

05.1-65 STRUCTURAL STUDY OF THE N-ISOPROPYLOCARBAZOLE PHASE TRANSITION. By E. Baert and A. Mierzejewski U.E.R. de Physique Fondamentale, U.S.T.L., 59655 Villeneuve d'Ascq, France.
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N-isopropylcarbazole is a piezo and pyroelectric substance exhibiting strong triboluminescence. The compound shows a reversible single crystal to single crystal phase transition at 130 K. Crystal structures of the high and low temperature phases have been solved. Both structures are orthorhombic and crystal data are as follow.

	high temperature phase	low temperature phase
a =	16.808 (5) Å	16.842 (4) Å
b =	17.984 (8) "	17.463 (3) "
c =	7.983 (3) "	7.863 (4) "
V =	2413.1 Å ³	2312.2 Å ³
D _x =	1.15 Mg m ⁻³	1.20 Mg m ⁻³
Z =	8	8
Space Group	Iba2	Pbc2 ₁
Temperature	294 (2) K	130 (.5) K

A least squares analysis of the rigid body motion (Schomaker and Trueblood, Acta Cryst. (1968) B24 63), of the molecule in both phases shows that the HC(CH₃)₂ groups undergoes large libration motions in the high temperature phase. At 130 K the HC(CH₃)₂ group is quite stable with a different orientation with respect to the mean plane of the other fragment of the molecule. Drawings and details are presented to explain this second order phase transition.

05.1-66 PHASE TRANSITIONS IN BETAININE COMPOUNDS. By W. Schildkamp, W. Brill, J. Spilker, Fachrichtung Kristallographie, Univ. des Saarlandes, D-6600 Saarbrücken, Federal Republic of Germany.

Several simple amino acids crystallize with inorganic compounds to form dielectrically interesting substances (e.g. Triglycine Sulfate, Trisarcosine Calcium Chloride, etc.). Structural results will be presented for Betaine Phosphate (BP), Betain Arsenate (BA), and Betaine Calcium Chloride Dihydrate (BCC).

BP performs a phase transition from a paraelectric high temperature phase (P₂₁/m; z=2) to an antiferrodistortive phase (P₂₁/c; z=4) and to an antiferroelectric phase (P₂₁/c; z=8). The high temperature phase is described by a molecular disorder, which orders in the antiferrodistortive phase. Three of four hydrogen atoms of the phosphate group remain disordered. The structure of the antiferroelectric phase is highly pseudosymmetric and cannot be solved by classical crystallographic methods.

BA is ferroelastic at ambient temperature (P₂₁/n; z=4) and ferroelectric below 119 K. The ferroelastic phase has also disordered hydrogen atoms. Both in BP and BA the inorganic components are chained in the direction becoming antiferroelectric or ferroelectric by disordered hydrogen bonds.

In BCC (Pnma; z=4) we have found a sheet structure where the organic and the inorganic component alternate. The calcium atom is octahedrally surrounded by two para-sited oxygen atoms of two different betaine molecules, two ortho-sited oxygen atoms of the water of crystallization, and two ortho-sited chlorine atoms.

The structural results are described in terms of rigid body motion parameters.

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05.1-67 TRANSFORMATION PROCESSES IN AN Al-Zn-Cu ALLOY. By M. Šimerská and P. Bartuška, Institute of Physics, Czechoslovak Academy of Sciences, 180 00 Praha, Czechoslovakia.

Structure changes in the supersaturated Al-30wt%Zn-5wt%Cu alloy were examined by X-ray diffraction and TEM in the temperature range from 373 to 733 K. Isothermal annealing of investigated coarse-grained polycrystalline samples was preceded by their solution-treatment (1 hour at 753 K) and water-quenching to 273 K. The phases identified within the fcc α matrix during the decomposition processes were: G-P zones, fcc α' , hcp β (\approx Zn), hcp ϵ (\approx CuZn₅), bct θ (\approx CuAl₂) as reported by

Mondolfo (Aluminium Alloys, Butterworths, London-Boston, 1976), and rhombohedral T' (\approx Al₁₂Cu₉Zn₂) found by Murphy (Metal.Sci.

J.(1975)9,163) in Al-Cu-Zn alloys with 13-56wt%Cu as the superstructure form of T phase with the CsCl structure type. Results of our study revealed both the transformation sequences of phases in dependence on the annealing temperature and the mechanisms of their formation and decomposition as well as the regions of existence and stability of the investigated phases.

The decomposition of fcc α matrix starts up to 498 K with the homogeneous nucleation of Zn- and Cu-rich spherical G-P zones coherent with α . They change later their shape into flat ellipsoids due to the rhombohedral distortion of their structure along one of the elastically soft $\langle 111 \rangle$ directions as found in Al-Zn alloys (Šimerská and Synček, Acta metall.(1967)15,223). The α matrix containing G-P zones is gradually converted into the lamellar product. Cellular reaction starts at grain boundaries by the formation of ϵ lamellae within α and proceeds very fast into the grains. G-P zones were found up to 498 K. Above this temperature up to 713 K, the decomposition of α starts with the homogeneous formation of T' by the nucleation of a pair of inserted 001 atomic planes in regions enriched in Cu. T' forms elongated precipitates which have the distinct orientation relationship to α . This phase is the only equilibrium phase within α between 548 and 593 K. Above 593 K T' is metastable and is decomposed by the formation of θ precipitates on T'/ α interfaces and by their very fast penetration into the interior of T' particles. θ is then the only equilibrium phase within α up to 713 K. Only the equilibrium α solid solution was found above 713 K which is the common solvus temperature of both θ and T'. θ is also formed by the heterogeneous nucleation on dislocation loops, vacancy clusters, and at grain boundaries. It appears as the metastable phase around 593 K and at lower temperatures between 373 and 423 K. T' is the equilibrium phase also below 548 down to 373 K with the simultaneous presence of the equilibrium β which has its solvus close below 548 K. Below 498 K, where the decomposition of α starts by the formation of G-P zones, the equilibrium T' phase is formed later. Though the mechanism of its formation is the same as mentioned above, the shapes of T' precipitates change due to the formation of ϵ at T'/ α interfaces. This leads to necking and subsequent spheroidization of T' precipitates. The metastable α' was observed between 498 and 538 K only, i.e. α' has a very limited range of existence as compared to the Al-30wt%Zn alloy. It is formed by the heterogeneous nucleation on dislocations by the same mechanism we have found recently in Al-Zn alloys at temperatures at which the homogeneous mode of decomposition is retarded. It has the parallel orientation to α . The metastable ϵ phase participates in the decomposition process between 373 and 538 K; its solvus is close above 538 K. As already mentioned, ϵ appears mainly in the form of lamellae. Small precipitates of ϵ are nucleated also on dislocation loops and on dislocated phase interfaces of existing precipitates, i.e. on T'/ α , α' / α , and θ / α . Such ϵ precipitates have the epitaxial orientation to α . The equilibrium β is predominantly formed from ϵ in the parallel orientation. This transformation is supported by the similar structure of both ϵ and β phases. Similarly to Al-Zn alloys, β is formed also by the decomposition of α' in the epitaxial orientation to α , and at grain boundaries.