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Structural Redetermination of the ThNi Phase

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Abstract. $M_r = 290.8$, orthorhombic, *Pnma*, $a = 14.146\,(6)$, $b = 4.286\,(3)$, $c = 5.702\,(3)$ Å, $V = 345.7$ Å^3, $Z = 8$, $D_x = 11.17$ Mg m^{-3}, $F(000) = 944$, room temperature, $\lambda(\text{Mo }K\alpha) = 0.71069$ Å, $\mu(\text{Mo }K\alpha) = 138$ mm^{-1}, final $R = 0.049$ for 306 observed reflections. Contrary to the report of Florio, Baenziger & Rundle [*Acta Cryst.* (1956), **9**, 367–372], ThNi was found to crystallize in a stacking variant of the CrB–FeB types with trigonal-prismatic coordination of the Ni atoms, and recognized to be isotypic with the SrAg phase, having stacking code $(hc)_2$.

Introduction. The crystal structure of the orthorhombic ThNi was described by Florio, Baenziger & Rundle (1956). During a study on the structures of phases formed by the alkaline-earth elements with Cu and Ag (Merlo & Fornasini, 1981), it was noted that ThNi had the same space group and number of atoms per cell, and very similar lattice-constant ratios as SrAg, a stacking variant of the CrB–FeB types, whereas atomic positions and coordination were different. A sample of ThNi was then prepared and the observed powder intensities were compared with the values calculated both for the original proposition by Florio *et al.* (1956) and for the SrAg model. As the latter gave a significantly better agreement, a single-crystal refinement was undertaken and this paper reports the results obtained.

Experimental. Metals supplied by Koch-Light: Th 99·8 and Ni 99·999 wt % pure; the sample prepared by melting under vacuum the two elements in an alumina crucible in an induction furnace, and then annealed in an evacuated silica tube at 1073 K for 20 d. The alloy (brittle, well crystallized, air-resistant) checked by micrographic examination proved to be a homogeneous phase. A plate-like single crystal with dimensions $0.08 \times 0.07 \times 0.03$ mm isolated and mounted on a Enraf–Nonius CAD-4 automatic diffractometer; lattice constants determined by least-squares refinement of the angular values of 25 diffractometer-measured reflections. Systematic extinctions confirmed the space group *Pnma* and reflections from three octants of reciprocal lattice were collected; graphite-monochromated Mo $K\alpha$ radiation, ω–θ scan mode up to $2\theta = 60°$. Intensities processed for Lp and absorption effects, spherical ($\mu r = 3.45$) and semi-empirical correction based on the ψ-scan data of two top reflections (North, Phillips & Mathews, 1968), maximum transmission-factor ratio 12·5; 555 unique reflections ($R_{\text{int}} = 0.084$), 306 with $F_o > 2\sigma(F_o)$ used in the structure refinement.

The parameters of SrAg (Merlo & Fornasini, 1981) were assumed as starting values for a full-matrix least-squares refinement (on *F*) in *Pnma* with *SHELX76* (Sheldrick, 1976), taking atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Isotropic cycles, $R = 0.071$; anisotropic refinement over 25 parameters with weights $w = 1/\sigma^2(F_o)$, $R = 0.049$, $wR = 0.039$, maximum shift to e.s.d. in the last cycle 0·3; maximum and minimum height in final difference Fourier map 7·4 and −4·2 e Å^{-3}, respectively. No correction for secondary extinction.

Discussion. The final atomic parameters are listed in Table 1.* Table 2 gives the interatomic distances in ThNi. The Th–Ni contacts seem to play an important

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38531 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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role in stabilizing this structure, showing a maximum contraction of 4% with respect to the sum of the metallic radii for coordination number (CN) 12 (Teatum, Gschneidner & Waber, 1960), whereas the distances Th–Th and Ni–Ni are always larger than the corresponding metallic diameter. The coordination is very similar to that of the isotypic SrAg phase. The Th atoms are surrounded by seven Ni and eight Th; the Ni atoms are at the centre of a Th trigonal prism with its lateral faces capped by a Th and two Ni atoms. This coordination is typical for all the compounds crystallizing in the stacking variants of the CrB–FeB types, as found for the dimorphic TbNi (Lemaire & Paccard, 1970), for several ternary rare-earth–transition-metal alloys (Klepp & Parthé, 1980, 1981, 1982) and for some alkaline-earth equiatomic compounds with Cu and Ag (Merlo & Fornasini, 1981). ThNi is the first representative phase formed by an actinide element.

As remarked by Klepp & Parthé (1980), a useful way to classify these stacking variants is the Jagodzinski notation, connected with the interpretation of structures based on trigonal prisms in terms of the periodic microtwinning concept. In this respect, Klepp & Parthé (1982) point out that in alloys $R_{1-x}R_x'$Ni and $RT_{1-x}T_x'$ (R = rare-earth elements; T = transition elements), the Jagodzinski formula contains either no *h* symbol or pairs of *h* symbols only. This rule is not followed by the stacking variants found with the alkaline earths, namely α- and β-CaCu and SrAg, with stacking code $(hch_2c)_2$, hc_2hc and $(hc)_2$, respectively, so that the hitherto identified phases seem to belong to two different families of structures. In order to study the limit for existence of these two families, the ternary Th–rare-earth–Ni alloys could provide an interesting combination, since ThNi is in an intermediate position: as in the rare-earth alloys mentioned above the more electronegative partner is again a transition metal, whilst its structure is the same as that of an alkaline-earth phase.

Table 1. *Atomic parameters for* ThNi *with e.s.d.'s in parentheses*

The thermal factors are defined as $T = \exp[-8\pi^2 10^{-2} U_{\rm eq}(\sin\theta/\lambda)^2]$ with $U_{\rm eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	*y*	*z*	$U_{\rm eq}$(Å^2)
Th(1)	0·2847 (2)	0·25	0·5366 (4)	1·4 (1)
Th(2)	0·0344 (2)	0·25	0·7479 (7)	1·2 (1)
Ni(1)	0·3543 (6)	0·25	0·031 (2)	2·2 (5)
Ni(2)	0·1050 (5)	0·25	0·256 (2)	1·7 (4)

Table 2. *Interatomic distances* (Å) *in* ThNi

E.s.d.'s are ≤ 0·01 Å.

Th(1)–2Ni(1)	2·91	Th(2)–2Ni(2)	2·91
–2Ni(2)	2·93	–2Ni(1)	2·93
–Ni(1)	2·99	–Ni(2)	2·98
–Ni(2)	3·00	–Ni(1)	3·00
–Ni(1)	3·05	–Ni(2)	3·06
–4Th(1)	3·70	–2Th(2)	3·68
–2Th(2)	3·72	–2Th(2)	3·72
–Th(2)	3·74	–2Th(1)	3·72
–Th(2)	3·74	–Th(1)	3·74
		–Th(1)	3·74
Ni(1)–2Ni(2)	2·72		
–2Th(1)	2·91	Ni(2)–2Ni(1)	2·72
–2Th(2)	2·93	–2Th(2)	2·91
–Th(1)	2·99	–2Th(1)	2·93
–Th(2)	3·00	–Th(2)	2·98
–Th(1)	3·05	–Th(1)	3·00
		–Th(2)	3·06

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Structure de l'Octachlorure de Tricadmium et de Calcium 8,5-Hydraté, $2[Ca(H_2O)_7].[Cd_6Cl_{16}(H_2O)_2]_\infty.H_2O$

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Abstract. $Cd_3CaCl_8.8{\cdot}5H_2O$, $M_r = 814{\cdot}02$, $P\bar{1}$, $a = 12{\cdot}257$ (2), $b = 12{\cdot}212$ (2), $c = 14{\cdot}790$ (1) Å, $\alpha = 83{\cdot}28$ (1), $\beta = 73{\cdot}75$ (1), $\gamma = 78{\cdot}12$ (1)°, $V = 2075{\cdot}67$ Å^3, $Z = 4$, D_m(flotation) $= 2{\cdot}59 \pm 1$, $D_x = 2{\cdot}606$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 4{\cdot}29$ mm^{-1}, $T = 293$ K, $F(000) = 1540$. The structure

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