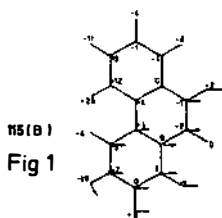


TEMPERATURE DEPENDENCE OF INTENSITY FOR SOME LOW-FREQUENCY RAMAN BANDS IN CRYSTALLINE PHENANTHRENE

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Among several investigations performed by different techniques in order to confirm the existence of the phase transition in phenanthrene or to explain its nature, the results obtained by Spielberg et al. /1/ in neutron inelastic measurements represent a challenge to molecular spectroscopists. He assumed that at 68°C molecular conformational changes in crystal lattice give rise to a new degree of freedom. The intramolecular regrouping proposed involves the positions of the two overcrowded H atoms /2/. The molecular symmetry C_2 is expected to change to the symmetry C_s . The number of Raman active modes remains the same in both phases, but the proposed conformational change should affect some of the low-frequency torsional modes /3/. The torsional mode, which is roughly drawn in Fig. 1 and which



was assigned to the bands 112A and 116B, should, in our opinion, be very sensitive to conformational changes assumed by Spielberg. As shown in Fig. 2, no abrupt change in frequency was observed for these bands, although they are temperature-sensitive in the range from 45° to 72°C. This fact and the absence of new bands seems to indicate that there is no conformational molecular change, at least not such as could be observed by vibrational spectroscopy. The band 116B exhibits a large variation in intensity with temperature, as shown in Fig. 3. The intensity of the band decreases with increasing temperature. It must be emphasized that the band 116B does not disappear and its frequency can be measured up to melting point. Fig. 4 shows the comparison between temperature dependence of intensities for the torsional mode 116 cm^{-1} and the librational mode 99 cm^{-1} . The intensities of both bands were measured relative to the band 63 cm^{-1} . The integral in-

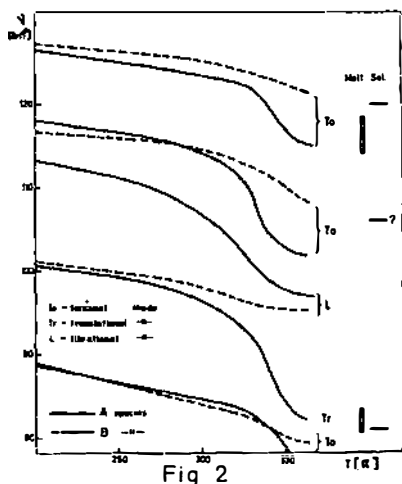


Fig 2

intensity had to be considered due to the considerable broadening of the bands with temperature. The observed intensity variation occurs in the temperature range far from the phase transition.

References

1. D.H. Spielberg et al., J. Chem. Phys. 54 (1971) 2597.
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3. J. Godec et al., J. Chem. Phys., in press.

