octahedral and the other tetrahedral holes of the close-packed metal configuration.

The structure thus arrived at is

Space group $R\bar{3}m$

Hexagonal Description $(000)(\frac{1}{3}\frac{2}{3}\frac{1}{3})(\frac{2}{3}\frac{1}{3}\frac{2}{3})^+$		Rhombohedral Description	
3 Th (I)	(000)	1 Th (I)	(000)
6 Th (II)	$\pm(00z_1)$	2 Th (II)	$\pm(z_1z_1z_1)$
6 N (I)	$\pm(00z_2)$	2 N (I)	$\pm(z_2z_2z_2)$
6 N (II)	$\pm(00z_3)$	2 N (II)	$\pm(z_3z_3z_3)$

with $z_1 = 0{\cdot}222 \pm 0{\cdot}003$, $z_2 \simeq 0{\cdot}137$, $z_3 \simeq 0{\cdot}389$.

The interatomic distances for this assumed structure are

Th (I)–6 N (II) 2·70 Å
–6 Th (II) 3·77
–6 Th (I) 3·87

Th (II)–4 N (I) 2·34 Å
–3 N (II) 2·70
–3 Th (I) 3·77
–3 Th (II) 3·77
–6 Th (II) 3·87

The Th_3N_4 structure is closely related to that of Th_2N_2O previously reported (Zachariasen, 1949) as Th_2N_3. In the latter structure the metal atoms are in simple hexagonal close-packing so that the *c* axis is twice the separation of hexagonal layers, whereas the *c* axis is nine times the layer distance in the Th_3N_4 structure. As shown below, the hexagonal *a* axis and the layer separation are slightly smaller for the Th_3N_4 phase:

Th_2N_2O	Th_3N_4
$a_0 = 3{\cdot}8833$ Å	$a_0 = 3{\cdot}871$ Å
$c_0 = 6{\cdot}1870 \simeq 2 \times 3{\cdot}0935$ Å	$c_0 = 27{\cdot}385 \simeq 9 \times 3{\cdot}043$ Å

The atomic positions of the Th_2N_2O structure are

2 Th in $\pm(\frac{1}{3}\frac{2}{3}z_1)$ with $z_1 = 0{\cdot}250 \pm 0{\cdot}006$
2 N in $\pm(\frac{1}{3}\frac{2}{3}z_2)$ with $z_2 \simeq 0{\cdot}631$
1 O in (000).

The N atoms occupy tetrahedral and the O atoms octahedral holes of the close-packed metal structure. The interatomic distances are

Th–4 N 2·35 Å
–3 O 2·72
–6 Th 3·81
–6 Th 3·88

Thus, the configuration about the Th (II) atoms of the Th_3N_4 structure is almost identical with that of the Th_2N_2O phase. However, the Th (I) atoms form only six bonds to nitrogen atoms, all occupying octahedral holes.

References

MATIGNON, C. & DELÉPINE, M. (1907). *Ann. Chim. Phys.* **8**, 130.

NEUMANN, B., KROEGER, C. & HAEBLER, H. (1932). *Z. anorg. allgem. Chem.* **207**, 145.

ZACHARIASEN, W. H. (1949). *Acta Cryst.* **2**, 388.

Acta Cryst. (1966). **21**, 840

X-ray examination of some rare-earth-containing binary alloy systems.

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Despite the intensive efforts which have been expended on the study of rare earth intermetallic compounds in recent years, there remains a large number of binary alloy systems yet to be investigated. Upon reviewing compendia by Gschneidner (1961) and McMasters & Gschneidner (1964), certain patterns of omission were observed, these usually occurring where one or both of the component elements are difficult to handle with ordinary melting techniques. In particular, most investigators seem to have avoided lanthanides with: high vapor pressures, high oxygen affinity, high melting points, divalent character, and those which are relatively scarce. The general approach followed during the present study was that described in earlier work by Moriarty (1960). Structural data for compounds formed in similar systems with gadolinium and dysprosium, and holmium and erbium can be found in reports by Baenziger & Moriarty (1961) and Moriarty, Gordon & Humphreys (1965) respectively.

Alloys were prepared by blending stoichiometric proportions of the components and either arc-melting them on a water cooled copper hearth or encapsulating them in tantalum crucibles and heating these in a tube or induction furnace. All procedures employed a protective atmosphere of dry argon gas. Each specimen was repeatedly remelted to improve homogeneity. Final weights differed from initial weights by less than 1·0 %. Purities of the metals used were: rare earths, at least 99·8 %; all others greater than 98·5 %.

In all cases the phases herein reported were identified by indexing the X-ray diffraction powder patterns. Diffraction equipment included a basic Norelco X-ray unit, using either filtered copper $K\alpha$ (Cu $K\alpha_1 = 1{\cdot}54051$, Cu $K\alpha_2 = 1{\cdot}54433$ Å) or iron $K\alpha$ (Fe $K\alpha_1 = 1{\cdot}93597$, Fe $K\alpha_2 = 1{\cdot}93991$ Å) radiation, 114·6 mm Debye–Scherrer cameras, and either Ansco Superay C or Kodak Type KK film. Suitable photographs were made at 20 to 25°C of the alloy specimens in an annealed condition. Filings were annealed in Vycor capillaries previously 'gettered' with zirconium wire to minimize oxidation. Some alloys were 'bulk' annealed in small sealed Vycor tubes and then crushed.

Results of this study are given in Tables 1 through 4. The lattice constants were calculated under the direction of one of us (N.C.B.) with an IBM 7044 computer from back-reflection data, with the use of an analytical least-squares program written by Miss Carol Valley at State University of Iowa.

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Table 1. CsCl *structure type*(a)

	a (Å)		*a* (Å)
YCu	3·4757 (2)(b)	YbAu	3·5634 (7)
YCu(c)	3·477	YIn	3·806 (2)
YCu(d)	3·474	LaIn	3·985 (1)
EuCu	3·479 (3)	PrIn	3·955 (4)
YAg	3·6196 (7)	TmIn	3·739 (1)
YAg(c)	3·617	YbIn	3·8138 (5)
YAg(e)	3·619	TmTl	3·670 (2)
YbAg	3·6787 (4)	TmTl(f)	3·711 (3)

Efforts to prepare YCo resulted in no such compound being formed.

(*a*) *Strukturbericht*, **1**, 74 (1931).
(*b*) Calculated standard deviations are given in parentheses.
(*c*) Dwight (1959).
(*d*) Domagala, Rausch & Levinson (1961).
(*e*) Bruzzone & Ferro Ruggiero (1962–63).
(*f*) Iandelli & Palenzona (1965).

Table 2. $MgCu_2$ *structure type*(a)

	a (Å)
$TmPt_2$	7·556 (2)(b)
$YbPt_2$	7·381 (4)
$TbFe_2$	7·368 (3)
$TbFe_2$(c)	7·369

Efforts to prepare $YbFe_2$, $EuFe_2$, $YbMn_2$, $EuMn_2$, $SmMn_2$, $EuCo_2$, and $EuNi_2$ resulted in no such compounds being formed.

(*a*) *Strukturbericht*, **1**, 490 (1931).
(*b*) Calculated standard deviations are given in parentheses.
(*c*) Krip'yakevich, Teslyuk & Frankevich (1965).

Table 3. $MoSi_2$ *structure type*(a)

	a (Å)	*c* (Å)
$YbAu_2$	3·6274 (7)(b)	8·889 (6)
$YbAg_2$	3·624 (2)	8·88 (2)

(*a*) *Strukturbericht*, **1**, 741 (1931).
(*b*) Calculated standard deviations are given in parentheses.

Table 4. $AuCu_3$ *structure type*(a)

	a (Å)		*a* (Å)
$YbAl_3$	4·2036 (3)(b)	$PrPt_3$	4·0650 (4)
$YbAl_3$(c)	4·202	$NdPt_3$	4·0590 (8)
$TbIn_3$	4·5896 (3)	$SmPt_3$	4·0633 (7)
$TbIn_3$(d)	4·588	$TbPt_3$	4·0839 (6)
$TmIn_3$	4·561 (1)	$TmPt_3$	4·0423 (4)
$TmIn_3$(d)	4·554	$YbPt_3$	4·0455 (1)
$YbIn_3$	4·6164 (4)	La_3In	5·075 (1)
$YbIn_3$(d)	4·620	La_3In(e)	5·07
$EuTl_3$	4·718 (5)	Ce_3In	5·0006 (7)
$TbTl_3$	4·679 (1)	Ce_3In(f)	4·9610 (5)
$TmTl_3$	4·6554 (3)	Pr_3In	4·9636 (8)
$LaPt_3$	4·0745 (8)	Pr_3In(g)	4·93
$CePt_3$	4·162 (1)	Nd_3In	4·9296 (6)

(*a*) *Strukturbericht*, **1**, 486 (1931).
(*b*) Calculated standard deviations are given in parentheses.
(*c*) van Vucht & Buschow (1964).
(*d*) Kuz'ma & Markiv (1964).
(*e*) McMasters & Gschneidner (1964).
(*f*) Dariel (1966).
(*g*) Iandelli (1947).

References

Baenziger, N. C. & Moriarty, J. L. (1961). *Acta Cryst.* **14**, 948.

Bruzzone, G. & Ferro Ruggiero, A. (1962–63). *Atti accad. naz. Lincei, Rend. Classe sci. fis. mat. nat.* **33**, no. 5, 312.

Dariel, M. (1966). *Acta Cryst.* **20**, 586.

Domagala, R. F., Rausch, J. J. & Levinson, D. W. (1961). *Trans. ASM*, **53**, 137.

Dwight, A. E. (1959). *Trans. AIME*, **215**, 283.

Gschneidner, K. A., Jr. (1961). *Rare Earth Alloys.* New York: Van Nostrand.

Iandelli, A. & Palenzona, A. (1965). *J. Less-Common Metals*, **9**, 1.

Iandelli, A. (1947). *Atti accad. naz. Lincei, Rend. Classe sci. fis. mat. nat.* **2**, 327.

Krip'yakevich, P. I., Teslyuk, M. Yu. & Frankevich, D. P. (1965). *Kristallografiya*, **10**, no. 3, 422.

Kuz'ma, Yu. B. & Markiv, V. Ya. (1964). *Kristallografiya*, **9**, no. 2, 279.

McMasters, O. D. & Gschneidner, K. A., Jr. (1964). *Nuclear Metallurgy Series*, X, 93.

Moriarty, J. L. (1960). Ph.D. Thesis; *Diss. Abstr.* **21**, 1391.

Moriarty, J. L., Gordon, R. O. & Humphreys, J. E. (1965). *Acta Cryst.* **19**, 285.

Vucht, J. H. N. van & Buschow, K. H. J. (1964). *Phillips Res. Repts.* **19**, 319.

Acta Cryst. (1966). **21**, 841

Reinvestigation of the crystal structure of lithium iodate.

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Discussion of the structure

From their early X-ray study of lithium iodate Zachariasen & Barta (1931) concluded that the iodine atoms were regularly surrounded by six oxygen atoms. Irregular coordination polyhedra were observed, however, in iodates which were investigated more accurately later on ($NaIO_3$, MacGillavry & Panthaleon van Eck, 1943; $Ce(IO_3)_4$, Cromer & Larsson, 1956; $Ce(IO_3)_4.H_2O$, Ibers, 1956; Ibers & Cromer, 1958). During the present reinvestigation of the crystal structure of lithium iodate we found that the symmetry of the crystals is lower than was assumed by Zachariasen & Barta (Table 1). The hexagonal close packing *ABABAB* with the iodine atoms in the centres of regular octahedra