

Rhodium Diyttrium Disilicide, Y_2RhSi_2

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Abstract. $M_r = 336.88$, monoclinic, $C2/m$, $a = 10.517$ (2), $b = 4.1990$ (5), $c = 10.515$ (2) Å, $\beta = 123.02$ (1)°, $V = 389.3$ Å³, $Z = 4$, $D_x = 5.75$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 349.18$ cm⁻¹, $\mu R = 1.0$, $F(000) = 604$, room temperature, final $R = 0.050$ for 525 unique reflections. The structure is made up of Y and Rh trigonal prisms centred by Si atoms and is isotypic with Sc_2CoSi_2 .

Introduction. To obtain new materials with possible superconducting properties a systematic X-ray investigation of the ternary Y–Rh–Si system was carried out. A new phase has been identified with composition Y_2RhSi_2 and a structure isotypic with Sc_2CoSi_2 (Gladyshevskii & Kotur, 1978).

Experimental. Alloys made from commercially available elements of high purity (Y:99.9%, Rh:99.99%, Si:99.999%). Samples prepared by conventional arc-melting techniques. D_m not determined. Small crystals of Y_2RhSi_2 suitable for X-ray analysis isolated by mechanical fragmentation from crushed melt. Weissenberg photographs showed crystals to have space group $C2/m$. Single crystal $35 \times 50 \times 60$ µm. Intensities measured with graphite-monochromated Mo $K\alpha$ radiation on a CAD-4 Enraf–Nonius diffractometer. $\theta/2\theta$ scan mode. Accurate cell dimensions determined by least-squares analysis of 25 θ values. Three standard reflections monitored at intervals of 3600 s, intensity variation during the data collection < 1%. Intensities of 664 independent reflections, to limit of $\theta = 35^\circ$, measured and corrected for background, Lorentz and polarization factors with *START* (Frenz, 1983). $-12 < h < 14$, $0 < k < 5$, $-14 < l < 0$. No absorption correction. Structure solved by direct methods with *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Positions of Y, Rh and Si atoms revealed in corresponding E map for space group $C2/m$. Full-matrix least-squares refinement of 31 positional and anisotropic thermal parameters converged after a few cycles using F values of 525 reflections with $I > 3\sigma(I)$; $wR = 0.050$; $w = 1/\sigma^2(F)$. In final least-squares cycle $(\Delta/\sigma)_{\max} = 3 \times 10^{-3}$. Peak height in final difference map < 15.0 e Å⁻³. No correction for secondary extinction. All calculations performed on PDP 11/23 computer using *SDP* (Frenz,

1983). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Atomic positions and equivalent isotropic temperature factors are listed in Table 1; * interatomic distances are in Table 2.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39949 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic positions and equivalent isotropic thermal parameters

E.s.d.'s are given in parentheses. $B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

	<i>x</i>	<i>y</i>	<i>z</i>	B_{eq} (Å ²)
Y(1)	0.0769 (1)	0	0.8909 (2)	0.77 (3)
Y(2)	0.3257 (1)	0	0.3247 (2)	0.73 (2)
Rh	0.3552 (1)	0	0.6279 (1)	0.82 (2)
Si(1)	0.6324 (4)	0	0.1220 (5)	0.86 (8)
Si(2)	0.0767 (4)	0	0.4360 (4)	0.81 (8)

Table 2. Interatomic distances (Å) in Y_2RhSi_2 up to 4.0 Å

Rh–Si(2)	2.428 (1)	Y(1)–Si(2)	2.894 (3)
–Si(2)	2.492 (3)	–Si(1)	2.990 (2)
–Si(1)	2.561 (3)	–Si(1)	3.017 (2)
–Y(2)	3.030 (1)	–Si(1)	3.134 (3)
–Y(2)	3.051 (1)	–Rh	3.235 (1)
–Y(2)	3.112 (1)	–Y(2)	3.551 (1)
–Rh	3.170 (1)	–Y(2)	3.623 (1)
		–Y(2)	3.827 (1)
Y(2)–Si(1)	2.892 (2)		
–Si(2)	2.996 (2)	Si(1)–Si(1)	2.559 (6)
–Rh	3.030 (1)	–Rh	2.561 (3)
–Rh	3.051 (1)	–Y(2)	2.892 (2)
–Si(2)	3.062 (2)	–Y(1)	2.990 (4)
–Rh	3.112 (1)	–Y(1)	3.017 (2)
–Si(2)	3.401 (3)	–Y(1)	3.134 (3)
–Y(2)	3.507 (2)	–Si(2)	3.933 (4)
–Y(1)	3.551 (1)	–Si(2)	3.990 (4)
–Y(1)	3.623 (1)		
–Y(1)	3.827 (1)	Si(2)–Rh	2.428 (1)
		–Rh	2.492 (3)
		–Si(2)	2.604 (6)
		–Y(1)	2.894 (3)
		–Y(2)	2.996 (2)
		–Y(2)	3.062 (2)
		–Y(2)	3.401 (3)
		–Si(2)	3.763 (5)
		–Si(1)	3.933 (4)
		–Si(1)	3.990 (4)

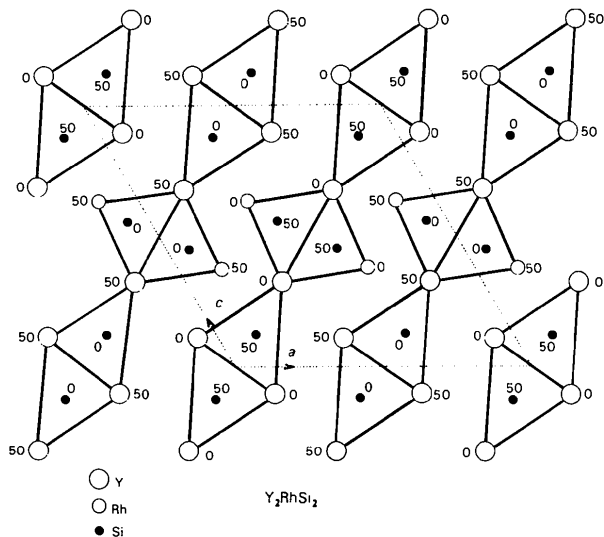


Fig. 1. Projection along the b axis for Y_2RhSi_2 . Numbers correspond to y parameters multiplied by 100. All Si atoms are at the centres of trigonal prisms with Y or Rh atoms at the six vertices.

The structure of Y_2RhSi_2 is shown (Fig. 1) in projection along the b axis. All Y and Rh atoms participate in the formation of trigonal prisms centred by Si atoms. The atomic model is isotypic with Sc_2CoSi_2 (Gladyshevskii & Kotur, 1978). Two columns of Y prisms with formula Y_3Si_2 are connected with two columns of Y and Rh prisms with formula $Y_3Rh_2Si_2$ to form the whole structure with formula $Y_3Si_2 + YRh_2Si_2$

$= Y_4Rh_2Si_4$ or Y_2RhSi_2 . If the columns of Y prisms only are considered, it is possible to join n prisms together to form a band with formula $Y_{n+1}Si_n$ and thus compounds with formula $Y_{n+1}Si_n + YRh_2Si_2 = Y_{n+2}Rh_2Si_{n+2}$. Some structures have already been identified with this composition. $YRhSi$ with $n=0$ (Hovestreydt, Engel, Klepp, Chabot & Parthé, 1982), $Y_3Rh_2Si_3$ with $n=1$ (Paccard, Le Roy & Moreau, 1982), and Y_3RhSi_3 with $n=4$ (Paccard, Paccard & Moreau, 1985). Similar structures have been recognized in the Sc-Fe-Si system (Chabot, Engel & Parthé, 1984): $ScFeSi$, $Sc_3Fe_2Si_3$ and Sc_2FeSi_2 .

References

- CHABOT, B., ENGEL, N. & PARTHÉ, E. (1984). *J. Less-Common Met.* **96**, 331–340.
- FRENZ, B. A. (1983). *Structure Determination Package*. Enraf-Nonius, Delft, Holland.
- GLADYSHEVSKII, E. I. & KOTUR, B. A. (1978). *Sov. Phys. Crystallogr.* **23**, 533–535.
- HOVESTREYDT, E., ENGEL, N., KLEPP, K., CHABOT, B. & PARTHÉ, E. (1982). *J. Less-Common Met.* **85**, 247–274.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
- MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.
- PACCARD, D., LE ROY, J. & MOREAU, J. M. (1982). *Acta Cryst.* **B38**, 2448–2449.
- PACCARD, L., PACCARD, D. & MOREAU, J. M. (1985). *J. Less-Common Met.* To be published.

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Multiple Hydrogen Positions in the Zeolite Brewsterite, $(Sr_{0.95}, Ba_{0.05})Al_2Si_6O_{16} \cdot 5H_2O$

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Abstract. $M_r = 658.64$, monoclinic, $P2_1/m$, $a = 6.767$ (2), $b = 17.455$ (2), $c = 7.729$ (1) Å, $\beta = 94.40$ (2)°, $V = 910.2$ Å³, $Z = 2$, $D_x = 2.40$ g cm⁻³, Be-monochromatized neutrons, $\lambda = 1.05097$ (6) Å, $\mu = 0.616$ cm⁻¹, $T \sim 295$ K, $R(F^2) = 0.098$ (1880 reflections). Multiple proton positions occur for three out of the four types of water molecules, and they cannot be

related to models of short-range Al,Si order. There is greater freedom of proton positions for water molecules lying well inside the cavity. The $T-O$ distances correlate with $T-O-T$ angle, and inferred Al contents are $T(1)$ 0, $T(2)$ 25, $T(3)$ and $T(4)$ 37%. Sr is coordinated to five water oxygens at 2.56–2.74 Å and five framework oxygens at 2.77–3.14 Å.