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X-ray and neutron diffraction studies of the MBe_{13} intermetallic compounds.*

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Recent interest in intermetallic compounds of beryllium has resulted in conflicting reports regarding phases near the high beryllium end of the phase diagrams. While compounds of clearly different structure have been observed, most reports mention a cubic phase variously designated MBe_9 (Battelle Memorial Institute, 1943; Hausner & Kalish, 1950), MBe_{13} (Baenziger & Rundle, 1949) or MBe_{14} (Vacher, private communication), but all apparently having a lattice constant of about 5·1 kX. Among the heavy metals represented were U, Th, Ce and Zr. At about the time a Los Alamos group was investigating a cubic phase in the vicinity of UBe_{14}, a report by Baenziger & Rundle (AECD-2506) was declassified. Their work showed that a cubic phase near the high beryllium end of the diagrams with U, Th, Ce, Zr should be indexed as face-centered cubic with lattice constants in the vicinity of 10·2 kX. The face centering was indicated by very weak reflections in the powder patterns, and was confirmed by single-crystal patterns of the zirconium compound. Further, Baenziger & Rundle computed structure factors based on the $NaZn_{13}$ structure (Baenziger & Rundle, 1949; Zintl & Hauche, 1937) and demonstrated that for this structure the Be contributions, while small, were in the right direction to give agreement with observed intensities.

To obtain better confirmation for the heavy-metal compounds, we carried this investigation further. Single crystals of the U–Be and Th–Be compounds were oscillated on the Unicam S. 25 goniometer through regions of the reciprocal lattice selected to include one or more points of the face-centered cell. The (531), (731) and (11,3,1) reflections were sought, and were obtained on the first and third layer lines with the expected (Baenziger & Rundle, 1949) relative intensities.

Table 1. *Calculated and observed intensities*

HKL	2θ	P_c (neutrons/min.)		P_o (neutrons/min.)
111	10° 0′	0		0
200	11° 32′	272		268
220	16° 20′	0·01		< 2*
311	19° 10′	0		0
222	20° 2′	63		19
400	23° 10′	39		16
331	25° 16′	0		0
420	25° 56′	330		314
422	28° 28′	765		798
511	30° 14′	0		0
333		0		0
440	33° 0′	64		
531	34° 32′	2115	2697	~ 2600
600	35° 4′	250		
442		268		
620	37° 2′	274		
533	38° 26′	0	309	~ 340
622	38° 54′	35		

* Contaminated by second order (531).

Neutron-diffraction studies were made on a powder sample of the U–Be compound using the apparatus of Wollan & Shull (1948). The more favorable ratio of the Be/U scattering for neutrons compared to X-rays offered the possibility of determining the Be positions with the required sensitivity. Intensities were calculated on the basis of the $NaZn_{13}$ structure with the 96-fold Be set having the parameters of that structure, namely $y=0{\cdot}112$, $z=0{\cdot}178$. Table 1 lists the observed and calculated intensities, the latter calculated according to

$$P_{HKL} = \frac{K j_{HKL} F^2_{HKL}}{n^2 \sin\theta \sin 2\theta},$$

where n = 8, the number of molecules per unit cell;
K = 0·4047, derived from apparatus constants and the nature of the sample;
j_{HKL} = the usual powder pattern multiplicity; and
F_{HKL} = the structure factor for neutron scattering in units of 10^{-12} cm. per unit cell.

The wave-length used was 1·030 kX.; a_0 was found to be 10·26 kX. No temperature factor was included in the calculations.

The agreement is satisfactory, although some change in parameters is indicated. In conclusion, our results seem to support strongly the generalization, first made by Baenziger & Rundle, that the cubic compounds which occur in high beryllium alloys are face centered, have the composition MBe_{13}, and are isomorphous with $NaZn_{13}$.

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References

Baenziger, N. C. & Rundle, R. E. (1949). *Acta Cryst.* **2**, 258; also AECD-2506.

Battelle Memorial Institute (1943). Manhattan Project Report CT-1009.

Hausner, H. H. & Kalish, H. S. (1950). *Trans. Amer. Inst. Min. (Metall.) Engrs.* **188**, 59.

Vacher, H. C. Bureau of Standards.

Wollan, E. O. & Shull, C. G. (1948). *Phys. Rev.* **73**, 830.

Zintl, E. & Hauche, W. (1937). *Naturwissenschaften*, **25**, 717.