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## Structures of the Rare-Earth–Platinum Compounds $R_7Pt_3$ , $R_2Pt$ , $R_5Pt_3$ and $RPt$

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Structures of rare-earth–platinum compounds are identified.  $R_7Pt_3$  compounds ( $R = La, Ce, Pr, Nd, Sm, Gd$ ) crystallize with the  $Th_7Fe_3$  structure type.  $PrPt$  and  $NdPt$  have a high-temperature modification which corresponds to the  $CrB$  type.  $R_2Pt$  and  $R_5Pt_3$  compounds crystallize with the  $Ni_2Si$  and  $Mn_5Si_3$  types, where  $R = Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Y$  for both structure types. Atomic parameters were refined from single-crystal intensities collected on  $Gd_2Pt$ . The coordination polyhedra of  $Ni_2Si$  are compared with those of the  $Fe_2P$  type. It is shown that a greatly idealized version of the  $Ni_2Si$  type can be derived by periodic unit-cell twinning of the cubic-close-packed element structure. A survey of the known  $R_xPt$  compounds ( $x \geq 1$ ) is given. These compounds are compared with those occurring in the corresponding  $Ni$  and  $Pd$  systems.

### Introduction

A survey of the crystal structures of rare-earth–transition-metal compounds  $R_xT$  with  $x \geq 1$  ( $T = Co, Rh, Ni, Pd$ ) has been made (Parthé & Moreau, 1977). These structures may be grouped into those where all  $T$  atoms are at the centres of trigonal prisms of  $R$  atoms and those where the  $T$  atoms are at the centres of either trigonal prisms, cubes, square antiprisms and/or truncated square antiprisms. To see if this classification is still valid for  $T = Pt$ , systematic studies of the  $R$ – $Pt$  systems have been made. We report in this paper the structure types and lattice parameters of some of the phases which have been identified. No phase diagram of any  $R$ – $Pt$  system was found in the literature except for  $Yb$  (Iandelli & Palenzona, 1975).

### Experimental

The alloys were made from commercially available elements of high purity: rare earth 99.9%,  $Pt$  99.99%. Samples were prepared by conventional arc-melting techniques. X-ray photographs from powdered samples were obtained on a Guinier camera with  $Cu K\alpha$  radiation and were calibrated with  $Si$  powder. Small single crystals of  $Gd_2Pt$  suitable for X-ray analysis were isolated by mechanical fragmentation and intensities were measured with graphite-monochromated  $Mo K\alpha$  radiation on a computer-controlled four-circle

goniometer in the  $\theta$ – $2\theta$  scan mode. All computer programs used were those of the XRAY system (1976), except for the program calculating intensities for X-ray powder-diagram identification (Yvon, Jeitschko & Parthé, 1977).

### Structure determination

In the rare-earth-rich part of the  $R$ – $Pt$  systems new compounds have been identified with the following structure types:  $Th_7Fe_3$ ,  $Ni_2Si$ ,  $Mn_5Si_3$  and  $CrB$ .

$Sm_7Pt_3$  and  $Gd_7Pt_3$  crystallize with the hexagonal  $Th_7Fe_3$  structure type. This type has already been found with  $La_7Pt_3$ ,  $Ce_7Pt_3$ ,  $Pr_7Pt_3$  and  $Nd_7Pt_3$  (Olcese, 1973). The atomic parameters for  $Gd_7Pt_3$  (Moreau & Parthé, 1973) were used in the calculation of the powder diffraction intensities [ $P6_3mc$ ; two  $Gd(1)$  in  $2(b)$ :  $z = 0.06$ ; six  $Gd(2)$  in  $6(c)$ :  $x = 0.125$ ,  $z = 0.25$ ; six  $Gd(3)$  in  $6(c)$ :  $x = 0.5395$ ,  $z = 0.0499$ ; and six  $Pd$  in  $6(c)$ :  $x = 0.8102$ ,  $z = 0.3125$ ]. No efforts were made to refine the atomic parameters of  $Sm_7Pt_3$  and  $Gd_7Pt_3$ . Lattice parameters of all  $R_7Pt_3$  compounds are reported in Table 1.

The orthorhombic  $Ni_2Si$  (or anti- $PbCl_2$ ,  $C23$ ) type was found to occur with all elements from  $Gd$  to  $Lu$  and  $Y$ . A single crystal of  $Gd_2Pt$  has been isolated and X-ray intensities were collected. Space group  $Pnma$  with point positions similar to  $Ni_2Si$  were assumed (Toman, 1952). Positional and isotropic thermal

Table 1. Lattice parameters of  $R_7Pt_3$  compounds with the  $Th_7Fe_3$  structure type (space group  $P6_3/mc$ )

E.s.d.'s are in parentheses;  $V$  = volume of the unit cell;  $n$  = number of atoms in the unit cell.

	$a$ (Å)	$c$ (Å)	$(V/n)^{1/3}$ (Å)	References
$La_7Pt_3$	10.336	6.516	3.11	(a)
$Ce_7Pt_3$	10.204	6.399	3.07	(a)
$Pr_7Pt_3$	10.137	6.376	3.05	(a)
$Nd_7Pt_3$	10.099	6.351	3.04	(a)
$Sm_7Pt_3$	10.017 (3)	6.298 (3)	3.01	(b)
$Gd_7Pt_3$	9.977 (5)	6.275 (5)	3.00	(b)
$Y_7Pt_3$	9.864	6.299	2.98	(c)

References: (a) Olcese (1973). (b) This work. (c) Geballe, Matthias, Compton, Corenzwit, Hull & Longinotti (1965).

Table 2. Atomic parameters for  $Gd_2Pt$  crystallizing in the  $Ni_2Si$  structure type, with e.s.d.'s in parentheses

The Debye-Waller factor is defined as  $\exp[-2\pi^2 10^{-2} U(2 \sin \theta/\lambda)^2]$ .  
The space group is  $Pnma$ .

	Equipoint	$x$	$y$	$z$	$U$ (Å <sup>2</sup> )
Gd(1)	4(c)	0.8538 (7)	$\frac{1}{4}$	0.0810 (6)	0.7
Gd(2)	4(c)	0.9883 (7)	$\frac{3}{4}$	0.6705 (6)	0.7
Pt	4(c)	0.2576 (6)	$\frac{1}{4}$	0.0953 (5)	0.8

Table 3. Lattice parameters of  $R_2Pt$  compounds with the  $Ni_2Si$  structure type (space group  $Pnma$ )

E.s.d.'s are in parentheses;  $V$  = volume of the unit cell;  $n$  = number of atoms in the unit cell.

	$a$ (Å)	$b$ (Å)	$c$ (Å)	$(V/n)^{1/3}$	References
$Gd_2Pt$	7.186 (5)	4.813 (3)	8.854 (8)	2.95	(a)
$Tb_2Pt$	7.147 (5)	4.772 (3)	8.763 (9)	2.92	(a)
$Dy_2Pt$	7.101 (7)	4.747 (4)	8.731 (8)	2.91	(a)
$Ho_2Pt$	7.054 (7)	4.722 (4)	8.686 (8)	2.89	(a)
$Er_2Pt$	7.037 (4)	4.705 (3)	8.668 (7)	2.88	(a)
$Tm_2Pt$	7.008 (5)	4.688 (5)	8.619 (9)	2.87	(a)
$Yb_2Pt$	7.614	4.400	8.957	2.92	(b)
$Lu_2Pt$	6.978 (4)	4.630 (9)	8.584 (9)	2.85	(a)
$Y_2Pt$	7.141 (4)	4.764 (3)	8.753 (6)	2.92	(a)

References: (a) This work. (b) Iandelli & Palenzona (1975).

parameters of the structure refined satisfactorily. Relativistic Hartree-Fock scattering factors were used (Cromer & Mann, 1968) and anomalous-dispersion corrections were made with values taken from *International Tables for X-ray Crystallography* (1974).  $R = \sum | \Delta F | / \sum | F_o |$  was 0.10 for 468 observed reflexions.\* The final positional and thermal parameters

\* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32858 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 4. Lattice parameters of  $R_5Pt_3$  compounds with the  $Mn_5Si_3$  structure type (space group  $P6_3/mcm$ )

E.s.d.'s are in parentheses.  $V$  = volume of the unit cell;  $n$  = number of atoms in the unit cell.

	$a$ (Å)	$c$ (Å)	$c/a$	$(V/n)^{1/3}$	References
$Gd_5Pt_3$	8.479 (4)	6.275 (7)	0.740	2.90	(a)
$Tb_5Pt_3$	8.415 (5)	6.230 (8)	0.740	2.88	(a)
$Dy_5Pt_3$	8.367 (4)	6.210 (7)	0.742	2.87	(a)
$Ho_5Pt_3$	8.319 (5)	6.191 (8)	0.744	2.85	(a)
$Er_5Pt_3$	8.298 (2)	6.181 (4)	0.745	2.85	(a)
$Tm_5Pt_3$	8.252 (3)	6.128 (5)	0.743	2.83	(a)
$Yb_5Pt_3$	8.337	6.251	0.750	2.87	(b)
$Lu_5Pt_3$	8.183 (1)	6.155 (9)	0.752	2.82	(a)
$Y_5Pt_3$	8.370 (3)	6.276 (5)	0.749	2.88	(a)

References: (a) This work. (b) Iandelli & Palenzona (1975).

are listed in Table 2. Lattice parameters of  $R_2Pt$  compounds are reported in Table 3. The decrease of the lattice constants from  $Gd_2Pt$  to  $Lu_2Pt$  is a consequence of the lanthanide contraction. The deviations for  $Yb_2Pt$  ( $a$  and  $c$  larger,  $b$  smaller than expected) are probably correlated with the divalent character of Yb in this compound. A similar deviation has been observed for  $Yb_2Au$  in comparison with the other  $R_2Au$  compounds which all have the  $Ni_2Si$  crystal structure (McMasters, Gschneidner, Bruzzone & Palenzona, 1971).

The hexagonal  $Mn_5Si_3$  ( $D_8^8$ ) type with point positions similar to  $Gd_5Bi_3$  [Hohnke & Parthé, 1969;  $P6_3/mcm$ ; six Gd(1) in 6(g):  $x = 0.25$ ; four Gd(2) in 4(d) and six Bi in 6(g):  $x = 0.61$ ] has been found to occur with all rare-earth elements from Gd to Lu and Y. The atomic parameters were not refined, but the refined lattice parameters are reported in Table 4.

PrPt and NdPt are known to crystallize with the FeB structure type (Dwight, Conner & Downey, 1965). However, it was found that samples quenched from high temperatures have the CrB structure type. For the intensity comparison we used the atomic parameters of GdNi determined by Dwight, Conner & Downey (1965) [ $Cmcm$ ; four Gd in 4(c):  $x = 0.135$ ; and four Ni in 4(c):  $x = 0.435$ ]. The refined unit-cell parameters of these high-temperature modifications are: PrPt:  $a = 3.891$  (2),  $b = 10.899$  (7),  $c = 4.569$  (3) Å; NdPt:  $a = 3.846$  (3),  $b = 10.769$  (9),  $c = 4.542$  (4) Å.

## Discussion

The  $Th_7Fe_3$  structure type has already been observed with  $R_7Rh_3$ ,  $R_7Ir_3$ ,  $R_7Ni_3$  and  $R_7Pd_3$  (Olcese, 1973; Moreau & Parthé, 1973). The  $Mn_5Si_3$  type has also been found with  $R_5Rh_3$  (Raman & Ghassem, 1973; Le Roy, Moreau, Paccard & Parthé, 1977a). These compounds together with  $R_5Pt_3$  are examples of the second branch of the  $Mn_5Si_3$  type where the second

alloying partner is also a transition element. The first compounds of this branch to be discovered were  $Zr_3Ir_3$ ,  $Hf_3Ir_3$  and  $Zr_3Pt_3$  (Biswas & Schubert, 1967). The axial ratios  $c/a$  for  $R_5Pt_3$  and  $R_5Si_3$  are about the same ( $\sim 0.74$ ). This is also true for  $Zr_5Ir_3$  and  $Zr_5Si_3$  ( $\sim 0.69$ ). Thus with this structure type one does not find the characteristic relative unit-cell changes known, for example, with the CrB, FeB or  $U_3Si_2$  types which occur when the alloying partner is a transition element in one case or a  $b$  element (those with filled  $d$  shells) in the other. It seems that the value of the  $c/a$  ratio of the  $Mn_5Si_3$  phases becomes larger if there are fewer valence electrons available. The highest value known occurs with  $Ba_5As_3$ , where  $c/a = 0.832$  (Better, Hütz & Nagorsen, 1976). However, the size of the atoms is also an influence on the  $c/a$  ratio.

The common presence of the two geometrically related structure types has been observed in the equiatomic  $RNi$  and  $RAu$  compounds. Based on the structure block stacking model it was possible to derive equations which allow a calculation of the unit-cell parameters of one type to be made if the data are known for the other (Hohnke & Parthé, 1966). To calculate the CrB unit cell from the FeB cell one finds that

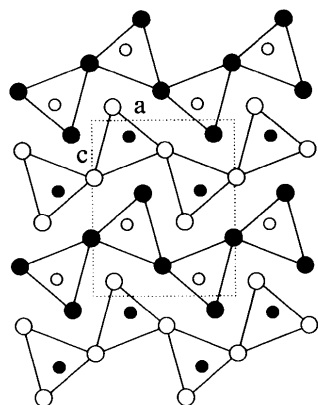
$$a_{CrB} = c_{FeB} \sqrt{\left\{ 2 - \sqrt{\left[ 4 - \left( \frac{a_{FeB}}{c_{FeB}} \right)^2 \right]} \right\}} \quad (1)$$

$$b_{CrB} = c_{FeB} \sqrt{\left\{ 2 + \sqrt{\left[ 4 - \left( \frac{a_{FeB}}{c_{FeB}} \right)^2 \right]} \right\}} \quad (2)$$

$$c_{CrB} = b_{FeB} \quad (3)$$

The theoretical CrB cell data for PrPt and NdPt based on the FeB data published by Dwight, Conner & Downey (1965) are: PrPt:  $a = 3.88$ ,  $b = 10.72$ ,  $c = 4.56$  Å; and NdPt:  $a = 3.86$ ,  $b = 10.67$ ,  $c = 4.55$  Å, which may be compared with the experimental values listed in the previous section.

Compounds with the composition  $R_2T$ , except  $Yb_2Pt$  (Iandelli & Palenzona, 1975), have not yet been found. For compounds of this composition which are built up exclusively of trigonal prisms, the trigonal-prism linkage coefficient has to be three (Parthé & Moreau, 1977). Different geometrical realizations are possible. Three are shown in Fig. 1: the orthorhombic  $Ni_2Si$  (or anti-PbCl<sub>2</sub>) type, the hexagonal  $Fe_2P$  type and the monoclinic  $Ge_2Os$  type. In Fig. 1 the tables used to calculate the trigonal-prism linkage coefficients are shown. All these structures have infinite columns of trigonal prisms, stacked on their triangular faces. The  $Ge_2Os$  structure is unique because there are double columns, formed by joining two columns along a common face. The  $Ni_2Si$  structure has prism columns which are joined along two edges to other prism columns, while in  $Fe_2P$  one finds isolated prism columns and a column assembly where each prism column is joined along three edges to other prism columns. The  $Ni_2Si$  and  $Fe_2P$  structures are closely related. One finds that exactly the same coordination figures (Fig. 2) occur in both. The  $Ni_2Si$  and  $Fe_2P$  structures have therefore to be considered as homotectic. However, it does not seem possible here to transform one into the other by a layer-stacking mechanism. This close geometrical relationship is perhaps also the reason why



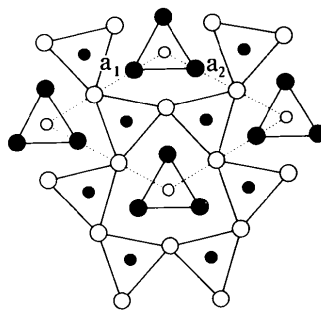
$Ni_2Si$   
 $Pnma$

All atoms in equipoint 4(c)

	Ni(1)	Ni(2)	Number
Si	2	4	=6
$p$	2	4	

$$LC = 4 \times (2 + 4)/8 = 3$$

$$R_6T_{LC} = R_6T_3 \equiv R_2T$$

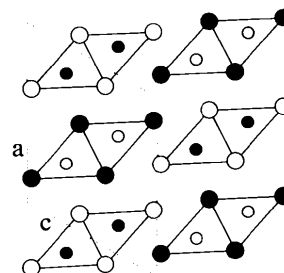


$Fe_2P$   
 $P6_2m$

	Fe(1) in 3(f)	Fe(2) in 3(g)	Number
P(1) in 2(c)	0	6	=6
P(2) in 1(b)	6	0	=6
$p$	$\frac{1}{3} \times 6 = 2$	$\frac{2}{3} \times 6 = 4$	

$$LC = 3 \times (2 + 4)/6 = 3$$

$$R_6T_{LC} = R_6T_3 \equiv R_2T$$



$Ge_2Os$   
 $C2/m$

All atoms in equipoint 4(f)

	Ge(1)	Ge(2)	Number
Os	4	2	=6
$p$	4	2	

$$LC = 4 \times (4 + 2)/8 = 3$$

$$R_6T_{LC} = R_6T_3 \equiv R_2T$$

Fig. 1. Three possible structure types for  $R_2T$  compounds which consist exclusively of  $T$  centred trigonal prisms of  $R$  atoms. Filled circles correspond to atoms at a height of 0 or  $\frac{1}{2}$  and empty circles to those at a height of  $\frac{1}{3}$  or  $\frac{2}{3}$ .

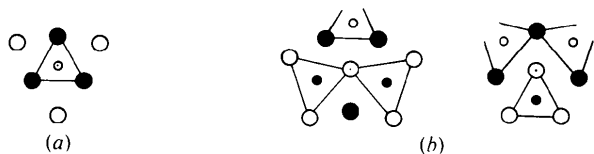


Fig. 2. The three coordination figures which occur in  $\text{Ni}_2\text{Si}$  and  $\text{Fe}_2\text{P}$  as seen along the orthorhombic  $b$  or hexagonal  $c$  axes respectively. Large circles correspond to Ni or Fe atoms and small circles to Si or P atoms. The full circles are displaced by  $(0, \frac{1}{2}, 0)$  or  $(0, 0, \frac{1}{2})$  respectively from the plane of the open circles. (a) The Si(P) atom environment in  $\text{Ni}_2\text{Si}(\text{Fe}_2\text{P})$ . (b) The two kinds of Ni(Fe) atom environment in  $\text{Ni}_2\text{Si}(\text{Fe}_2\text{P})$ .

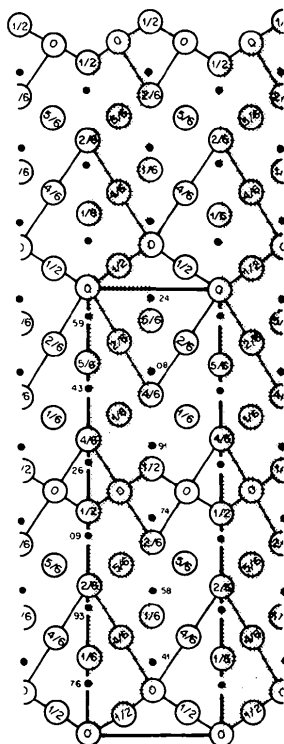


Fig. 3. A hypothetical  $R_2T$  structure derived by periodic unit-cell twinning of a cubic-close-packed element structure and occupation of the trigonal-prismatic holes by the  $T$  atoms. The untwinned segments have been alternately stippled or left clear.

Table 5. Theoretical structure data for a  $R_2T$  structure similar to  $\text{Ni}_2\text{Si}$  derived by periodic unit-cell twinning of the cubic-close-packed element structure

Space group  $Pnma$

Unit-cell dimensions

$$a_{\text{Ni}_2\text{Si}} = 4(\sqrt{2}/\sqrt{1})a_H = 1.705 a_H$$

$$b_{\text{Ni}_2\text{Si}} = a_H$$

$$c_{\text{Ni}_2\text{Si}} = \sqrt{11}a_H = 3.316 a_H$$

Idealized point positions

	$x$	$z$
4 Ni(1) in 4(c)	$\frac{3}{4}$	$\frac{1}{4} = 0.022$
4 Ni(2) in 4(c)	0	
4 Si in 4(c)	$\frac{1}{4}$	0.154

both structure types have been found with transition-metal silicides:  $\text{Co}_2\text{Si}$ ,  $\text{Ni}_2\text{Si}$ ,  $\text{Ru}_2\text{Si}$ ,  $\text{Rh}_2\text{Si}$  and  $\text{Ir}_2\text{Si}$  adopt the  $\text{Ni}_2\text{Si}$  type, while  $\text{Pd}_2\text{Si}$  and  $\text{Pt}_2\text{Si}$  adopt the  $\text{Fe}_2\text{P}$  type.

Recently, it has been shown how structures with trigonal prisms can be derived by periodic unit-cell twinning of close-packed structures (Andersson & Hyde, 1974; Parthé, 1976). Following the procedure and notation used by Parthé (1976), the twinning along every second possible twin plane and occupation of trigonal-prismatic holes by  $T$  atoms must lead to a

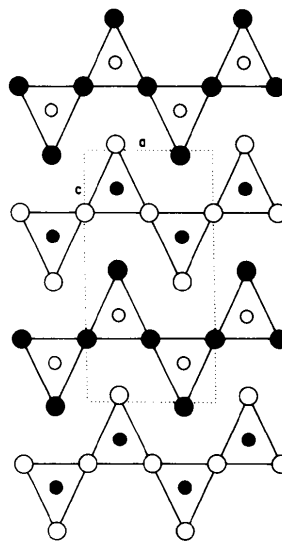


Fig. 4. Hypothetical, greatly idealized  $\text{Ni}_2\text{Si}$  structure identical to that shown in Fig. 3, but now described with the proper unit cell and shown in a projection along the axes of the trigonal-prism columns.

Table 6. Survey of compounds in  $R$ -Pt up to 50 at.% Pt

	Structure types						
	$\text{Mn}_3\text{C}_2$	$\text{Th}_7\text{Fe}_3$	$\text{Ni}_2\text{Si}$	$\text{Mn}_2\text{Si}_3$	$\text{Er}_3\text{Ni}_2$	$\text{Sm}_5\text{Ge}_4$	CrB FeB
La		(a)			(b)		(c)
Cc		(a)			(b)		(c)
Pr		(a)			(b)		$h(f)$ (c)
Nd		(a)			(b)		$h(f)$ (c)
Sm		(f)					(c)
Eu							
Gd		(f)	(f)	(f)			(c)
Tb			(f)	(f)			(c)
Dy			(f)	(f)			(c)
Ho			(f)	(f)			(c)
Er			(f)	(f)			(c)
Tm			(f)	(f)			(c)
Yb	(d)		(d)	(d)		(d)	(d)
Lu			(f)	(f)			(c)
Y		(e)	(f)	(f)		(g)	(c)

References: (a) Olcese (1973). (b) Le Roy, Moreau, Paccard & Parthé (1977b). (c) Dwight, Conner & Downey (1965). (d) Iandelli & Palenzona (1975). (e) Geballe, Matthias, Compton, Corenzwit, Hull & Longinotti (1965). (f) This work. (g) Le Roy, Moreau, Paccard & Parthé (1977a).

structure of composition  $R_2T$ . The result for a cubic-close-packed base structure is shown in Fig. 3. After a unit-cell transformation, similar to that used in the derivation of the CrB structure, the hypothetical structure shown in Fig. 4 can be recognized as a greatly idealized  $Ni_2Si$  structure. The corresponding theoretical structural data are given in Table 5. A comparison between real and idealized structures shows that the  $T$  atom coordinations (six  $R$  atoms in the surrounding trigonal prism and three extra  $R$  atoms in the plane of projection) are identical, but that the  $R$  atom environments are different. It seems to be characteristic of the real  $Ni_2Si$  structure type (and also of the  $Fe_2P$  structure type) that the  $R$  atoms tend to adopt the atomic arrangement found in the W structure. This is supported by the observation that in other structure types found with other rare-earth-transition-metal compounds, e.g. the  $U_3Si_2$  and  $Er_3Ni_2$  types, one can observe  $R_6T$  trigonal prisms together with complete  $R_8R$  tungsten-like cubes.

A survey of all known  $R$ -Pt compounds up to 50 at.% Pt is given in Table 6. The structures of the  $R$ -Pt compounds may be compared with those of the  $R$ -Ni and  $R$ -Pd compounds for which surveys have already been published (Parthé & Moreau, 1977). Nearly all structure types occurring in  $R$ -Ni are built up of trigonal prisms, the exceptions being in the  $R$ -Pd system where both the  $Ho_5Pd_2$  and CsCl types are found, and in the  $R$ -Pt system where the  $Mn_5Si_3$  type is also found. Only the heavy, small rare-earth elements participate in the formation of these abnormal structure types. In the group of structure types which are built up of trigonal prisms there are a few that are found in compounds with Ni, Pd or Pt (e.g.  $Th_7Fe_3$ ,  $Er_3Ni_2$  or CrB), while others occur only with one particular alloying partner (e.g.  $Fe_3C$ ,  $Dy_3Ni_2$ ,  $Y_3Ni_2$  only with  $R$ -Ni compounds,  $U_2Si_2$  only with  $R_3Pd_2$  compounds and  $Ni_2Si$  exclusively with  $R_2Pt$  compounds). At the present time we do not know the reasons for these occurrences.

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