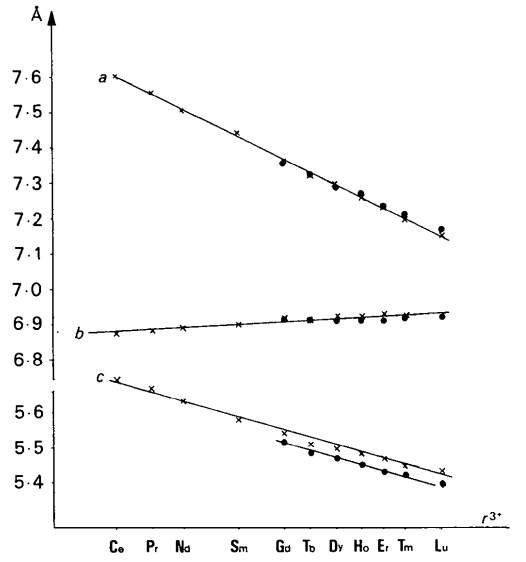

Fig. 2. Unit-cell parameters a, b, c, for orthorhombic RPd_2Si(×) and RPt_2Si(●) compounds *versus* ionic radius r^{3+} for rare-earth elements.

almost independent and it can be concluded that the bigger the rare earth, the shorter is the Pd–Pd distance along the b axis.

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Orthorhombic Palladium Yttrium Silicide $Y_3Pd_2Si_3$ and Rhodium Yttrium Silicide $Y_3Rh_2Si_3$ with $Hf_3Ni_2Si_3$ Structure Type

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Abstract. $Y_3Pd_2Si_3$ is orthorhombic, space group *Cmcm* with $a = 4{\cdot}251$ (3), $b = 10{\cdot}406$ (8), $c = 14{\cdot}123$ (7) Å, $\mu R = 1{\cdot}4$, $Z = 4$. The structure was determined by direct methods; final $R = 0{\cdot}08$ for 182 independent intensities. $Y_3Rh_2Si_3$ is isotypic; $a = 4{\cdot}174$ (2), $b = 10{\cdot}598$ (4), $c = 13{\cdot}726$ (5) Å. Both structures are isotypic with $Hf_3Ni_2Si_3$.

Introduction. In the ternary system Y–Pd–Si we investigated first the system YPdSi–YSi to see whether it would be possible to find structures based on trigonal prisms of Y and Pd atoms surrounding Si atoms. A phase corresponding to 2(YPdSi) + YSi, or $Y_3Pd_2Si_3$, was found and the structure was solved.

The alloys were made from commercially available elements of high purity (Y 99·9, Pd 99·99, Rh 99·99, Si 99·999%). Samples were prepared by conventional arc-melting techniques. Small crystals of $Y_3Pd_2Si_3$ and $Y_3Rh_2Si_3$ suitable for X-ray analysis were isolated by mechanical fragmentation from the crushed melt. Weissenberg photographs showed the crystals to have space group *Cmcm*.

$Y_3Pd_2Si_3$ single-crystal intensities were measured with Zr-filtered Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å) radiation on a computer-controlled three-circle goniometer in the θ–2θ scan mode. Intensities of 231 independent reflections, to a limit of $\sin\theta/\lambda = 0{\cdot}30$ Å^{-1}, were measured and corrected for background, Lorentz and polarization factors and 182 reflections with $I > 3\sigma(I)$ were considered as observed. X-ray photographs from powdered samples were obtained on a Guinier camera with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) and were calibrated with Si powder. Lattice parameters (see *Abstract*) were refined by least squares to fit values for 23 independent reflections observed on films from powdered samples.

All the computer programs used were from the XRAY system (Stewart, Kruger, Ammon, Dickinson

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Table 1. *Atomic positions for* $Y_3Pd_2Si_3$, *space group Cmcm*

E.s.d.'s are given in parentheses. The isotropic temperature factors for $Y_3Pd_2Si_3$ are expressed as $\exp[-2\pi^2 \times 10^{-2}U(2\sin\theta/\lambda)^2]$.

	x	y	z	U (Å^2)
Pd	0	0·7024 (7)	0·094 (3)	0·6 (1)
Y(1)	0	0·4091 (5)	0·1117 (4)	1·1 (1)
Y(2)	0	0·1337 (7)	$\frac{1}{4}$	0·9 (2)
Si(1)	0	0·105 (1)	0·037 (1)	0·5 (3)
Si(2)	0	0·834 (3)	$\frac{1}{4}$	0·6 (4)

Table 2. *Interatomic distances in* $Y_3Pd_2Si_3$ *up to* 3·45 Å

E.s.d.'s are in parentheses.

Pd	−2Si(1)	2·487 (8)	Y(2)	−2Si(2)	2·98 (2)
	− Si(2)	2·60 (1)		−2Si(1)	3·02 (1)
	− Si(1)	2·73 (2)		− Si(2)	3·12 (2)
	−2Y(1)	3·034 (5)		−4Pd	3·146 (4)
	− Y(1)	3·063 (7)			
	− Y(1)	3·126 (8)	Si(1)	− Si(1)	2·42 (2)
	− Y(2)	3·146 (4)		−2Pd	2·487 (8)
				− Pd	2·73 (2)
Y(1)	−2Si(2)	2·989 (7)		−2Y(1)	2·99 (1)
	−2Si(1)	2·99 (1)		− Y(2)	3·02 (1)
	−2Pd	3·034 (5)		−2Y(1)	3·13 (1)
	− Pd	3·063 (7)		− Y(1)	3·33 (2)
	− Pd	3·126 (8)			
	− Si(1)	3·13 (1)	Si(2)	−2Pd	2·60 (1)
	− Si(1)	3·33 (2)		−2Y(2)	2·98 (2)
				−4Y(1)	2·989 (7)
				− Y(2)	3·12 (2)

& Hall, 1972). The crystal structure of $Y_3Pd_2Si_3$ was solved by direct methods with the programs *SINGEN* and *PHASE*, which generated the phases with $|E(hkl)| > 1·3$. The positions of the Y and Pd atoms were revealed in the corresponding E map, while the Si positions were obtained by difference Fourier syntheses. Full-matrix least-squares refinement converged after a few cycles to a conventional $R(\equiv\sum|\Delta F|/\sum|F_o|)$ of 0·08.* Scattering factors were taken from *International Tables for X-ray Crystallography* (1974).

The final positional parameters are listed in Table 1, interatomic distances in Table 2. Weissenberg photographs of $Y_3Rh_2Si_3$ single crystals being identical to those of $Y_3Pd_2Si_3$, both structures can be considered as isotypic.

Discussion. A projection of the crystal structure of $Y_3Pd_2Si_3$ along its short axis is shown in Fig. 1. The structure is easily described by Si-centred trigonal prisms of Y and Pd atoms. First-neighbour atoms of Si are at the six vertices of trigonal prisms with three additional atoms outside the rectangular faces of the prisms. Two types of centred trigonal prisms can be distinguished. Those centred by Si(1) form pairs having in common one rectangular face of four Y atoms, the other edge being formed by two Pd atoms. Those prisms centred by Si(2) have Y atoms only at the corners of the prisms. The ratio of the prism height to the prism width (distances averaged) is 1·29 for Si(1) and 1·17 for Si(2) prisms respectively, which is usual for Si-centred prisms. This model should be compared to members of the $R_{n+2}T_n$ structure series having bands of trigonal prisms (Parthé & Moreau, 1977). The Re_3B type ($n = 1$) is made of isolated infinite columns of trigonal prisms and the Ge_2Os type ($n = 2$) is made of isolated infinite columns of double prisms. The $Y_3Pd_2Si_3$ model can be obtained by alternately connecting bands of trigonal prisms from the Re_3B and Ge_2Os models, the connection being made through common prism edges. Other compounds reported in the literature are $Hf_3M_2Si_3$ with M = Ni, Fe, Co and $Zr_3M_2Si_3$ with M = Co, Fe, by Yarmolyuk, Grin' & Gladyshevskii (1977) and $Sc_3Co_2Si_3$ by Gladyshevskii & Kotur (1978).

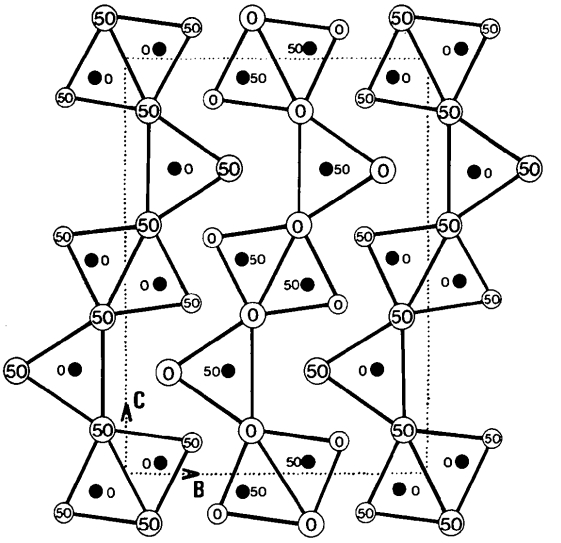

Fig. 1. The linkage of trigonal prisms in $Y_3Pd_2Si_3$ in projection down **a**. Numbers are x parameters multiplied by 100. Large circles are Y atoms, small circles Pd atoms and filled circles Si atoms.

* A list of structure factors for $Y_3Pd_2Si_3$ has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36865 (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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