

Table 2. Structural data for ThX compounds having the CrB structure

ThX	'a' (Å)	'b' (Å)	'c' (Å)	y_{Th}	y_X	X-X		Th-X		Th-Th in ThX
						in ThX	for C.N.12	in ThX	for C.N.12	
ThCo	3.74	10.88	4.16	0.136	0.416	2.77	2.50	2.86	3.05	3.62
ThRu	3.878	11.29	4.071	0.144	0.410	2.86	2.67	2.87	3.13	3.75
ThRh	3.866	11.24	4.220	0.140	0.410	2.92	2.68	2.92	3.14	3.78
ThIr	3.894	11.13	4.266	0.140	0.410	2.93	2.70	2.94	3.15	3.79
ThPt	3.900	11.09	4.454	0.140	0.410	2.99	2.77	2.99	3.18	3.82
ThAl	4.42	11.45	4.19	0.147	0.443	2.46	2.85	3.22	3.22	3.85

structures of ThAl₃ and Th₃Al₂, the present author (Murray, 1955) found that since the scattering powers of thorium and aluminium differ by a factor of about 8, it was not possible to determine the aluminium atomic parameters in those compounds from intensity calculations. Accordingly, the aluminium parameters suggested for ThAl₃ and Th₃Al₂ were derived from geometrical considerations. In a recent paper, van Vucht (1961) has confirmed that his aluminium parameter for ThAl was also derived from geometrical considerations on the assumption that each large (Th) atom had 6 equidistant small (Al) neighbours. Since this condition is not satisfied in several other compounds with this structure (e.g. ThCo, PuNi, CeNi, DyGa and HfAl) it may not be necessary in ThAl. A small decrease in the Al parameter would lead to an increase in Al-Al and a rather smaller decrease in Th-Al.

In a recent survey of borides and silicides of the transition metals, Aronsson (1960) has pointed out that the occurrence of the CrB structure depends to a rather large extent on a favourable radius ratio $r_x/r_M \cong 0.7$. He also suggested that, since the same structure is found among intermetallic compounds, 'electronic' factors may not be of primary importance in its formation. In the present series of compounds, the radius ratio varies between 0.69 for ThCo to 0.79 for ThAl in general agreement with Aronsson's observations, but the decreased Th-X distances suggest that there may be appreciable Th-X interaction.

Frank & Kasper (1958, 1959) and Kripyakevich (1960) have noted that there is often a high coordination around the larger atoms in intermetallic compounds and they suggested that this might contribute to the stability of certain structures. In the present ThX series the coordination around the larger, thorium atom is $(4 + 2 + 1)X +$

$(4 + 2 + 2 + 2)Th = 17$ whilst that around the smaller, X, atom is $2X + (4 + 2 + 1)Th = 9$ in support of this suggestion.

Grateful acknowledgement is made to Prof. J.G. Ball under whose supervision this work was carried out and also to the Atomic Energy Research Establishment, Harwell, for financial support and for allowing the author to make use of some of their experimental facilities.

References

- ARONSSON, B. (1960). *Ark. Kemi*, **16**, 379.
 BAENZIGER, N. C. & MORTARTY, J. L. (1961). *Acta Cryst.* **14**, 946.
 BRAUN, P. B. & VUCHT, J. H. N. VAN (1955). *Acta Cryst.* **8**, 246.
 CROMER, D. T. & ROOF, R. B. (1959). *Acta Cryst.* **12**, 942.
 EDHAMMAR, L.-E. (1961). *Acta Chem. Scand.* **15**, 403.
 FERRO, R. & RAMBALDI, G. (1961). *Acta Cryst.* **14**, 1094.
 FINNEY, J. J. & ROSENZWEIG, A. (1961). *Acta Cryst.* **14**, 69.
 FLORIO, J. V., BAENZIGER, N. C. & RUNDLE, R. E. (1956). *Acta Cryst.* **9**, 367.
 FRANK, F. C. & KASPER, J. S. (1958). *Acta Cryst.* **11**, 184.
 FRANK, F. C. & KASPER, J. S. (1959). *Acta Cryst.* **12**, 483.
 KRIPYAKEVICH, P. I. (1960). *Soviet Phys. Cryst.* **5**, 69.
 KRIPYAKEVICH, P. I. (1962). *Soviet Phys. Cryst.* **6**, 501.
 MURRAY, J. R. (1955-56). *J. Inst. Metals*, **84**, 91.
 PAULING, L. (1956). *Theory of Alloy Phases*, Amer. Soc. Met., p. 232.
 PEARSON, W. B. (1958). *Handbook of Lattice Spacings and Structures of Metals*. London: Pergamon Press.
 THOMSON, J. R. (1961). *Nature, Lond.* **189**, 217.
 THOMSON, J. R. (1962). *Nature, Lond.* **194**, 465.
 VUCHT, J. H. N. VAN (1961). *Philips Res. Rep.* **14**, 1.

Acta Cryst. (1962). **15**, 1309

The crystal structure of Ti₂Ni. (A correction). By G. A. YURKO, J. W. BARTON and J. GORDON PARR, Department of Mining and Metallurgy, University of Alberta, Edmonton, Alberta, Canada

Dr. Linus Pauling has written to us to point out an anomaly in Table 2 of the paper by G. A. Yurko, J. W. Barton, and J. Gordon Parr (1959).

Only two titanium positions are required (as the paper itself stated), and the table should be amended to include:

Atom	Bond	Num. of bonds	Distance
Ti(48f)	Ti-Ni	2	2.57 ± 0.05 Å
	Ti-Ni	2	2.91 ± 0.05
	Ti-Ti	2	2.93 ± 0.02
	Ti-Ti	4	2.95 ± 0.05
	Ti-Ti	4	2.91 ± 0.05
		<u>4</u>	

14

Atom	Bond	Num. of bonds	Distance
Ti(16c)	Ti-Ni	6	2.49 ± 0.02 Å
	Ti-Ti	6	2.93 ± 0.00
		<u>12</u>	

Some changes relating to coordination numbers mentioned in the discussion must therefore be made, but the rest of the paper is unaffected. We do, however, apologize for our error, and are grateful to Dr. Pauling for drawing our attention to it.

J. Gordon Parr

Reference

- YURKO, G. A., BARTON, J. W. & PARR, J. GORDON (1959). *Acta Cryst.* **12**, 909.