APPENDIX

The treatment in § 2 can be extended to allow for the change of layer spacing accompanying segregation. Let A_3, $A_3(1+\varepsilon/2\pi)$, $A_3(1+\varepsilon/\pi)$ be the spacings between layers with average scattering factors of f_1 and f_1, f_1 and f_2, f_2 and f_2. It is easily shown that formula (15) for the intensity of the $3M\pm1$ reflexions is then modified, assuming $\varepsilon \ll 1$, to

$$\begin{aligned} I(h_3) &= 1+2\alpha(1-\alpha)\beta(\beta+2)-2S\cos(2\pi h_3+s) \\ &\quad +\tfrac{1}{2}T\cdot\frac{\cos(4\pi h_3+t)+P\cos(2\pi h_3+t-p)}{1+P^2+2P\cos(2\pi h_3+p)}, \end{aligned} \tag{17}$$

where

$$\begin{aligned} S\cos s &= \tfrac{1}{2}+\tfrac{1}{2}\alpha(1-\alpha)\beta(4+\beta) \\ &\quad \pm\sqrt{3}\alpha(1-\alpha)(1-2\alpha)\beta(1+\beta)\varepsilon h_3, \\ S\sin s &= \pm\tfrac{1}{2}\sqrt{3}(1-2\alpha)(1-\alpha\beta^2+\alpha^2\beta^2) \\ &\quad +\alpha(1-\alpha)(1+\beta)(2+\beta)\varepsilon h_3; \\ Q\cos q &= 1-2\alpha+2\alpha^2\mp\sqrt{3}\alpha(1-\alpha)(1-2\alpha)\varepsilon h_3, \\ Q\sin q &= \pm\sqrt{3}(1-2\alpha)+\alpha(1-\alpha)\varepsilon h_3; \\ R\cos r &= -1\mp\tfrac{1}{2}\sqrt{3}(1-2\alpha)\varepsilon h_3, \\ R\sin r &= -\tfrac{3}{2}\varepsilon h_3; \\ P\cos p &= \tfrac{1}{2}, \\ P\sin p &= \pm\tfrac{1}{2}\sqrt{3}(1-2\alpha)+2\alpha(1-\alpha)\varepsilon h_3; \\ T\cos t &= Q^2\cos 2q-4\alpha(1-\alpha)(1+\beta)QR\cos(q+r) \\ &\quad +4\alpha^2(1-\alpha)^2(1+\beta)^2R^2\cos 2r, \\ T\sin t &= Q^2\sin 2q-4\alpha(1-\alpha)(1+\beta)QR\sin(q+r) \\ &\quad +4\alpha^2(1-\alpha)^2(1+\beta)^2R^2\sin 2r. \end{aligned}$$

For a given alloy, with finite values of α, β and ε, the profiles of the $3M+1$ and $3M-1$ reflexions are no longer equivalent; moreover, these profiles are different for the successive peaks occurring with increasing h_3. Evaluation of (17) with the aid of the Mercury computer for the case $\varepsilon = 0{\cdot}02$ showed that the values of the points on the curves in Figs. 4(*a*) and 4(*b*) (corresponding to $\varepsilon = 0$) were changed by about 7% for the first order peak and 22% for the second order peak. For many alloys, in particular those such as Ag–Au and Co–Ni with a wide range of solid solution, ε is practically zero and the simpler theory of S_2 is then adequate.

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The Crystal Structures of $PuNi_3$ and $CeNi_3$*

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The structure of $PuNi_3$ and the structure and composition of $CeNi_3$ have been determined by single crystal X-ray methods. $PuNi_3$ has three formula units in a rhombohedral unit cell with $a = 6{\cdot}22$ Å and $\alpha = 33°\ 44'$, probable space group $R\bar{3}m$. $CeNi_3$ has six formula units in a hexagonal cell with $a = 4{\cdot}98$ and $c = 16{\cdot}54$ Å, probable space group $P6_3/mmc$. These structures are both derived from stacking single layers of the MNi$_5$ structure ($CaCu_5$-type) and double layers of the MNi$_2$ structure (Cu_2Mg-type).

Introduction

Because of the many similarities between the plutonium–nickel and cerium–nickel binary phase diagrams, structures of compounds in these two systems are simultaneously being investigated. The plutonium–nickel phase diagram, published originally by Wensch & Whyte (1951), shows the existence of the compounds PuNi, $PuNi_2$, $PuNi_3$, $PuNi_4$, $PuNi_5$ and Pu_2Ni_{17}. The structures of $PuNi_2$, $PuNi_5$ and Pu_2Ni_{17} have been reported in a review by Coffinberry & Ellinger (1956) to be of the Cu_2Mg, $CaCu_5$ and Th_2Ni_{17} structure types, respectively. Vogel (1947), in a study of the cerium–nickel phase diagram, lists the compounds Ce_3Ni,

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CeNi, $CeNi_2$, $CeNi_3$(?), $CeNi_4$(?) and $CeNi_5$. The compounds $CeNi_3$ and $CeNi_4$ were of uncertain composition. Nowotny (1942) had previously found that $CeNi_2$ and $CeNi_5$ had the Cu_2Mg and $CaCu_5$ structures. No other structure analysis of compounds in this system has been reported.

In this paper, the structure of $PuNi_3$ and the structure and verification of the composition of $CeNi_3$ are reported.

Experimental

A plutonium–nickel alloy containing 74·3 at.% nickel (by chemical analysis) yielded good crystals of $PuNi_3$. The alloy was prepared by vacuum induction melting of the components followed by slow cooling. The purity of the plutonium was at least 99·9 wt.%, and that of the nickel was 99·99 wt.%. Carbon and silicon were the major impurities in the plutonium, and 125 p.p.m. carbon was the principal contaminant in the nickel. The alloy specimen was crushed and, after considerable searching among the pieces, a fragment was found that produced good single crystal X-ray photographs. The crystal was of somewhat irregular shape and had the approximate average dimensions 90 × 25 × 15 microns. Weissenberg photographs were originally indexed on the basis of a monoclinic unit cell with

$$a = 8{\cdot}57,\quad b = 5{\cdot}00,\quad c = 8{\cdot}62\ \text{Å};\quad \beta = 109^\circ\ 40'.$$

The extinctions were characteristic of space group $C2$ or $C2/m$. The true, primitive unit cell is, however, rhombohedral with $a = 6{\cdot}22$ Å, $\alpha = 33^\circ\ 44'$ and probable group $R\bar{3}m$. The non-primitive hexagonal cell has $a = 5{\cdot}00 \pm 0{\cdot}02$ and $c = 24{\cdot}35 \pm 0{\cdot}10$ Å. The cell dimensions were measured from resolved α_1, α_2 reflections on zero-level Weissenberg photographs (Cu $K\alpha_1$, $\lambda = 1{\cdot}54050$ Å). The calculated density with 3 $PuNi_3$ in the rhombohedral cell is 11·8 g.cm.$^{-3}$. The measured density of the bulk specimen (by displacement of bromobenzene) was 11·8 g.cm.$^{-3}$. For the intensity data, Mo $K\alpha$ radiation and a scintillation counter attached to a Weissenberg camera were used (Evans, 1953). The crystal was rotated about the monoclinic b axis and intensities on the zero level were measured to $\sin\theta/\lambda = 0{\cdot}746$. The long dimension of the crystal coincided closely with the rotation axis. Of the 122 reflections within this circle, 80 were observed to be greater than zero. No absorption corrections were made.

A cerium–nickel alloy of gross stoichiometry $CeNi_3$ was prepared by melting the elements in a helium atmosphere at 1600 °C. and cooling fairly rapidly. Cerium of 99·86 and nickel of 99·99 wt.% purity were used. A fragment of this alloy specimen was identified by its diffraction pattern as being $CeNi_5$. The alloy was reheated in vacuum to 940 °C., held at that temperature for 72 hr., and then cooled to room temperature at the rate of 4°/min. Fragments were then examined with a precession camera. Two different crystalline species were found. Both were hexagonal with $a = 4{\cdot}98 \pm 0{\cdot}02$ Å but one had $c = 16{\cdot}54 \pm 0{\cdot}06$ and the other had $c = 24{\cdot}52 \pm 0{\cdot}08$ Å. Both crystals showed the following systematic extinctions: The classes of reflections $00l$, hhl and hkl with $h-k=3n$ were absent with l odd. These extinctions are characteristic of certain special positions of space group $P6_3/mmc$ or the non-centric space group $P\bar{6}2c$. By determining its structure, the smaller of these cells was identified as $CeNi_3$. The calculated density, with 6 formula units per unit cell is 8·87 g.cm.$^{-3}$. The measured density of the bulk specimen was 8·48 g.cm.$^{-3}$. It is worth noting that the cell constants of the larger cell are close to those reported by Florio *et al.* (1956) for $ThFe_3$ and $ThCo_{2-3}$. A crystal of $CeNi_3$ with the approximate average dimensions of 40 × 20 × 15 microns was mounted on the a axis and intensity data for $h = 0$ to 5 were obtained with a scintillation counter on a Weissenberg camera. The long dimension of the crystal was approximately parallel to a^*. There were 389 out of approximately 775 non-equivalent reflections within a sphere of radius $\sin\theta/\lambda \approx 1{\cdot}078$ that were observed to be greater than zero. No absorption corrections were made.

Determination of the structure of $PuNi_3$

The xz parameters of the trial structure were deduced from inspection of the Patterson projection of the monoclinic, non-primitive cell on (010). The intensity distributions on the odd k layers were essentially identical. The zero and the 4th layers were the same but the 2nd layer was different. The relationship of these layers indicated that atoms were at $y = 0$, $\frac{1}{4}$ and $\frac{1}{2}$ and hence the y parameters of the various atoms could be determined.

This trial structure had such marked threefold symmetry, with the threefold axis coinciding with c^*, that it prompted further investigation of the crystal with a precession camera, and the true rhombohedral cell was quickly revealed. The probable space group is $R\bar{3}m$ with

1 Pu in $1a$ (0, 0, 0, 2 Pu in $2c$ (x, x, x) with $x \approx \frac{1}{7}$;
1 Ni in $1b$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; 2 Ni in $2c$ (x, x, x) with $x \approx \frac{1}{3}$;
and 6 Ni in $6h$ (x, x, z) with $x \approx \frac{7}{12}$ and $z \approx \frac{1}{12}$.

The exact location of the sixfold set of nickel atoms assigned to positions xxz determines whether the space group is $R\bar{3}$ or $R\bar{3}m$. If they are not in positions where $x = y$, the space group is $R\bar{3}$. Within the accuracy of our data, these nickel atoms are in set $6h$ of $R\bar{3}m$.

In order to somewhat simplify the calculations, all further work was done using the non-primitive hexagonal cell. A least-squares refinement was made. All non-zero $F_o(h0l)$ (hexagonal indices) were equally weighted and the zero F_o were omitted. Off-diagonal terms of the normal equations were omitted. Usually, this omission is not possible with two-dimensional data, but in this case the structure is well resolved in projection. Individual isotropic temperature factors were assigned to each crystallographically different atom and these parameters were refined simultaneously with the atomic positions and the scale factor. The Thomas–Fermi form factor was used for plutonium, and the form factor of Viervoll & Øgrim (1949) was used for nickel.

The refinement of the atomic positions proceeded satisfactorily. The x parameter of the nickel atoms in 18h did not change significantly from $\frac{1}{2}$. The positions of these nickel atoms are analogous to the positions of the threefold set of nickel atoms in the $PuNi_5$ structure and these atoms are ideally arranged in a sheet of regular hexagons, a condition realized only if $x=\frac{1}{2}$. However, the temperature factor parameters of Ni_1 and Ni_2 would have become negative had the program allowed this to happen. This situation can be explained by saying that the nickel form factor should have been much larger or that the plutonium form factor should have been much smaller. There is no physical reason for the former case but there is for the latter. The wavelength of Mo $K\alpha$ radiation is just on the long wavelength side of the L_{III} absorption edge of plutonium and hence there should be a large anomalous dispersion correction to the form factor. Methods for calculating this correction are only approximate. By the method of Parratt & Hempstead (1954), a value of $\Delta f=-10$ electrons was calculated, but this procedure gives results admittedly on the low side.

The Patterson projection has a number of well resolved peaks. Inspection of the relative magnitudes of these peaks suggested that $\Delta f \approx -16$ to -20 electrons, depending on which peaks were compared.

The least-squares calculations were repeated with various values of Δf applied to the plutonium form factor. The sum of the squares of the residuals became a minimum with $\Delta f=-20$ electrons. A curve of the residuals *vs.* Δf is shown in Fig. 1. The slope of the curve is small in the region of the minimum so that values of Δf from -17 to -23 electrons give essentially the same results.

In all these calculations, the positional parameters changed very little and therefore the derived structure is independent of the plutonium form factor over fairly wide limits. The final results with $\Delta f_{Pu}=-20$ electrons are given in Table 1. The corresponding structure factors are listed in Table 2. The reliability index with $F_o=0$ excluded is 6·4%. Work is underway in this laboratory to experimentally measure the plutonium form factor on an absolute scale.

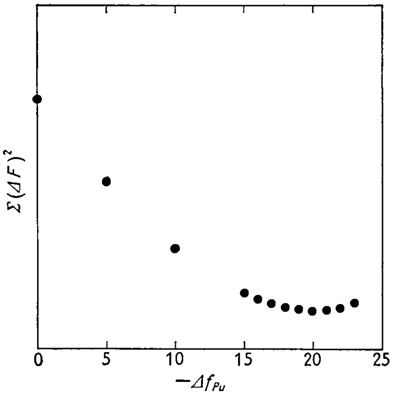

Fig. 1. A plot of the sum of the squares of residuals from the least-squares refinement of $PuNi_3$ *vs.* the anomalous dispersion correction applied to the Thomas–Fermi form factor of plutonium.

Table 1. *Results of the least-squares refinement of* $PuNi_3$ *with* $\Delta f_{Pu}=-20$ electrons

Atom	x	y	z	B (Å^2)
Pu_1	0	0	0	0·37 ± 0·11
Pu_2	0	0	0·1414 ± 0·0002	0·59 ± 0·08
Ni_1	0	0	$\frac{1}{2}$	0·58 ± 0·30
Ni_2	0	0	0·3336 ± 0·0005	0·45 ± 0·20
Ni_3	0·5002 ± 0·0013	$-x$	0·0829 ± 0·0002	1·10 ± 0·11

Table 2. *Observed and calculated structure factors for* $PuNi_3$ *with* $\Delta f_{Pu}=-20$ *electrons*

h	ℓ	F_o	F_c	h	ℓ	F_o	F_c	h	ℓ	F_o	F_c	h	ℓ	F_o	F_c
0	3	0	-81	1	23	0	-22	3	-21	258	269	4	11	0	8
0	6	239	215	1	26	0	-13	3	-18	0	81	4	14	312	322
0	9	213	185	1	29	142	170	3	-15	266	272	4	17	-205	-216
0	12	603	573	1	32	0	-30	3	-12	87	87	4	20	0	68
0	15	449	402	1	35	114	92	3	- 9	126	129	4	23	126	111
0	18	233	-217	2	-32	130	-105	3	- 6	485	474	4	26	0	68
0	21	350	337	2	-29	0	29	3	- 3	0	7	5	-20	132	128
0	24	270	231	2	-26	96	92	3	0	456	452	5	-17	0	-46
0	27	192	189	2	-23	156	158	3	3	0	-47	5	-14	168	172
0	30	0	34	2	-20	119	85	3	6	471	474	5	-11	102	-138
0	33	0	21	2	-17	-341	-319	3	9	130	129	5	- 8	172	191
0	36	301	292	2	-14	524	491	3	12	87	87	5	- 5	0	23
1	-34	0	82	2	-11	0	24	3	15	255	272	5	- 2	0	25
1	-31	0	-41	2	- 8	197	186	3	18	0	81	5	1	0	74
1	-28	209	233	2	-5	312	-322	3	21	262	269	5	4	0	-33
1	-25	190	-189	2	-2	263	277	3	24	0	4	5	7	178	200
1	-22	217	214	2	1	521	554	3	27	134	141	5	10	0	-64
1	-19	0	11	2	4	-257	-296	3	30	150	164	5	13	0	51
1	-16	156	146	2	7	86	62	4	-28	126	112	5	16	0	71
1	-13	88	100	2	10	0	38	4	-25	0	-2	5	19	0	3
1	-10	197	-171	2	13	390	389	4	-22	243	212	6	-12	146	175
1	-7	500	516	2	16	0	-8	4	-19	148	-148	6	-9	0	65
1	-4	75	-93	2	19	223	-223	4	-16	0	1	6	-6	0	92
1	-1	183	180	2	22	296	295	4	-13	249	246	6	-3	0	-12
1	2	44	46	2	25	0	4	4	-10	0	22	6	0	340	341
1	5	80	69	2	28	144	145	4	-7	0	51	6	3	0	-12
1	8	402	474	2	31	182	-166	4	-4	168	-165	6	6	0	92
1	11	344	-338	2	34	115	126	4	-1	321	312	6	9	0	65
1	14	345	360	3	-30	181	164	4	2	154	155	6	12	155	175
1	17	72	-91	3	-27	134	141	4	5	182	-179				
1	20	234	246	3	-24	0	4	4	8	128	124				

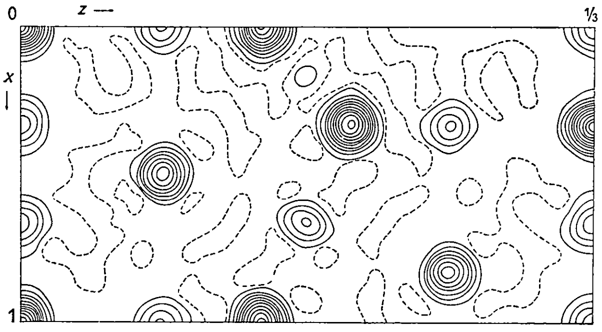

Fig. 2. Fourier projection of $PuNi_3$ on a plane normal to the hexagonal b axis. The zero contour is dashed. The contour interval is 20 e.Å^{-2}.

Fig. 2 shows a Fourier projection of the hexagonal cell of $PuNi_3$. The scaling of this Fourier was derived from the least-squares results with $\Delta f_{Pu} = -20$ electrons.

Determination of the structure of $CeNi_3$

Two different crystalline species were obtained from the cerium–nickel alloy, but the amount of either compound available in pure form was far too small for chemical analysis or density measurement. Speculations as to the identities of these crystals had to be based on their unit-cell volumes and the published phase diagram, which, in this composition region, indicated the uncertain existence of $CeNi_3$ and $CeNi_4$.

Knowing the volumes of $CeNi_2$ and $CeNi_5$ one can calculate atomic volumes for cerium and nickel and hence compute the approximate volume of any other cerium–nickel compound. The cerium and nickel atomic volumes are 22·6 and 12·0 Å^3. The volumes of the two unknown compounds are 355 and 524 Å^3.

At first, the assumption was made that the compounds listed by Vogel (1947) were correct. Of these compounds, 6 $CeNi_3$ (352 Å^3) or 5 $CeNi_4$ (353 Å^3) fit the smaller cell and only 9 $CeNi_3$ (527 Å^3) fit the larger cell. Structures for the compositions 5 $CeNi_4$ and 9 $CeNi_3$ were extensively studied. Even though the space groups indicated by the systematic extinctions do not permit odd numbers of atoms, arrangements could be found that made the 'extinct' reflections uniformly weak because $2f_{Ni} \approx f_{Ce}$.

No structures for 5 $CeNi_4$ or 9 $CeNi_3$ could be found that satisfactorily accounted for all of the observed intensities. Finally, a three-dimensional Patterson was computed for the smaller cell. Inspection of the Patterson quickly showed that this cell contained 6 $CeNi_3$ in space group $P6_3/mmc$ with

2 Ce_1 in $2c$, 4 Ce_2 in $4f$ with $z \approx 0{\cdot}042$, 2 Ni_1 in $2a$, 2 Ni_2 in $2b$, 2 Ni_3 in $2d$ and 12 Ni_4 in $12k$ with $x \approx \frac{5}{6}$ and $z \approx \frac{1}{8}$.

The least-squares refinement of all data yielded the results shown in Table 3. The cerium form factors were taken from *Internationale Tabellen* (1935). The other features of the least-squares calculations were as described in the section on $PuNi_3$. The complete set of observed and calculated structure factors is given in Table 4. With the $F_o = 0$ omitted, the reliability index is 6·6%. This excellent agreement is convincing evidence for both the structure and composition of this compound. The twelvefold set of nickel atoms is analogous to the threefold set in $CeNi_5$ and their position determines whether the space group is $P6_3/mmc$ or $P\bar{6}2c$. The fact that these nickel atoms ideally form a regular hexagonal network, a condition realized if they are in set $12k$ of space group $P6_3/mmc$ with $x = \frac{5}{6}$, and also the structure factor agreement indicates that $P6_3/mmc$ is the most probable space group. A Fourier projection of $CeNi_3$ is shown in Fig. 3.

Table 3. *Results of the least-squares refinement of* $CeNi_3$

Atom	x	y	z	B (Å^2)
Ce_1	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0·45 ± 0·03
Ce_2	$\frac{1}{3}$	$\frac{2}{3}$	0·04178 ± 0·00004	0·58 ± 0·02
Ni_1	0	0	0	0·83 ± 0·08
Ni_2	0	0	$\frac{1}{4}$	0·38 ± 0·06
Ni_3	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0·57 ± 0·07
Ni_4	0·8334 ± 0·0002		0·12715 ± 0·00005	0·54 ± 0·02

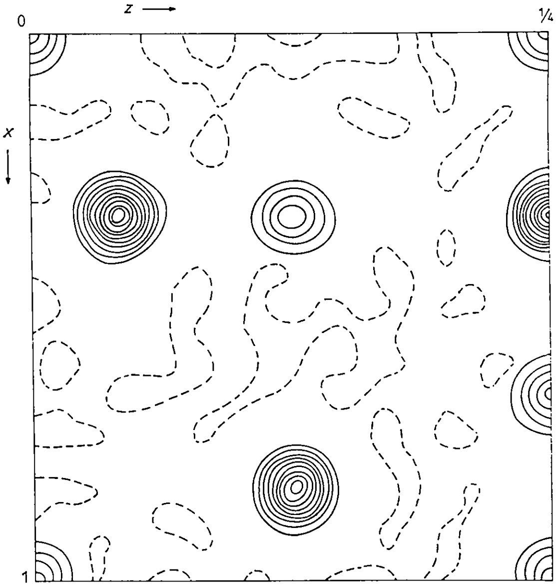

Fig. 3. Fourier projection of $CeNi_3$ on a plane normal to the b axis. The zero contour is dashed. The contour interval is 25 e.Å^{-2}.

At this writing, the composition and structure of the larger cell have not been definitely established.

Discussion of the structure

These structures represent two new structure types for MX_3 compounds. They are a combination of the Cu_2Mg and $CaCu_5$ structures. In $CeNi_3$, the Ce_1 atoms have surroundings identical to those of the cerium atoms in $CeNi_5$. The Ce_2 atoms have surroundings identical to those of the cerium atoms in $CeNi_2$. The structure is built up of alternating single layers of $CeNi_5$ and double layers of $CeNi_2$. A drawing of the $CeNi_3$ structure is shown in Fig. 4.

$PuNi_3$ is similar to $CeNi_3$ except that the third $PuNi_5$-type layer, rather than being directly above the first is displaced from it by $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$, and thus $PuNi_3$ has a rhombohedral lattice.

Table 5 lists the various interatomic distances. The estimated error for any of these distances is ± 0·01 Å, and results almost entirely from errors in the cell dimensions. All distances are close to the corresponding ones in $CeNi_2$, $CeNi_5$, $PuNi_2$ and $PuNi_5$

Table 4. *Observed and calculated structure factors for* CeNi$_3$

The column headings are h, k, l, F_o and F_c

1	0	0	29	-32
2	0	0	194	-185
3	0	0	243	233
4	0	0	139	-119
5	0	0	41	-23
6	0	0	235	241
7	0	0	56	-17
8	0	0	59	-52
9	0	0	61	62
1	0	1	32	-32
2	0	1	230	222
3	0	1	0	0
4	0	1	148	-139
5	0	1	36	19
6	0	1	0	0
7	0	1	0	-14
8	0	1	57	58
9	0	1	0	0
0	0	2	0	18
1	0	2	15	-14
2	0	2	14	-6
3	0	2	20	19
4	0	2	0	-3
5	0	2	0	-4
6	0	2	0	7
7	0	2	0	-1
8	0	2	0	1
9	0	2	0	3
1	0	3	22	-21
2	0	3	199	196
3	0	3	0	0
4	0	3	125	-121
5	0	3	21	9
6	0	3	0	0
7	0	3	0	-6
8	0	3	49	48
9	0	3	0	0
0	0	4	56	58
1	0	4	68	-72
2	0	4	95	86
3	0	4	274	275
4	0	4	54	49
5	0	4	37	-37
6	0	4	28	28
7	0	4	31	-27
8	0	4	0	16
9	0	4	60	74
1	0	5	222	-247
2	0	5	22	25
3	0	5	0	-0
4	0	5	49	-23
5	0	5	114	117
6	0	5	0	0
7	0	5	66	-76
8	0	5	0	12
9	0	5	0	-0
0	0	6	124	-115
1	0	6	64	68
2	0	6	47	48
3	0	6	95	-95
4	0	6	32	34
5	0	6	33	34
6	0	6	51	-44
7	0	6	0	24
8	0	6	0	17
9	0	6	0	-28
1	0	7	136	-142
2	0	7	30	-23
3	0	7	0	-0
4	0	7	0	14
5	0	7	62	66
6	0	7	0	-0
7	0	7	38	-43
8	0	7	0	-6
9	0	7	0	-0
0	0	8	319	346
1	0	8	89	90
2	0	8	49	-48
3	0	8	25	26
4	0	8	37	-34
5	0	8	32	39
6	0	8	116	123
7	0	8	0	24
8	0	8	0	-18
9	0	8	0	9
1	0	9	73	-79
2	0	9	228	234
3	0	9	0	0
4	0	9	166	-165
5	0	9	46	46
6	0	9	0	0
7	0	9	34	-31
8	0	9	68	73
0	0	10	261	-263
1	0	10	103	110
2	0	10	111	114
3	0	10	164	-167
4	0	10	82	84
5	0	10	57	62
6	0	10	100	-112
7	0	10	48	42
8	0	10	32	39
1	0	11	39	34
2	0	11	84	80
3	0	11	0	0
4	0	11	58	-55
5	0	11	25	-20
6	0	11	0	0
7	0	11	0	13
8	0	11	0	24
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2	0	12	142	140
3	0	12	59	60
4	0	12	101	100
5	0	12	25	22
6	0	12	73	-65
7	0	12	0	13
8	0	12	50	43
1	0	13	44	-39
2	0	13	102	-102
3	0	13	0	-0
4	0	13	78	72
5	0	13	0	23
6	0	13	0	-0
7	0	13	0	-16
8	0	13	35	-34
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2	0	14	71	72
3	0	14	150	-155
4	0	14	57	57
5	0	14	54	60
6	0	14	74	-78
7	0	14	33	42
8	0	14	0	28
1	0	15	70	70
2	0	15	146	-148
3	0	15	0	-0
4	0	15	111	115
5	0	15	42	-46
6	0	15	0	-0
7	0	15	31	31
8	0	15	54	-54
0	0	16	210	204
1	0	16	62	52
2	0	16	43	-33
3	0	16	22	21
4	0	16	30	-26
5	0	16	32	28
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7	0	16	0	18
8	0	16	0	-16
1	0	17	88	87
2	0	17	37	32
3	0	17	0	0
4	0	17	25	-24
5	0	17	50	-53
6	0	17	0	0
7	0	17	37	37
8	0	17	0	14
0	0	18	123	-96
1	0	18	44	30
2	0	18	46	46
3	0	18	49	-48
4	0	18	35	37
5	0	18	0	21
6	0	18	43	-51
7	0	18	0	16
8	0	18	0	21
1	0	19	109	111
2	0	19	42	-45
3	0	19	0	0
4	0	19	39	37
5	0	19	69	-73
6	0	19	0	-0
7	0	19	52	50
0	0	20	70	37
1	0	20	47	-36
2	0	20	39	28
3	0	20	142	145
4	0	20	28	21
5	0	20	0	-25
6	0	20	0	21
7	0	20	0	-19
1	0	21	0	2
2	0	21	96	-94
3	0	21	0	-0
4	0	21	74	76
5	0	21	0	-1
6	0	21	0	-0
7	0	21	0	-0
0	0	22	57	38
1	0	22	0	2
2	0	22	0	-15
3	0	22	0	1
4	0	22	0	-12
5	0	22	0	3
6	0	22	0	20
7	0	22	0	3
1	0	23	23	22
2	0	23	66	-64
3	0	23	0	-0
4	0	23	55	53
5	0	23	0	-15
6	0	23	0	-0
7	0	23	0	10
0	0	24	218	223
1	0	24	0	-20
2	0	24	65	-69
3	0	24	101	101
4	0	24	52	-57
5	0	24	0	-15
6	0	24	124	130
1	0	25	0	-12
2	0	25	87	88
3	0	25	0	0
4	0	25	72	-73
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6	0	25	0	0
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2	0	26	0	11
3	0	26	0	13
4	0	26	0	11
5	0	26	0	-2
6	0	26	0	-13
1	0	27	0	-11
2	0	27	46	42
3	0	27	0	0
4	0	27	37	-35
5	0	27	0	8
6	0	27	0	0
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1	0	28	0	-24
2	0	28	0	16
3	0	28	100	94
4	0	28	0	14
5	0	28	0	-17
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3	0	29	0	-0
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2	0	30	0	9
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5	0	30	28	19
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3	0	31	0	-0
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1	0	32	0	17
2	0	32	0	-14
3	0	32	0	10
4	0	32	0	-13
1	0	33	0	-19
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1	0	35	0	6
1	1	0	324	307
2	1	0	36	-28
3	1	0	23	-25
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5	1	0	35	-22
6	1	0	0	-19
7	1	0	77	87
8	1	0	0	-13
2	1	1	33	-26
3	1	1	21	22
4	1	1	0	-0
5	1	1	0	-18
6	1	1	0	15
7	1	1	0	-0
8	1	1	0	-9
1	1	2	25	24
2	1	2	0	-9
3	1	2	0	-7
4	1	2	0	14
5	1	2	0	-3
6	1	2	0	-2
7	1	2	0	6
8	1	2	0	1
2	1	3	0	-15
3	1	3	0	12
4	1	3	0	-0
5	1	3	0	-8
6	1	3	0	6
7	1	3	0	-0
8	1	3	0	-3
1	1	4	352	362
2	1	4	57	-55
3	1	4	48	-46
4	1	4	198	194
5	1	4	38	-34
6	1	4	0	-29
7	1	4	99	102
8	1	4	0	-19
2	1	5	187	-187
3	1	5	159	153
4	1	5	0	0
5	1	5	112	-104
6	1	5	79	84
7	1	5	0	0
8	1	5	57	-53
1	1	6	118	-121
2	1	6	52	53
3	1	6	44	44
4	1	6	66	-70
5	1	6	30	31
6	1	6	28	26
7	1	6	41	-38
8	1	6	0	18
2	1	7	108	-108
3	1	7	92	89
4	1	7	0	0
5	1	7	56	-59
6	1	7	46	47
7	1	7	0	0
8	1	7	31	-30
1	1	8	32	33
2	1	8	69	67
3	1	8	58	55
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5	1	8	35	33
6	1	8	0	26
7	1	8	0	11
8	1	8	0	16
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3	1	9	55	57
4	1	9	0	-0
5	1	9	40	-42
6	1	9	32	35
7	1	9	0	-0
8	1	9	0	-21
1	1	10	190	-201
2	1	10	89	90
3	1	10	75	78
4	1	10	122	-128
5	1	10	48	56
6	1	10	42	46
7	1	10	67	-71
8	1	10	35	31
2	1	11	30	28
3	1	11	29	-25
4	1	11	0	-0
5	1	11	0	18
6	1	11	0	-15
7	1	11	0	-0
8	1	11	0	10
1	1	12	79	73
2	1	12	36	36
3	1	12	32	30
4	1	12	45	43
5	1	12	27	19
6	1	12	0	15
7	1	12	0	26
8	1	12	0	8
2	1	13	36	-33
3	1	13	30	29
4	1	13	0	0
5	1	13	0	-21
6	1	13	0	17
7	1	13	0	0
8	1	13	0	-12
1	1	14	174	-178
2	1	14	80	83
3	1	14	72	74
4	1	14	116	-123
5	1	14	50	54
6	1	14	44	45
7	1	14	62	-70
8	1	14	38	31
2	1	15	59	62
3	1	15	55	-56
4	1	15	0	0
5	1	15	35	41
6	1	15	0	-34
7	1	15	0	0
1	1	16	0	24
2	1	16	48	43
3	1	16	45	37
4	1	16	0	17
5	1	16	27	25
6	1	16	0	20
7	1	16	0	11
2	1	17	75	76
3	1	17	66	-67
4	1	17	0	-0
5	1	17	48	48
6	1	17	33	-40
7	1	17	0	-0
1	1	18	58	-54
2	1	18	36	27
3	1	18	23	25
4	1	18	40	-39
5	1	18	0	20
6	1	18	0	17
7	1	18	26	-24
2	1	19	95	99
3	1	19	82	-89
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5	1	19	66	66
6	1	19	55	-55
7	1	19	0	-0
1	1	20	163	163
2	1	20	36	-33
3	1	20	28	-30
4	1	20	113	119
5	1	20	0	-24
6	1	20	0	-20
7	1	20	76	72
2	1	21	0	1
3	1	21	0	-1
4	1	21	0	0
5	1	21	0	0
6	1	21	0	-0
1	1	22	0	2
2	1	22	0	2
3	1	22	0	2
4	1	22	0	0
5	1	22	0	3
6	1	22	0	3
2	1	23	0	20
3	1	23	0	-18
4	1	23	0	0
5	1	23	0	13
6	1	23	0	-11
1	1	24	112	112
2	1	24	0	-19
3	1	24	0	-17
4	1	24	82	84
5	1	24	0	-14
6	1	24	0	-11
2	1	25	0	-11
3	1	25	0	9
4	1	25	0	-0
5	1	25	0	-7
6	1	25	0	5
1	1	26	0	15
2	1	26	0	-4
3	1	26	0	-3
4	1	26	0	10
5	1	26	0	-2
2	1	27	0	-10
3	1	27	0	9
4	1	27	0	-0
5	1	27	0	-7
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2	1	28	0	-22
3	1	28	0	-20
4	1	28	90	80
5	1	28	0	-16
2	1	29	65	-65
3	1	29	59	60
4	1	29	0	0
1	1	30	43	-43
2	1	30	31	23
3	1	30	0	21
4	1	30	30	-34
2	1	31	0	-28
3	1	31	33	25
4	1	31	0	0
1	1	32	0	11
2	1	32	0	16
3	1	32	0	14
2	1	33	29	-17
1	1	34	55	-51
2	1	34	31	27
2	2	0	442	426
3	2	0	26	-23
4	2	0	98	-92
5	2	0	118	117
6	2	0	63	-62
7	2	0	0	-14
8	2	0	115	119
3	2	1	23	-20
4	2	1	111	105
5	2	1	0	0
6	2	1	68	-69
7	2	1	0	10
8	2	1	0	0
2	2	2	16	11
3	2	2	0	-5
4	2	2	0	-2
5	2	2	0	10
6	2	2	0	0
7	2	2	0	0
8	2	2	0	1
3	2	3	0	-11
4	2	3	94	89
5	2	3	0	0
6	2	3	56	-58
7	2	3	0	4
8	2	3	0	0
2	2	4	51	39
3	2	4	41	-41
4	2	4	40	32
5	2	4	128	136
6	2	4	22	19
7	2	4	0	-21
8	2	4	0	12
3	2	5	132	-132
4	2	5	24	23
5	2	5	0	-0
6	2	5	0	-16
7	2	5	0	58
8	2	5	0	0
2	2	6	68	-70
3	2	6	37	38
4	2	6	24	27
5	2	6	42	-50
6	2	6	0	20
7	2	6	0	19
3	2	7	77	-76
4	2	7	0	-9
5	2	7	0	-0
6	2	7	0	7
7	2	7	0	33
2	2	8	216	211
3	2	8	42	46
4	2	8	35	-27
5	2	8	0	14
6	2	8	0	-20
7	2	8	0	17
3	2	9	57	-51
4	2	9	127	128
5	2	9	0	0
6	2	9	87	-86
7	2	9	0	23
2	2	10	174	-178
3	2	10	68	69
4	2	10	63	67
5	2	10	88	-93
6	2	10	50	46
7	2	10	0	33
3	2	11	29	22
4	2	11	40	42
5	2	11	0	0
6	2	11	0	-28
7	2	11	0	-11
2	2	12	105	-105
3	2	12	28	25
4	2	12	78	77
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6	2	12	54	51
7	2	12	0	9
3	2	13	0	-26
4	2	13	63	-56
5	2	13	0	-0
6	2	13	40	39
7	2	13	0	13
2	2	14	116	-118
3	2	14	65	66
4	2	14	42	47
5	2	14	84	-91
6	2	14	0	33
7	2	14	0	33
3	2	15	48	51
4	2	15	93	-93
5	2	15	0	-0
6	2	15	60	64
7	2	15	0	-23
2	2	16	148	151
3	2	16	33	32
4	2	16	0	-22
5	2	16	0	13
6	2	16	0	-17
7	2	16	0	14
3	2	17	53	59
4	2	17	0	20
5	2	17	0	0
6	2	17	0	-15
2	2	18	73	-75
3	2	18	0	23
4	2	18	0	31
5	2	18	0	-30
6	2	18	0	23
3	2	19	75	80
4	2	19	27	-30
5	2	19	0	0
6	2	19	0	20
2	2	20	0	31
3	2	20	33	-28
4	2	20	0	17
5	2	20	83	91
6	2	20	0	12
3	2	21	0	1
4	2	21	67	-63
5	2	21	0	-0
6	2	21	46	46
2	2	22	32	30
3	2	22	0	2
4	2	22	0	-9
5	2	22	0	-1
6	2	22	0	-5
3	2	23	0	16
4	2	23	46	-44
5	2	23	0	-0
2	2	24	188	183
3	2	24	0	-16
4	2	24	42	-49
5	2	24	68	65
3	2	25	0	-8
4	2	25	63	62
5	2	25	0	0
2	2	26	0	-16
3	2	26	0	-3
4	2	26	0	10
5	2	26	0	7
3	2	27	0	-8
4	2	27	29	30
2	2	28	0	21
3	2	28	0	-19
4	2	28	0	12
3	2	29	54	-55
4	2	29	0	1
2	2	30	0	-11
3	2	30	0	20
3	2	31	29	-23
2	2	32	74	66
3	3	0	150	146
4	3	0	29	-20
5	3	0	0	-18
6	3	0	76	79
7	3	0	0	-11
4	3	1	0	-17
5	3	1	0	14
6	3	1	0	-0
7	3	1	0	-8
3	3	2	0	12
4	3	2	0	-3
5	3	2	0	-1
6	3	2	0	5
7	3	2	0	1
4	3	3	0	-7
5	3	3	0	6
6	3	3	0	-0
7	3	3	0	-3
3	3	4	175	170
4	3	4	30	-31
5	3	4	32	-26
6	3	4	89	94
7	3	4	0	-18
4	3	5	94	-94
5	3	5	77	77
6	3	5	0	0
7	3	5	52	-49
3	3	6	62	-62
4	3	6	39	28
5	3	6	29	24
6	3	6	28	-35
7	3	6	0	17
4	3	7	52	-52
5	3	7	41	43
6	3	7	0	0
7	3	7	0	-28
3	3	8	0	17
4	3	8	33	29
5	3	8	33	23
6	3	8	0	11
7	3	8	0	14
4	3	9	40	-38
5	3	9	33	31
6	3	9	0	-0
7	3	9	38	-19
3	3	10	110	-115
4	3	10	44	51
5	3	10	41	42
6	3	10	61	-65
7	3	10	0	29
4	3	11	0	16
5	3	11	0	-13
6	3	11	0	-0
3	3	12	47	38
4	3	12	0	17
5	3	12	0	13
6	3	12	0	24
4	3	13	0	-19
5	3	13	0	16
6	3	13	0	0
3	3	14	105	-111
4	3	14	44	50
5	3	14	46	42
6	3	14	65	-64
4	3	15	37	37
5	3	15	0	-31
6	3	15	0	0
3	3	16	0	15
4	3	16	0	22
5	3	16	0	18
6	3	16	0	10
4	3	17	43	44
5	3	17	40	-37
6	3	17	0	-0
3	3	18	39	-36
4	3	18	0	18
5	3	18	0	16
6	3	18	28	-22
4	3	19	56	60
5	3	19	51	-50
3	3	20	107	108
4	3	20	0	-22
5	3	20	0	-19
4	3	21	0	0
5	3	21	0	0
3	3	22	0	-0
4	3	22	0	3
5	3	22	0	3
4	3	23	0	12
5	3	23	0	-10
3	3	24	73	77
4	3	24	0	-12
4	3	25	0	-6
3	3	26	0	9
4	3	26	0	-1
3	3	28	85	74
4	4	0	201	196
5	4	0	0	-14
6	4	0	36	-45
5	4	1	0	-11
6	4	1	49	49
4	4	2	0	5
5	4	2	0	-0
6	4	2	0	2
5	4	3	0	-4
6	4	3	44	41
4	4	4	0	23
5	4	4	0	-23
6	4	4	0	14
5	4	5	62	-63
6	4	5	0	9
4	4	6	28	-36
5	4	6	0	21
6	4	6	0	15
5	4	7	40	-36
6	4	7	0	-6
4	4	8	102	102
5	4	8	0	19
6	4	8	0	-16
5	4	9	0	-25
6	4	9	60	62
4	4	10	89	-93
5	4	10	33	36
6	4	10	37	34
5	4	11	0	11
6	4	11	0	21
4	4	12	58	-53
5	4	12	0	10
6	4	12	39	36
5	4	13	0	-14
4	4	14	61	-64
5	4	14	35	36
5	4	15	0	25
4	4	16	78	85
5	4	16	0	15
5	4	17	0	31
4	4	18	50	-44
5	4	18	0	14
5	4	19	42	42
4	4	20	0	17
4	4	22	0	17
5	5	0	59	67
5	5	2	0	4
5	5	4	81	80
5	5	6	0	-30
5	5	8	0	10
5	5	10	50	-55

Table 5. *Interatomic distances in* CeNi$_3$ *and* PuNi$_3$

CeNi$_3$

Atom	Neighbor	Number	Distance
Ce$_1$	Ce$_2$	2	3·44 Å
	Ni$_2$	3	2·88
	Ni$_3$	3	2·88
	Ni$_4$	12	3·22
Ce$_2$	Ce$_1$	1	3·44
	Ce$_2$	3	3·19
	Ni$_1$	3	2·96
	Ni$_4$	3	3·14
	Ni$_4$	6	2·86
Ni$_1$	Ce$_2$	6	2·96
	Ni$_4$	6	2·55
Ni$_2$	Ce$_1$	3	2·88
	Ni$_3$	3	2·88
	Ni$_4$	6	2·49
Ni$_3$	Ce$_1$	3	2·88
	Ni$_2$	3	2·88
	Ni$_4$	6	2·49
Ni$_4$	Ce$_1$	2	3·22
	Ce$_2$	1	3·14
	Ce$_2$	2	2·86
	Ni$_1$	1	2·55
	Ni$_2$	1	2·49
	Ni$_3$	1	2·49
	Ni$_4$	4	2·49

PuNi$_3$

Atom	Neighbor	Number	Distance
Pu$_1$	Pu$_2$	2	3·44 Å
	Ni$_2$	6	2·89
	Ni$_3$	12	3·21
Pu$_2$	Pu$_1$	1	3·44
	Pu$_2$	3	3·14
	Ni$_1$	3	2·95
	Ni$_3$	3	3·02
	Ni$_3$	6	2·88
Ni$_1$	Pu$_2$	6	2·95
	Ni$_3$	6	2·50
Ni$_2$	Pu$_1$	3	2·89
	Ni$_2$	3	2·89
	Ni$_3$	6	2·50
Ni$_3$	Pu$_1$	2	3·21
	Pu$_2$	1	3·02
	Pu$_2$	2	2·88
	Ni$_1$	1	2·50
	Ni$_2$	2	2·50
	Ni$_3$	4	2·50

except for the Ce$_1$–Ce$_2$ and Pu$_1$–Pu$_2$ distances which are 3·44 Å in these compounds and about 4 Å in the *M*Ni$_5$ structures.

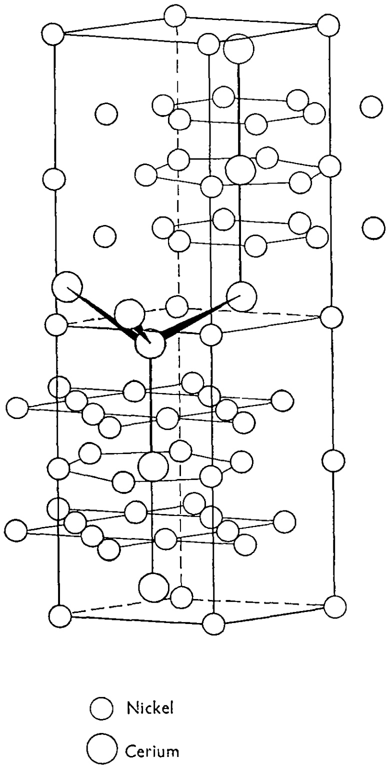

Fig. 4. Drawing of the CeNi$_3$ structure.

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