

plane; in the **b** direction, we meet in succession two sheets of steroid molecules and one sheet made up of the included solvent. The steroid molecules in the same sheet are linked in the **a** direction by a hydrogen bond ($O \cdots O = 2.75 \text{ \AA}$, $O-H \cdots O = 166^\circ$). Each inclusion molecule is linked to a steroid molecule by a hydrogen bond involving the 17β -ol function ($O \cdots O = 2.86 \text{ \AA}$, $O-H \cdots O = 158^\circ$).

In the **b** and **c** directions, crystal cohesion is ensured by attractive van der Waals forces. No repulsive contacts are observed.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Acta Cryst. (1976). B32, 1298

Reply to Comment on 'Struktur des tetragonalen $(B_{12})_4B_2Ti_{1.3-2.0}$ ' by E. Amberger and K. Polborn. By E. AMBERGER and K. POLBORN, *Institut für Anorganische Chemie der Universität, D-8000 München 2, Meiserstrasse 1, Deutschland (BRD)*

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Reduction of BCl_3 and $TiCl_4$ with H_2 on boron nitride substrate produces the analytically controlled carbon-free $(B_{12})_4B_2Ti_{1.3-2.0}$. Therefore the tetragonal unit cell contains boron on special equivalent point $2(b)$ and titanium on $2(a)$.

In the paper *Struktur des tetragonalen $(B_{12})_4B_2Ti_{1.3-2.0}$* (Amberger & Polborn, 1975) the synthesis and structure of the berthollide titanium boride were described. The unit cell was found to contain four B_{12} icosahedra, two single boron atoms on special equivalent point $2(b)$, and a maximum of two titanium atoms on $2(a)$. Now Ploog (1976) in a comment on this paper argues that carbon is more likely to occupy the $2(b)$ position than boron.

But there are convincing arguments against this: (i) The crystal used for X-ray investigation was taken from a certain crystalline region of the boride deposit. The chemical analysis showed that this region was free from carbon. (ii) Furthermore each synthesis (reduction of gaseous BCl_3 and $TiCl_4$ with H_2) yielded the carbon-free titanium boride. An *I*-tetragonal titanium boride carbide $(B_{12})_4C_{\sim 2}Ti_{1.5-2.0}$ (Amberger, Polborn & Gerster, in preparation) was pro-

duced – and in fact is reproducible – under these conditions but only with an additional amount of CCl_4 . In the latter cell, carbon occupies the $2(b)$ position and titanium the $2(a)$. (iii) The structure of the titanium boride was derived from photometrically measured X-ray patterns. The figures resulting from this procedure are not precise enough to signify a formula of the investigated compound other than the formula $(B_{12})_4B_2Ti_{1.3-2.0}$, derived from chemical and analytical findings.

References

- AMBERGER, E. & POLBORN, K. (1975). *Acta Cryst.* B31, 949–953.
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