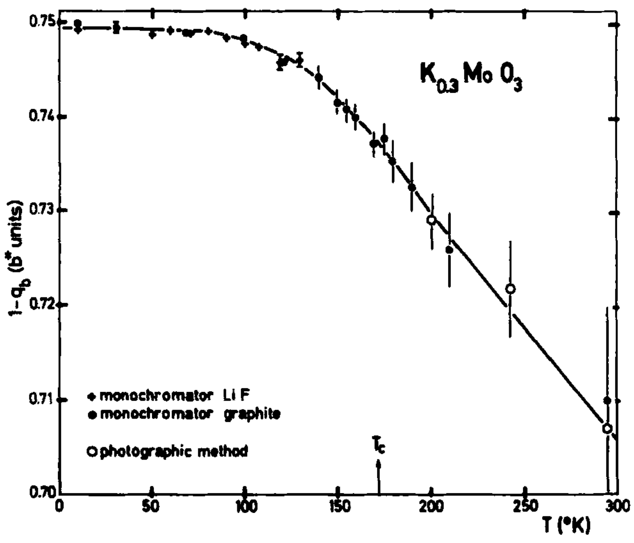

FIGURE 5 Temperature dependence of the wave vector component $1-q_b$ ($\equiv 2k_F$), measured by X ray scattering above and below T_c.

Fig. 5, 0.748 ± 0.001 for the neutron data of ref. 3 and 4 and X ray data of ref. 5, which is systematically found below the commensurate value 3/4. None of these data show the well defined 110K incommensurate-commensurate phase transition quoted in ref. 6. The temperature dependence of $2k_F$, which value is generally determined by the band filling, is not clearly understood. It might be related to the presence of the 2 quasi one dimensional bands suggested in ref. 1, which crosses the Fermi level at very close k_F values.

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