Acta Cryst. (1961). **14**, 69

The crystal structure of CeNi.

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(*Received* 28 *December* 1959)

Previous structural investigations of compounds in the cerium–nickel system have been adequately discussed in recent papers by Cromer & Larson (1959) and Cromer & Olsen (1959). The structure of Ce_3Ni is currently being studied. No previous structure studies have been reported for the compound CeNi.

Samples of CeNi were prepared by melting the constituent elements in stoichiometric proportions in vacuo. The melt was cooled slowly to allow for better crystallization. A portion of one sample was annealed but this treatment gave no improvement in the crystallization.

Investigations of CeNi were made using oscillation and Weissenberg photographs (Mo $K\alpha$). CeNi was found to be orthorhombic with

$$a_0 = 3{\cdot}77 \pm 0{\cdot}01,\ b_0 = 10{\cdot}46 \pm 0{\cdot}02,\ c_0 = 4{\cdot}37 \pm 0{\cdot}01\ \text{Å}\ .$$

Only the following reflections were observed:

Table 1. *Observed and calculated structure factors for* CeNi

k	l	F_o	F_c
0	2	273	−223
0	4	94	105
0	6	53	−42
2	0	0	23
4	0	148	−177
6	0	0	16
8	0	41	39
10	0	51	60
12	0	0	−13
14	0	56	43
2	1	127	−115
4	1	112	124
6	1	104	127
8	1	64	−78
10	1	59	−66
12	1	52	32
2	2	28	−14
4	2	129	133
6	2	0	−15
8	2	45	−33
10	2	47	50
2	3	60	71
4	3	69	−70
6	3	69	−80
8	3	50	52
10	3	50	45
2	4	0	3
4	4	64	−69
6	4	0	12
8	4	0	−22
10	4	0	30
2	5	0	−37
4	5	48	30
6	5	0	−39
8	5	0	−26
2	6	0	0

Where $F_o = 0$, the reflection was not observed.

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$$hkl,\ h+k=2n;\ \ h0l,\ l=2n\ .$$

Space groups displaying these conditions for non-extinction are $Cmc2_1$ and $Cmcm$. From the observed density and cell dimensions, $Z = 4$. The calculated density of 7·65 g.cm.$^{-3}$ is in good agreement with the observed density, 7·51 g.cm.$^{-3}$.

The axial ratio and cell contents suggest a similarity to the TlI structure with the space group $Cmcm$ (Helmholtz, 1936). Atoms of cerium and nickel were placed in positions $0y\frac{1}{4}$, $0y\frac{3}{4}$, $(+000, \frac{1}{2}\frac{1}{2}0)$ to correspond to the TlI structure. $0kl$ reflections were visually estimated from the Weissenberg photograph and corrected for the Lorentz-polarization factor (Buerger, 1941), but not for absorption. Various y parameters were tried until a general agreement with the estimated intensities was reached. The trial parameters were $y_{Ce} = 0{\cdot}14$ and $y_{Ni} = 0{\cdot}42$.

The y parameters were refined by the least-squares method using the Maniac II computer. The form factor for cerium was taken from *Internationale Tabellen* (1935) and the form factor of Viervoll & Øgrim (1949) was used for nickel. The simultaneous refinement of two position parameters, two isotropic temperature factors and a scale factor was carried through five cycles at which point the parameter shifts became less than the standard deviation. The final results of the least-squares refinement are:

$$y_{Ce} = 0{\cdot}139 \pm 0{\cdot}002,\ y_{Ni} = 0{\cdot}428 \pm 0{\cdot}004\ ,$$
$$B_{Ce} = 2{\cdot}3 \pm 0{\cdot}5 \times 10^{-16}\ \text{cm.}^2,\ B_{Ni} = 3{\cdot}12 \pm 1{\cdot}1 \times 10^{-16}\ \text{cm.}^2,$$

$R = 15{\cdot}8\%$. The observed and calculated structure factors are given in Table 1. The high residual error can be accounted for since only 24 $0kl$ reflections were actually observed and all reflections were somewhat broadened.

The interatomic distances for near neighbors are as follows: Ce–Ce, 3·63, 3·70 and 3·77 Å; Ni–Ni, 2·66 and 3·77 Å; Ce–Ni, 2·91, 2·97 and 3·01 Å.

The CeNi structure corresponds closely to that of PuNi as reported by Cromer & Roof (1959).

The authors are indebted to R. E. Tate, D. T. Cromer and A. C. Larson of the Los Alamos Scientific Laboratory for preparation of the samples and computations.

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