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The unit cell and space group of neopentyl alcohol. By G. B. CARPENTER, *Metcalf Research Laboratory, Brown University, Providence, Rhode Island 02912, U.S.A.*

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Neopentyl alcohol crystallizes in space group $Fm\bar{3}m$ with 4 molecules in a cell of edge $a=8.83$ Å. The molecules are thus highly disordered about cubic close-packed centers.

Neopentyl alcohol, $C(CH_3)_3CH_2OH$, is of interest because its melting point of 53° is much higher than that of other five-carbon alcohols.

Single crystals were grown in capillaries of 0.2 mm internal diameter by slow cooling of melted samples. They were studied by Laue and precession methods with molybdenum radiation. The initial precession photographs showed a total of 14 reflections, which could be indexed on cubic axes as reflections of the two forms $\{111\}$ and $\{200\}$. Measurements on the precession photographs recorded on Polaroid film according to the method of Swink & Carpenter (1967) gave a cell edge of $a=8.83$ Å with a standard deviation of 0.02 Å. The standard deviation is so large because of the small number of measurable spots, all at low angles. More heavily exposed photographs revealed faint traces of reflections in the forms $\{220\}$ and $\{222\}$.

The density measured by flotation is 0.848 g.cm $^{-3}$, and the density calculated for four molecules in the unit cell is 0.850 g.cm $^{-3}$.

The simplest interpretation of these observations is that the structure is face-centered cubic, space group $Fm\bar{3}m$, with four molecules centered at positions $4(a)$. Therefore each molecule is disordered so as to exhibit $m\bar{3}m$ point symmetry. The structure thus appears to be the same cubic close-packed structure shown by neopentane (Mones & Post, 1952), carbon tetrachloride (Rudman & Post, 1966),

and other related substances, in the solid phase obtained from the melt.

With so few independent structure factors measurable, it seems unprofitable to try to learn more about the structure by X-ray diffraction at room temperature. Low temperature work on this substance is not now contemplated.

The infrared absorption spectrum was examined in an effort to determine the extent of hydrogen bonding in the highly disordered crystals. A sample of neopentyl alcohol was melted and then allowed to solidify between rocksalt windows, and the spectrum was recorded with a Perkin-Elmer model 621 spectrometer. An intense symmetrical band appeared in the O-H stretching region at about 3340 cm $^{-1}$ with a width at half height of approximately 340 cm $^{-1}$; this and the appearance of the rest of the spectrum indicate a moderate amount of hydrogen bonding.

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The crystal structure of Fe_2AlB_2 . By WOLFGANG JEITSCHKO, *Department of Metallurgy, University of Illinois, Urbana, Illinois, U.S.A.*

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Fe_2AlB_2 crystallizes in the orthorhombic space group $Cmmm$ (D_{2h}^{19}) with lattice constants $a=2.9233 \pm 0.0010$, $b=11.0337 \pm 0.0014$ and $c=2.8703 \pm 0.0003$ Å. This compound was found to be isostructural with Mn_2AlB_2 (Becher, Krogmann & Peisker, 1966, *Z. anorg. allg. Chem.* **344**, 140). The structure has been refined from single-crystal X-ray data, giving a final R value of 0.084 for the 140 independent structure factors observed. The structure is closely related to the CrB- and MoAlB-type structures. Fe_2AlB_2 is either strongly paramagnetic or ferromagnetic at room temperature.

Introduction

In a publication on the ternary system iron-aluminum-boron Stadelmaier, Burgess & Davis (1966) reported the existence of a ternary phase close to the composition ' Fe_3AlB_3 '. From a structure-chemical viewpoint, aluminoborides are of interest because of the possible participation of aluminum atoms in building elements in the form of chains, nets, etc., which are formed by the boron atoms in borides (Aronsson, Lundström & Rundqvist, 1965). Although the structures of the various binary aluminumborides, as far as they are known (for references see Hoard &

Hughes, 1967), do not imply a covalent bond Al-B, this could not be ruled out for MoAlB (Jeitschko, 1966). However, the Al-B distance in this structure could not be determined accurately because the large scattering power of molybdenum prevented refinement of the free parameter of the boron atom.

Experimental

In their paper Stadelmaier, Burgess & Davis (1966) reported that the new ternary compound was found at a composition which is within the range of the primary crystallization of FeB. Primary crystallization of the ternary phase was, in turn,