Acta Cryst. (1961). **14**, 1084

A note on the structure of Zr_2Co.*

By D. M. Bailey and J. F. Smith, *Institute for Atomic Research and Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A.*

(*Received* 14 *April* 1961 *and in revised form* 26 *May* 1961)

Weissenberg and precession diffraction data from a single crystal of Zr_2Co were found to corroborate the Strukturbericht Type C16 ($CuAl_2$) structure (Pearson, 1958) reported by Nevitt & Downey (1961):

Space group D_{4h}^{18}–$I4/mcm$,

4 Co at $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \pm (0, 0, \frac{1}{4})$,

8 Zr at $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \pm (x, \frac{1}{2}+x, 0; \frac{1}{2}+x, \bar{x}, 0)$.

Eighteen ($h0l$) reflections were used with a least-squares program to determine the single structural parameter as $x = 0{\cdot}1679 \pm 0{\cdot}0019$. Extrapolation of spacings obtained from Debye–Scherrer patterns against the Nelson–Riley function (1945) resulted in the tetragonal lattice parameters: $a_0 = 6{\cdot}363$ Å and $c_0 = 5{\cdot}469$ Å.

Table 1. *Comparison of observed and calculated structure factors for* Zr_2Co

$h0l$	$\|F_o\|$	F_c	$h0l$	$\|F_o\|$	F_c
002	41·0	+43·2	402	40·8	−37·0
004	60·6	+61·6	404	4·8	− 6·6
006	22·8	+24·4	406	20·6	−23·4
200	12·8	−12·2	600	53·4	+51·4
202	57·0	−48·2	602	27·0	+26·0
204	7·6	− 9·0	604	37·6	+41·8
206	26·2	−27·2	800	9·0	− 8·0
400	4·8	− 8·2	802	20·6	−25·0

The ($h0l$) intensities were visually estimated from a series of timed exposures of precession patterns obtained with Mo $K\alpha$ radiation. Lorentz and polarization corrections were made in the manner of Lu (1943), and absorption corrections were made in the manner of Bradley (1935) with the approximation of cylindrical symmetry for the needle-shaped crystal. The scattering factors of Thomas & Umeda (1957) were modified for dispersion corrections in the manner of Dauben & Templeton (1955), and the structure was refined on an IBM–650 with the least-squares program of Senko as modified by Fitzwater (1958). A comparison of observed and calculated structure factors per unit formula is shown in Table 1. The tabulated values give rise to the discrepancy indices:

$$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0{\cdot}089$$

and

$$R_2 = \Sigma(|F_o| - |F_c|)^2/\Sigma F_o^2 = 0{\cdot}009 .$$

Isotropic temperature factors, $B_{Co} = 4{\cdot}08$ Å^2 and $B_{Zr} = 3{\cdot}06$ Å^2, were obtained and are rather large. On this basis one would expect appreciable vibrational amplitudes in the compound with a relatively high value for the entropy of formation. No thermodynamic data are available for corroboration. However, it may be noted that the temperature factors for the isostructural compound, Zr_2Ni, (Kirkpatrick, Bailey & Smith, 1961) are of comparable magnitude.

* Contribution No. 1015. Work was performed in the Ames Laboratory of the U.S. Atomic Energy Commission.

References

Bradley, A. J. (1935). *Proc. Phys. Soc.* **47**, 879.

Dauben, C. H. & Templeton, D. H. (1955). *Acta Cryst.* **8**, 841.

Fitzwater, D. R. (1958). Unpublished Ph.D. Thesis. Iowa State University, Ames, Iowa.

Kirkpatrick, M. E., Bailey, D. M. & Smith, J. F. (1961). *Acta Cryst.* To be published.

Lu, C. S. (1943). *Rev. Sci. Instrum.* **14**, 331.

Nelson, J. B. & Riley, D. P. (1945). *Proc. Phys. Soc.* **57**, 160.

Nevitt, M. V. & Downey, J. W. (1961). *Trans. Amer. Inst. Min. (Metall.) Engrs.* To be published.

Pearson, W. B. (1958). *Handbook of Lattice Spacings and Structures of Metals and Alloys*, p. 99. New York: Pergamon.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Acta Cryst. (1961). **14**, 1084

The crystal structure of Ce_7Ni_3.*

By R. B. Roof, Jr., Allen C. Larson and Don T. Cromer, *University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.*

(*Received* 25 *January* 1961)

Vogel (1947), in a study of the Ce–Ni phase diagram, reported the existence of six binary compounds in this system. Of these, $CeNi_3$ and $CeNi_4$ were listed as having uncertain compositions. The existence of $CeNi_3$ has been verified (Cromer & Olsen, 1959), and what was thought to be $CeNi_4$ has been shown to be Ce_2Ni_7 (Cromer & Larson, 1959). The most Ce-rich compound was reported by Vogel to be Ce_3Ni. We find this compound to be Ce_7Ni_3. In attempting to prepare Ce_3Ni, Coffinberry (1960) was

Table 1. *Final least-squares parameters for* Ce_7Ni_3

	Position	x	z	B (Å^2)
Ce_1	2(*b*)	1/3	0·7888 ± 0·0024	1·87 ± 0·24
Ce_2	6(*c*)	0·1250 ± 0·0005	0·0	1·52 ± 0·14
Ce_3	6(*c*)	0·5391 ± 0·0005	0·8011 ± 0·0012	1·85 ± 0·14
Ni	6(*c*)	0·8118 ± 0·0011	0·0496 ± 0·0026	1·76 ± 0·32

* Work performed under the auspices of the United States Atomic Energy Commission.