05.1-20 DISORDER AND DIFFUSE SCATTERING IN 1-D SYSTEMS: DIETHYL-PHENAZINIUM-IODIDE($E_2PI_{1.6}$), K-HOLLANDITE($K_{1.54}Mg_{0.77}Ti_{7.23}O_{16}$). By U.Wildgruber, E.Roßhirt, F.Frey, H.Boysen, Institut für Kristallographie, Universität München, F.R.Germany.

X-ray and neutron investigations were carried out on compounds consisting of two incommensurate substructures which are weakly bound together: chains of molecules or ions- parallel to a unique axis- are embedded within a framework structure. Diffuse scattering methods give insight into order/disorder behaviour along the chains, short range correlations between them, and common superordering phenomena of framework and included chains. $E_2PI_{1.6}$ is pseudotetragonal with slight monoclinic distortions, stacks of organic E_2P molecules surround chains of I_3-molecules. A characteristic diffuse layer line system was interpreted earlier by 1-d liquid models of uncorrelated iodine chains (Roßhirt et al. Acta Cryst.B41(1985)66). This is an approximation even at r.t.: all diffuse layers exhibit short range modulations which become more pronounced at low temperatures (→25 K). A second layer line system is due to a doubled chain period and may be interpreted quantitatively by a displacement modulation where the I_3-units are distributed- on the average- along the generators of cones (cone axis parallel to the c-axis). Below 200 K further diffuse layers occur corresponding to a sixfold chain period. This period is in register with an 11-fold superperiod along the organic stacks as indicated by satellite sheets to the Bragg-layers. In consequence, both substructures have a tendency to commensuration along c and become stronger correlated in lateral directions. K-Hollandite has a tetragonal structure which may be considered as a rutile derivate: corner and edge sharing Mg/TiO_6-octahedra make up a framework with large square tunnels, i.e.strings of cavities parallel to c, where K^+-ions are located. From Bragg data a model of the K distribution in the cavities was given by Weber et al.(Sol.St.Ionics 9(1983)1337 by analysis of temperature factors. Diffuse X-ray and neutron experiments (r.t.) revealed a complicated pattern of diffuse sheets: a system which may be indexed with $l = n \cdot q$ ($q=0.782$ in units of c^* ; $n=1,2,3$) corresponding to an (averaged) incommensurate chain period, satellite sheets at $l = m \pm n \cdot q$ ($m=1,2,..$), and a weak diffuse intensity beneath the Bragg layers of the host. In a first approximation there is a system of uncorrelated chains: the period is modulated by commensurate and incommensurate superordering due to interaction with the host. An interpretation is carried out in frame of a Frenkel-Kontorova model (Beyeler et al.,Phys. Rev.B22(1980)2988;Geisel,Sol.St.Comm.32(1979) 739;Radons et al,Z.Phys.B.61(1985)319).A precise analysis, however, is strongly affected by lateral short range maxima in (part of) the diffuse sheets. Quasieelastic neutron data measured along 001 were compared with several models. Raising the temperature up to 900 K the diffuse sheets beneath the Bragg layers become stronger, all the layers broaden, and the short range peaks become weaker. Lowering the temperature down to 35 K these peaks become stronger, but - even more important- the diffuse layers are now located at $l = n \cdot 0.2$, i.e. the K-chains become commensurate with a fivefold period. As in case of $E_2PI_{1.6}$ the 1-d character is gradually lost towards a 3-d ordering.

The work was supported by funds of the BMFT of the F.R.Germany.

05.1-21 STUDY OF THE DISORDERED STRUCTURE OF p-IODOTOLUENE USING NONBONDED INTERATOMIC POTENTIALS, by S.K. Talapatra, S. Maity and S.B. Sarkar, X-ray Lab., Deptt. of Physics, Jadavpur University, Calcutta- 700 032, India.

The pairwise nonbonded interatomic potentials of the Buckingham 6-exp type(E. Giglio et al, Z. Kristallogr, 1970, 131, 385) were applied to the study of disorder in p-iodotoluene (C_7H_7I). The space group of the crystal is $P2_12_12_1$ with 4 molecules per unit cell. The X-ray studies revealed a planar structure of p-iodotoluene with the presence of disordered molecules having 16% occupancy, where the iodine and methyl ends were interchanged (B. Carpenter et al, Acta. Cryst., 1972, B 28, 2152). Hence it was considered interesting to study this case from the energy point of view.

The intermolecular energy, U(Kcal/mole) of p-iodotoluene was evaluated using our program for lattice energy calculation(S.K. Talapatra et al, Ind. J. Phys., 1981, 55A, 281) by rotating the molecule at an interval of 10 degrees about its best plane normal passing through the centre of the molecule (centre of the phenyl ring). The summation radius was taken as 10Å. The energy versus angle of rotation curve, as shown in the figure, revealed some interesting features. The p-iodotoluene molecule, has no two fold axis of symmetry about its plane normal, but the appearance of two nearly identical potential wells separated by an angle of 180° clearly indicated the presence of two configurations of the molecule in the lattice.

The higher occupancy molecule has been heavily outlined in the figure and it corresponds to the potential well at 0°, while the lightly outlined one i.e., the reversed molecule, corresponds to the other well at 180°. Possibly, their similar size (Van der Waals radii, iodine, 2.15Å, methyl, 2.0Å) allows the two species at the two ends of the molecule to interchange places at random without appreciable energy difference. Similar results were obtained from the study of indole, and 1:1 complex of indole with S-trinitrobenzene using the same program (S.K. Talapatra et al, Acta. Cryst., 1984 A-40, Suppl. C-121).