Short Communications

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Single crystals of $BaAl_2O_4$.

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$BaAl_2O_4$ single crystals are hexagonal with $a=10\cdot444\pm0\cdot002$, $c=8\cdot793\pm0\cdot002$ Å, the a axis being doubled compared with the previously reported value.

Single crystals of $BaAl_2O_4$ were grown from a barium borate flux. The starting materials were melted in a platinum crucible which was heated to 1275 °C in a globar furnace. The crystals were grown by slow cooling of the melt at a rate of 2 °C per hour. Single crystals grew in the shape of clear hexagonal rods (3 mm long × 0·5 mm diameter) parallel to the c axis and bounded by $\{10\bar{1}0\}$ and $\{0001\}$ faces.

Single-crystal X-ray photographs showed very weak additional reflections which required a doubling of the hexagonal a axis compared with the unit cell reported by previous workers on polycrystalline material (Wallmark & Westgren, 1937; Do Dinh & Bertaut, 1965)*. A similar doubling of the a axis in this structure type has been found in single crystals of $BaGa_2O_4$ (Hoppe & Schepers, 1960). Lattice constants $a=10\cdot444\pm0\cdot002$ Å, $c=8\cdot793\pm0\cdot002$ Å were obtained by a least-squares fit of the back reflection powder diffraction lines.

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* These authors reported space group $P6_322$. The structure is described (*Strukturbericht*, 1937) as type $H2_8$.

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The crystal structure of diaquobis(acetylacetonato)magnesium(II).*

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The crystal structure of diaquobis(acetylacetonato)-magnesium(II), $Mg(C_5H_7O_2)_2.2H_2O$, has been determined. The coordination polyhedron about the magnesium atom is tetragonally distorted (2.03, 2.04 and 2.15 Å) to a similar degree to that found in the corresponding isomorphous nickel and cobalt compounds. This suggests that the tetragonal distortion is due to a crystal structure (or packing) effect rather than the electronic structure of the metal ions. A tabulation of metal ion displacements from the least-squares plane formed by the atoms of the chelate ring in metal acetylacetonates is given.

Bullen (1959) and Montgomery & Lingafelter (1964) have reported the crystal structures of diaquobis(acetylacetonato)-cobalt(II) and -nickel(II) ($MQ_2.2H_2O$ where $M=Co$ or Ni and $Q=C_5H_7O_2$, respectively). In both compounds, the metal ion is surrounded by six oxygen atoms which form a tetragonally distorted octahedron. Covalent bonding involving hybridization with d orbitals or, in terms of ligand-field theory, asymmetric $d\gamma$ and $d\varepsilon$ subshells have been invoked to explain the tetragonal distortion. It has been suggested (Bullen, 1959) that the zinc analog, with a more symmetric electronic structure, should exhibit a more regular octahedral environment about the metal ion; however, the only reported zinc complex (Montgomery & Lingafelter, 1963) is a monohydrate in which the zinc ion is not octahedrally coordinated. We present here our structure results on $MgQ_2.2H_2O$ which show the environment about the magnesium ion to be tetragonally distorted and,

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