22.1–1 THE GENERALIZED CRYSTALLOGRAPHY.
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The wellknown intensity function $I(b) = 1/v \cdot f^2 \widehat{Z S}^2$ of the kinematic scattering of a crystal reported by Ewald (Proc. Phys. Soc.(London),(1940) 52, 167) was generalized in 1950 to the so-called ideal paracrystal (Hosemann, Z. Phys. (1960) 128, 465). Ewald's peak function Z(b) was replaced by the Fouriertransform of a convolution polynom which depends on at least nine parameters g_{ik} (i,k = 1,2,3) which define liquid-like relative distance variances of adjacent lattice bricks. The shape factor of a paracrystal with N_i-netplanes in the direction i is related to the value g_{ii} by $\sqrt{N_i} g_{ii} = \alpha^*$. In 20 years of systematic work this formula was established experimentally for real microparacrystals with a value $\alpha^* = 0.15 \pm 0.05$, including matter ranging from melts with values $g_{ik} \sim 0{,}10$ up to catalysts with $g_{ik} \sim 0{,}01$. Just recently statistical methods led to the proof that there exists a g_{ik}-conducted equilibrium state where the α^*-relation defines the average number of netplanes in an ensemble of microparacrystals (Hosemann et al., Colloid and Polymer Sci. (1981) 259, 1161). A novel tangential intermolecular potential energy A_o plays the dominant role and leads to the free enthalpy ΔG given for cubic microparacrystals by $\Delta G = N^{\frac{2}{3}} \sigma + N^3 G_v + N^4 A_o g_{ik}$. From line profile- and TEM-experiments two further direct evidences were obtained which confirm the reality of this new kind of equilibrium state (Hindeleh, Hosemann, Polymer (1982) 23, 1101) and the fundamental importance of the α^*-relation for all colloids (Hosemann, Colloid and Polymer Sci. (1982) 280, 864).

22.1–2 X-RAY STUDY OF PHASE TRANSITION IN FOUR RING AROMATIC ESTER. By B.Pura, J.Zacharski, J.Przedmojski, R.Dąbrowski and K.Pyc, Institute of Physics, Warsaw Technical University, Koszykowa 75, 00-662 Warszawa, Military Technical Academy, 00-908 Warszawa, Poland

The liquid crystal of C_8H_{17}-⟨⟩-⟨⟩-COO-⟨⟩-⟨⟩-CN has been investigated by DSC, by polarization microscopy and by X-ray diffraction. The following phase diagram has been determined:

Cr 118° N_{re} 160.5° S_A 190° N 343° Iso

The samples have been orientated in magnetic field of 7 kGs. X-ray experiments have been performed with the use of photographic and spectrometric method. In the S_A phase a single peak with wave vector $q_1 = 0.150$ Å^{-1} has been observed while in N_{re} phase two sharp peaks $q_2 = 0.132$ Å^{-1}, $q_3 = 0.188$ Å^{-1} at 110°C have been detected. The measurements of X-ray critical scattering near the S_A – N_{re} phase transition have been carried out on two – crystal spectrometer with the use of Cu_K radiation monochromatized with help of two Ge flat crystals. The longitudinal / $q_\perp = 0$, $q_\parallel$ – varying / and transverse / $q_\parallel = q_1$, $q_\perp$ – varying/ scans have been carried out in N_{re} phase. The longitudinal and transverse correlation lengths have been found to be equal to $\xi_\parallel = 280$ Å, $\xi_\perp = 30$ Å respectively for the fixed temperature $T = (T_c - 2)$°C. The temperature behaviour of the intensity of the peaks has been measured in the N, S_A and N_{re} temperature range.

22.1–3 CRITICAL SCATTERING CROSS-SECTION WITH LIQUID CRYSTAL POINT-GROUP SYMMETRY.
By J. Kociński, Warsaw Technical University Institute of Physics, Koszykowa 75 00-662 Warszawa, Poland.

Symmetry of liquid crystals has been recently discussed by W. Helfrich /J. de Physique /1979/ 40, C3-105/ and by V. L. Indenbom and E. B. Loginov /Kristallografiya /1981/ 26, 925/. Critical scattering of X-rays in a liquid crystal at temperatures above a phase transition point is caused by fluctuations of the corresponding low-temperature phase. Critical scattering data therefore could reveal the symmetry of the low-temperature phase if a scattering cross-section having the symmetry of that phase were available. A method of calculating critical scattering cross-section which has the point-group symmetry of the scattering system /J. Kociński, Theory of Symmetry Changes at Continuous Phase Transitions, Elsevier 1983/ has been applied to liquid crystals. This method consists in constructing a correlation function, which is invariant under the symmetry operations of the relevant point group, whose Fourier transform yields a cross-section with the same symmetry. Critical scattering cross-sections with 6/mmm and ∞/mmm symmetries have been determined. They enable the interpretation of the constant scattered intensity curves which have been determined by critical X-ray scattering in DHB smectic, at the phase transition smectic B → isotropic liquid /B. Pura and J. Przedmojski, Phys. Lett. /1983/ A96, 98/.

22.1–4 AN ANALYSIS OF THE DIFFUSE X-RAY SCATTERING IN THE ORIENTATIONALLY DISORDERED PHASE OF HEXACHLOROETHANE. By P. Gerlach[x+] and W. Prandl[x] x Inst. f. Kristallographie der Universität Tübingen Charlottenstr. 33, D-7400 Tübingen. + Institut Laue-Langevin, BP 156X, Centre de Tri, F-38042 Grenoble, France.

The high temperature phases of numerous molecular crystals are characterised by orientational disorder. Scattering patterns taken in these so-called plastic phases show only a few weak Bragg reflections superimposed on a strong continuum of diffuse scattering. We demonstrate using the example of hexachloroethane how the analysis of diffuse X-ray scattering in highly disordered systems can give corresponding and complementary information to a conventional structure determination using Bragg intensities. The work is divided into two parts.

A model structure generated by a Monte Carlo method is compared with the experimental data. The Fourier-transformed one-particle model scattering density describes very well the diffuse patterns coming from uncorrelated disordered molecules. By this simulation we demonstrate clearly the influence of the hard core repulsive force considered in the model on the rotational-translational distribution of the molecules.

Furthermore, the existence of a one-dimensional short range orientational order is proved. The corresponding planes of diffuse intensity can be described by using an extended Ising model for the orientation, which has several possible directions.