

**05.1-47** X-RAY INVESTIGATION OF THE INCOMMENSURATE PHASE OF  $\alpha$ -BIS-(N-METHYLSALICYLALDIMINATO)-COPPER [Cu-Sim]. By W. Adlhart, H. Blank and H. Jagodzinski, Institut für Kristallographie und Mineralogie der Universität München, München, Federal Republic of Germany.

The  $\alpha$ -modification of Cu-Sim crystallizes in the space group Iba2 at room temperature. The almost planar chelate molecules lie approximately within the plane  $z = 0$  and  $z = 1/2$ . Along the  $c$ -direction the Cu-ions form chains with a Cu-Cu distance of 5.52 Å (B. Meuthen and M. v. Stackelberg, Z. anorg. Chemie (1960) 305, 279). At  $T_i = 305(5)$  K a structural phase transition from the orthorhombic commensurate to the orthorhombic incommensurate phase is observed. Owing to a mainly transversal sinusoidal displacement of the atoms along the  $c$ -direction satellites occur with a wave vector  $\vec{q} = (0.297 \pm 0.002) \cdot \vec{a}^*$ . The intensity of the satellites increases rapidly with decreasing temperature. At  $T_c = 257(2)$  K we observe a first order phase transition (W. Adlhart and V.K. Syal, Z. Krist. (1981) 154, 227) to a monoclinic I-structure without any superstructure. The satellite vector remains constant between  $T_i$  and 260 K and then decreases continuously to about  $0.289 \cdot \vec{a}^*$  at  $T_c$ . Simultaneously, a broadening of the main and satellite reflections is observed. Within this temperature range the magnitude of the satellite vectors and the half-widths indicate hysteresis effects. An intense diffuse scattering around the satellite reflections can be explained by modulations of the phase of the sinusoidal atomic displacements.

**05.2-01** THE DEBYE TEMPERATURE OF SOME ORTHORHOMBIC CRYSTALS. By A. Garg and R.C. Srivastava, Department of Physics, Indian Institute of Technology, Kanpur 208 016, India.

Calculation of Debye temperature  $\Theta_D$  involves evaluation of the integral  $\sum_{i=1}^3 \int \frac{d\Omega}{V v_i}$  where  $v_i$  ( $i = 1, 2, 3$ ) are acoustic wave velocities in the crystal in different directions. Three different approximations have been adopted here to calculate  $\Theta_D$  of fifteen orthorhombic crystals from their experimentally determined elastic constants  $C_{ij}$ : (i) the expansion of the above integral in terms of harmonics  $F_{\ell m}(\theta, \phi)$  having the same symmetry as the Christoffel equation (Joshi, Phys. Rev. (1961) 40 121), (ii) the approximate numerical solution of the above integral (Robie and Edward, J. Appl. Phys. (1966) 37 2659), and (iii) the VRHG approximation of Anderson (J. Phys. Chem. Solids (1963) 24 909). These three approximations have been programmed for DEC-10 computer system and used to calculate the Debye temperature. The agreement in the values of  $\Theta_D$  is quite good (maximum variation 5%) for all the crystals except one, viz benzalazine, for which the difference is significantly greater.

To show the variation of velocities in different directions wave velocity surfaces have been plotted in different sections for two compounds: ammonium tetrafluoroberyllate and benzalazine. An attempt has been made to correlate Debye temperature, hardness and crystal structure in all of the above crystals.

**05.2-02** EXPERIMENTAL MOLECULAR DIAMAGNETIC ANISOTROPIES OF CONDENSED AROMATIC COMPOUNDS. By G. Van den Bossche and R. Sobry, Institut de Physique B5, Université de Liège au Sart Tilman, B - 4000 Liège, Belgique.

For explaining diamagnetic exaltation observed in condensed aromatic compounds, their molecular diamagnetic anisotropies must be known. A method is proposed which, on the basis of relatively accurate structural data and of two experimental crystal anisotropies, allows the determination of molecular anisotropies in the plane and perpendicularly to it. The proposed method is applied and discussed in the case of eleven condensed aromatic compounds. It yields, in some cases, molecular anisotropies very different from those suggested by different authors. One very simplified model produces results which fit in with the molecular anisotropies obtained as long as the arrangement of the rings is not too complex.

**05.2-03** REGULARITIES IN BINARY INTERMETALLIC COMPOUNDS by P. Villars, K. Giergis Institut für Kristallographie und Petrographie CH 8092 Zürich, Switzerland.

Examination of the 105 known binary structure types, containing more than 5 examples\* each, showed that 85% exhibited the following three regularities:

1. A linear  $d_{AB} - \bar{R}$  dependence\*\*.
2. A narrow spacefilling,  $c/a$  and  $b/a$  range for the given structure type.
- 3i. A dependence between the position of the elements in the periodic table and their equipoint occupation in the structure.
- 3ii The existence of a narrow grouping, for compounds of a given structure type, in an isostoichiometric diagram of binary element-combinations.

This diagram (3ii) has been used to put forward one or two possible structure types, with a high probability of existence, for synthesised binary intermetallic compounds. For example, up until 1970 there were 811 known intermetallic compounds with no assigned structure types, and during the past ten years, the structure types of 120 have been established. By using the above diagram, the correct structure type has been proposed for 110 of these.

Footnotes: \* W.B. Pearson, Handbook of Lattice spacings and structures of metals, 1967, Pergamon Press.

\*\*  $d_{AB}$  is the shortest distance between the elements A and B. This distance depends upon all the lattice constants and position parameters.  $\bar{R} = (nR_A + mR_B)/(n+m)$ ;  $R_A, R_B$  are the radii of the elements A and B (E. Teatum et al., LA 2345, June (1960)),  $n, m$  are the stoichiometric proportions.