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Order-Disorder Phase Transition in a Triiodide Chain Compound: $\text{DIPS}\varnothing_4 (\text{I}_3)_{0.76}$

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ORDER-DISORDER PHASE TRANSITION IN A TRIIODIDE CHAIN
COMPOUND : $\text{DIPS}\phi_4 (\text{I}_3)_{0.76}$

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Abstract The ordering process of triiodide chains in the organic conductor $\text{DIPS}\phi_4 (\text{I}_3)_{0.76}$ has been studied by X ray scattering.

STRUCTURE OF THE COMPOUND

$\text{DIPS}\phi_4 (\text{I}_3)_{0.76}$ is an organic conductor belonging to the radical-ion family¹. It is grown by the direct oxydation of $\text{DIPS}\phi_4$ molecules by iodine in a solvent.

$\text{DIPS}\phi_4$ columns running along the c-axis delimit parallel channels filled with I_3^- anions (see below).

Crystal system : tetragonal

Space group : $P 4b2$

Unit cell a : 19.74 Å

c : 3.721 Å

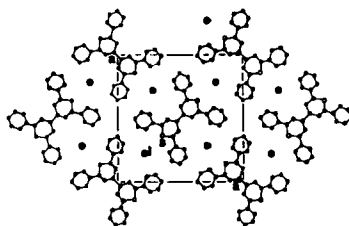


FIGURE 1. Projection of the structure along the c axis²

STRUCTURE OF THE TRIIODIDE CHAINS AT ROOM TEMPERATURE

At room temperature X ray photographs reveal intense diffuse lines perpendicular to the c axis³. It has been shown that these lines

were due to the disordered triiodide channels. Furthermore they present only small modulations, showing that the different I_3^- chains are very weakly correlated³. Fig. 2-a represents a microdensitometer scan of a photograph along the c-axis (1 index). We see well defined peaks which broaden as l^2 with increasing line index l . This broadening can be viewed as resulting from 1D liquid fluctuations; this is also encountered in other triiodide compounds⁴. A model in which the interactions between I_3^- units in a channel are assumed to be harmonic and between first neighbours has been used⁵⁻⁶. As can be seen on Fig.2-b, it accounts relatively well for the observed intensity. The additional lines (arrows) have been interpreted as a modulation of the I_3^- chains by the host lattice.

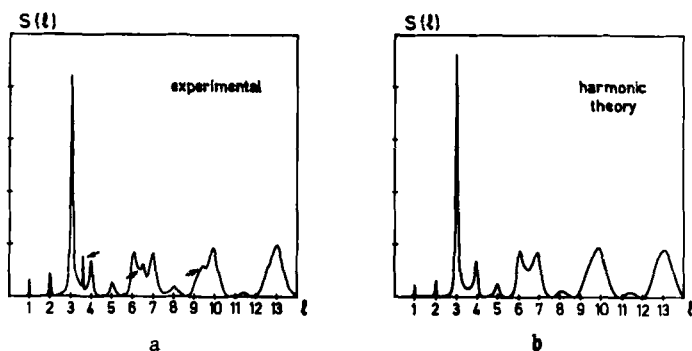


FIGURE 2.a. : Microdensitometer reading along the c axis.

(corrected for absorption and polarization)

FIGURE 2.b. : Theoretical intensity (harmonic model) corrected for the molecular factor of I_3^- .

EFFECT OF THE TEMPERATURE

As the temperature is lowered the first diffuse line becomes clearly modulated, this means that lateral correlations between triiodide chains develop. These precursor phenomena condense into

Bragg spots at about $T_c = 185$ K. Thus below T_c triiodide chains are laterally and longitudinally long-range ordered.

STUDY OF THE ORDERING PROCESS

The ordering process may be described by the Bragg spots appearing on the diffuse lines : the intensity of a Bragg spot appearing on the l^{th} line is proportional to the square of the l^{th} Fourier component of the mass-density. In Fig. 3 we have plotted the intensity of Bragg spots appearing on the first four lines ($l = 1$ to 4).

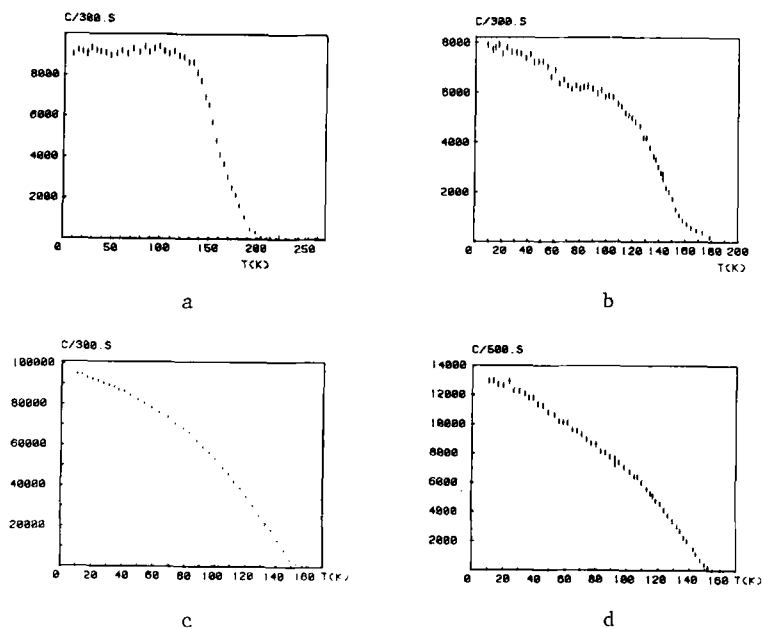


FIGURE 3.a.b.c.d. Intensity of Bragg spots appearing respectively on line 1, 2, 3, 4 versus temperature.

DISCUSSION

We see that Bragg spots develop first on the first line, then on the second one and the third and fourth ones; the last two intensities displaying practically the same behaviour. Furthermore the intensity of $\ell = 1$ Bragg spots saturates at about 100 K. A mean field theory of this transition, using the harmonic model has been developed by V.J. Emery and J.D. Axe⁵. It accounts well for the progressive apparition of the Bragg spots with increasing line index but not for the saturation of the $\ell = 1$ Bragg spots and the rapid growth of the others. A possible explanation could be in the broad conductor/semi-conductor phase transition that occurs at about T_C ⁷. As the conductivity of the $DIPS\phi_4$ columns diminishes, the screening between I_3^- chains decreases, which increases the coupling between them. This could lead to the observed avalanche effect.

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