SHORT COMMUNICATIONS

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Note on the Crystal Structure of Vanadium Dichloride
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In a paper on transition metal halides 1 Klemm and Grimm were unable to determine the structure of VCl₄ and TiCl₄. They stated, however, that VCl₄ was not isomorphous with TiCl₄ which was found to have the CdI₂-type structure. Later Baenziger and Rundh have found a preparation of TiCl₄ to be isomorphous with CdI₂.

We have carried out an X-ray investigation of VCl₄ prepared by K. Riishede of this laboratory by heating vanadium powder in a stream of dry HCl at 950°C. The product was obtained in the form of apple-green, muscovite-like leaflets of a more or less hexagonal appearance. The following data were obtained:

Unit cell dimensions: α₀ = 3.60 ± 0.01 Å, c₀ = 5.83 ± 0.01 Å. Observed density: 3.09 g/cm³, calculated density: 3.09 g/cm³. Diffraction symbol: 3m1P...; test for pyroelectricity: negative. Probable space group: P3m (No. 164). Arrangement of atoms:

1 V at 0,0,0
2 Cl at ± (1/3, 2/3, u) with u ~ 1/4.

Shortest V-Cl distance: 2.55 ± 0.05 Å. Structure type: CdI₂ (C6).

Experimental: Laue photographs were taken along the c-axis. The lattice constants were calculated from Debye-Scherrer diagrams taken in a 19 cm camera using CuKa radiation (λ = 2.2909 Å). Intensities were recorded on an X-ray diffractometer with CuKa radiation. The value of the parameter u was found to deviate only insignificantly from the ideal value 1/4 from a Fourier projection along the c-axis using the 00l reflections. The agreement between observed and calculated intensities of the 00l and 10l reflections is satisfactory but a different scaling factor had to be used because preferred orientation could not be totally depressed.

From the above it may be concluded either that TiCl₄ and VCl₄ both exist in two modifications or that the materials investigated by Klemm and Grimm have been partly decomposed before or during their X-ray exposure.

Added in proof: Very recently 2 Ehrlich and Seifert have recorded the structure of VCl₄ in complete agreement with the results given above.

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