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Short Communications

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The $M\mathrm{Be}_{13}$ compounds.*

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A series of intermetallic compounds of composition $M\mathrm{Be}_{13}$ has been found, where M is U, Th, Ce and Zr. Powder diagrams of the phases appear to be simple cubic, $a \doteqdot 5$ A., but rotation and Weissenberg diagrams of ZrBe_{13} reveal that the true unit is face-centered cubic, $a \doteqdot 10$ A., with 8 ZrBe_{13} per unit. Upon close inspection the (531) reflection, requiring the larger unit, can be seen on powder diagrams of all four compounds. The lattice constants reported in Table 1 are from back-reflections obtained with a symmetrical, self-focusing powder camera.

Table 1. *Lattice constants in Ångström units*†

CeBe_{13}	$10{\cdot}375 \pm 0{\cdot}001$
ThBe_{13}	10·395
UBe_{13}	10·256
ZrBe_{13}	10·047

The approximate composition, $M\mathrm{Be}_{13}$, was suggested from consideration of unit cell and atomic volumes. This has been confirmed by structural analysis of the single-crystal data from the zirconium compound; the beryllium compounds prove to be isomorphous with NaZn_{13} and similar compounds (Ketelaar, 1937; Zintl & Haucke, 1937, 1938).

In the structure (space group O_h^6–$Fm3c$) the face-centered positions are:

8 Zr in $\pm\frac{1}{8}, \frac{1}{4}, \frac{1}{4}$.

8 Be in $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

96 Be in $\pm 0, y, z$↖; $\pm 0, y, z$↖; $\pm\frac{1}{2}, \bar{z}, y$↖; $\pm\frac{1}{2}, \bar{z}, y$↖.

Only the 96 Be atoms contribute to reflections with odd indices, and these are of zero intensity for reflections (*hhl*). In Table 2 the observed intensities of the (*hkl*) reflections are compared with those calculated using parameter values found by Zintl & Haucke ($y = 0{\cdot}112$, $z = 0{\cdot}178$) for NaZn_{13}. The agreement is quite satisfactory.

Intensities have also been calculated for (*hk*0) reflections. These are influenced only moderately by the inclusion of the 8 Be atoms in special positions, but the intensities are improved by including their contributions, so it seems clear that they are present in the structure.

The composition of the uranium compound, as determined metallographically, was UBe_9 (Batelle Memorial Institute, 1943). The atomic weight ratio is such that the X-ray data provide a more unambiguous composition. Solid solubility in the phase is not excluded; lattice constants of the pseudo-unit have been observed to vary with composition from 5·125 to 5·133 A. (Gordon, 1946).

Table 2. *Reflections* (*hk*1) *for* ZrBe_{13}

(Observed and calculated reflections (*hhl*) are zero; these are not included in the table.)

Indices	$I_{\mathrm{calc.}}$	$I_{\mathrm{obs.}}$
531	1332	*s*
731	22	0
751	47	*w*
931	320	*m*
951	279	*m*
971	3	0
11.3.1	593	*m*
11.5.1	14	0
11.7.1	81	0

Ketelaar (1937) pointed out that NaZn_{13} and related compounds (zinc and cadmium compounds of alkali and alkaline earth metals are known) may be zone compounds. The zone bounded by (531), which is most prominent for these compounds, allows 234 electrons/unit cell, or 216·8 in the inscribed sphere, *v.* 216 electrons/unit for the alkali and 224 for the alkaline earth compounds. If U, Th, Ce and Zr are tetravalent, there are 240 electrons/unit in the beryllium compounds, exceeding that allowed for the filled zone. However, the (531) zone is not prominent for the beryllium compounds, leading to a smaller energy discontinuity. For NaZn_{13}, the electron:atom ratio is 27/14, one of the Hume-Rothery ratios. The ratio becomes 30/14 for the tetravalent elements reported here. The zone picture appears less satisfactory for the beryllium compounds.

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† Wave-lengths in true Ångström units, rather than kX., are used in this paper.