screw axes and connected to each other by hydrogen bonds through ammonium or water groups (Table 3). Of the six independent ammonium cations, N(3) has an exceptionally small temperature factor. It is coordinated by the three terminal O atoms bound to Se atoms.

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$Sc_5Re_8Si_{12}$, a New Orthorhombic Structure Type Related to $Sc_3Re_2Si_4$ and $Hf_2Ru_3Si_4$

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Abstract. $Sc_5Re_8Si_{12}$, $M_r = 2051{\cdot}4$, orthorhombic, *oS*100, *Amm*2, $a = 14{\cdot}475$ (4), $b = 19{\cdot}66$ (1), $c = 5{\cdot}237$ (2) Å, $V = 1490$ (1) Å^3, $Z = 4$, $D_x = 9{\cdot}14$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 713$ cm^{-1}, $F(000) = 3492$, $T = 293$ K, $wR = 0{\cdot}062$ for 2269 contributing reflections. The nearly face-centered structure is characterized by infinite parallel columns of face-joined Si-centered square antiprisms and infinite parallel columns of face-joined Re-centered deformed octahedra arranged in two structural slabs similar to those found in $Hf_2Ru_3Si_4$ and $Sc_3Re_2Si_4$. With respect to $Hf_2Ru_3Si_4$ or $Sc_3Re_2Si_4$ these two slabs are shifted in such a way that one is now the mirror image of the other; furthermore they are separated by additional atoms arranged in a plane and with composition $ScRe_2Si_4$. The $Sc_5Re_8Si_{12}$ structure is a correction of the previously published model of $ScRe_2Si_3$ in which four Sc atoms are missing in the unit cell.

Introduction. The phase diagram Sc–Re–Si has been investigated by Pecharskii (1979; cited by Rogl, 1984), who found five ternary phases: $Sc_2Re_3Si_4$, tetragonal, an ordered substitution variant of the Zr_5Si_4 type (Pecharskii, Bodak & Gladyshevskii, 1978); $Sc_3Re_2Si_3$, monoclinic, a new type (Pecharskii, Bodak & Gladyshevskii, 1979) for which a reinvestigation of the structure has shown that there are more Si atoms present, the true composition being $Sc_3Re_2Si_4$ (Chabot & Parthé, 1985); $ScRe_2Si_3$, orthorhombic, a new type (Pecharskii, Bodak & Gladyshevskii, 1979); '$ScReSi_2$' and '$Sc_8Re_3Si_9$' of unknown structures.

The structure model proposed for orthorhombic $ScRe_2Si_3$ attracted our attention because it contains holes which are not expected for this kind of compound. We decided thus to reinvestigate the composition and crystal structure of this phase.

Experimental. Samples of nominal compositions $Sc_4Re_9Si_{12}$, $Sc_5Re_8Si_{12}$, $Sc_4Re_8Si_{13}$ and $ScRe_2Si_3$ were prepared by arc melting under argon from Sc(99·99%), Re(99·99%) and Si(99·999%). Samples were X-ray powder analyzed both in their as-cast state and also after annealing (1070 K/7 d) and remelting, using a levitation technique to favor the crystal growth by slow cooling. None of the samples examined was single phase. Laue diffraction photographs showed a systematic splitting of the diffraction spots for most crystals selected. Good-quality single crystals were found in the $Sc_4Re_9Si_{12}$ as-cast sample only. The microchemical analysis of the majority phase of this sample was found, however, to be $Sc_{5.00(1)}Re_{7.85(1)}Si_{12.08(1)}$. The chemical analysis was performed on a Camebax MBX microprobe at 15 kV. The sample was analyzed simultaneously for Sc $K\alpha$, Re $M\beta$ and Si $K\alpha$ by wavelength dispersion and with $Sc_3Re_2Si_4$ (Chabot & Parthé, 1985) as standard. A single crystal of

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Table 1. *Atomic positional and displacement parameters for* $Sc_5Re_8Si_{12}$ (*space group Amm*2)

The isotropic atomic displacement factors are expressed as $T = \exp[-2\pi^2 U(2\sin\theta/\lambda)]$. E.s.d.'s are given in parentheses.

		x	y	z	U(Å^2 × 100)
Si(1)	8(*f*)	0·1490 (6)	0·0789 (5)	0·2798 (3)	1·0 (2)
Re(1)	8(*f*)	0·10785 (7)	0·20133 (6)	0·2709 (6)	0·70 (3)
Sc(1)	8(*f*)	0·1757 (4)	0·3660 (3)	0·274 (2)	0·8 (1)
Si(2)	8(*f*)	0·2415 (5)	0·2497 (5)	0·022 (2)	1·0 (1)
Sc(2)	8(*f*)	0·3255 (4)	0·1357 (3)	0·275 (2)	0·9 (1)
Si(3)	8(*f*)	0·3537 (5)	0·4185 (4)	0·282 (3)	0·8 (2)
Re(2)	8(*f*)	0·37519 (7)	0·29451 (7)	0·2690 (6)	0·74 (3)
Re(3)	4(*e*)	½	0·10081 (9)	0·0287 (7)	0·70 (4)
Si(4)	4(*e*)	½	0·2197 (8)	0·100 (3)	1·0 (3)
Si(5)	4(*e*)	½	0·3604 (6)	0·033 (3)	1·1 (3)
Si(6)	4(*d*)	0	0·1319 (7)	0·013 (4)	1·2 (2)
Si(7)	4(*d*)	0	0·2916 (7)	0·130 (3)	1·0 (3)
Re(4)	4(*d*)	0	0·41533 (9)	0·0276 (7)	0·85 (4)
Si(8)	4(*c*)	0·1208 (9)	0	0·655 (4)	1·1 (3)
Re(5)	4(*c*)	0·2308 (2)	0	0·0000 (7)	0·66 (4)
Re(6)	4(*c*)	0·2790 (2)	0	0·4911 (7)	0·65 (4)
Si(9)	4(*c*)	0·3969 (9)	0	0·137 (3)	0·9 (3)
Sc(3)	2(*b*)	½	0	0·566 (3)	0·6 (2)
Sc(4)	2(*a*)	0	0	0·043 (4)	1·3 (3)

irregular shape with 66 µm mean diameter was mounted on an automatic four-circle diffractometer (Philips PW 1100). Laue symmetry *mmm*, lattice parameters from 19 average reflection–antireflections with $26 < 2\theta < 44°$ and using Mo $K\alpha$.

Data collection: $(\sin\theta)/\lambda < 0·71$ Å^{-1}; spherical absorption correction 13·05–20·23; 1215 Friedel pairs measured $0 \leq h \leq 20$, $0 \leq k \leq 27$, $0 \leq l \leq 7$ and $-h-k-l$; 2 standard reflections ±(173); ±3·1% intensity variation; ω–2θ scan, ω-scan angle $(1·0 + 0·1\tan\theta)°$; 2269 contributing reflections [2071 with $|F| > 3\sigma(F)$]; systematic absences *hkl*: $k + l = 2n + 1$ leading to the four possible space groups *A*222, *Amm*2, *A*2*mm* and *Ammm*. The structure was solved in space group *Amm*2 using, as starting points, atom positions of the structure proposal for $ScRe_2Si_3$ (Pecharskii, Bodak & Gladyshevskii, 1979). Full-matrix least squares using $|F|$ values. 65 parameters refined: one scale factor, one extinction parameter, one absolute-structure parameter and 62 atomic positional and isotropic displacement parameters.* $R = 0·063$, $wR = 0·062$, $S = 2·74$, $w = 1/\sigma^2(F_{\rm rel})$; final max. shift/e.s.d. $\leq 3 \times 10^{-4}$; final residual electron density −15–17 e Å^{-3}; secondary isotropic extinction of type 1 with a Lorentzian distribution of 17·8 (9) × 10^{-6} (Becker & Coppens, 1974), absolute-structure parameter 0·02 (4) (Flack, 1983; Bernardinelli & Flack, 1985). Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); all programs used from *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). The origin of the polar space group was fixed by a restraint $\sum_i^N Z_i =$ constant (Flack & Schwarzenbach, 1987).

Table 2. *Interatomic distances up to* 3·3 Å *for* $Sc_5Re_8Si_{12}$

E.s.d.'s are all ≤ 0·02 Å.

Sc(1)—	Si(3)	2·78
	Si(2)	2·79
	Si(2)	2·80
	Si(8)	2·82
	Si(1)	2·83
	Si(6)	2·84
	Si(1)	2·89
	Re(5)	3·00
	Re(4)	3·01
	Si(7)	3·03
	Re(1)	3·08
	Re(1)	3·11
	Re(2)	3·21
Sc(2)—	Si(1)	2·79
	Si(3)	2·83
	Si(2)	2·87
	Si(5)	2·87
	Si(2)	2·87
	Si(3)	2·89
	Re(3)	2·92
	Si(9)	2·95
	Re(6)	2·97
	Re(2)	3·02
	Re(2)	3·06
	Si(4)	3·15
	Re(2)	3·20
Sc(3)—	2Si(9)$^{\alpha}$	2·69
	2Si(5)	2·75
	4Si(3)$^{\alpha}$	2·89
	2Re(3)	3·13
	2Re(6)	3·22
Sc(4)—	2Si(6)	2·60
	2Si(8)$^{\alpha}$	2·68
	4Si(1)$^{\alpha}$	2·93
	2Re(4)	3·04
	2Re(4)	3·17
Re(1)—	Si(7)$^{\beta}$	2·45
	Si(6)$^{\beta}$	2·48
	Si(7)$^{\beta}$	2·48
	Si(1)$^{\beta}$	2·48
	Si(2)$^{\beta}$	2·52
	Si(2)$^{\beta}$	2·53
	Sc(1)	3·08
	Re(4)	3·08
	Sc(1)	3·11
	Re(1)	3·12
	2Re(1)	3·24
Re(2)—	Si(3)$^{\beta}$	2·46
	Si(2)$^{\beta}$	2·49
	Si(4)$^{\beta}$	2·49
	Si(2)$^{\beta}$	2·50
	Si(4)$^{\beta}$	2·52
	Si(5)$^{\beta}$	2·54
	Sc(2)	3·02
	Re(3)	3·06
	Sc(2)	3·07
	2Re(2)	3·15
	Sc(2)	3·20
	Sc(1)	3·21
Re(3)—	Si(4)	2·37
	2Si(3)	2·51
	2Si(9)	2·55
	Si(5)	2·70
	Si(5)	2·75
	2Sc(2)	2·92
	2Re(2)	3·06
	Sc(3)	3·13
Re(4)—	Si(7)	2·49
	2Si(8)	2·50
	2Si(1)	2·52
	Si(6)	2·71
	Si(6)	2·85
	2Sc(1)	3·01
	Sc(4)	3·04
	2Re(1)	3·08
	Sc(4)	3·17
Re(5)—	Si(8)$^{\beta}$	2·41
	2Si(1)$^{\beta}$	2·44
	Si(9)$^{\beta}$	2·51
	2Si(3)$^{\beta}$	2·65
	Re(6)	2·66
	Re(6)	2·75
	2Sc(1)	3·00
Re(6)—	Si(8)$^{\beta}$	2·44
	2Si(3)$^{\beta}$	2·46
	Si(9)$^{\beta}$	2·52
	Re(5)	2·66
	2Si(1)$^{\beta}$	2·68
	Re(5)	2·75
	2Sc(2)	2·97
	Sc(3)	3·22
Si(1)—	Re(5)	2·44
	Re(1)	2·48
	Re(4)	2·52
	Si(8)	2·54
	Re(6)	2·68
	Si(6)	2·77
	Sc(2)	2·79
	Sc(1)	2·83
	Sc(1)	2·89
	Sc(4)	2·93
	Si(1)	3·10
Si(2)—	Re(2)$^{\gamma}$	2·49
	Re(2)$^{\gamma}$	2·50
	Re(1)$^{\gamma}$	2·52
	Re(1)$^{\gamma}$	2·53
	2Si(2)	2·62
	Sc(1)$^{\gamma}$	2·79
	Sc(1)$^{\gamma}$	2·80
	Sc(2)$^{\gamma}$	2·87
	Sc(2)$^{\gamma}$	2·87
Si(3)—	Re(2)	2·46
	Re(6)	2·46
	Re(3)	2·51
	Si(9)	2·54
	Re(5)	2·65
	Si(5)	2·73
	Sc(1)	2·78
	Sc(2)	2·83
	Sc(3)	2·89
	Sc(2)	2·89
	Si(3)	3·20
Si(4)—	Re(3)	2·37
	2Re(2)	2·49
	2Re(2)	2·52
	Si(5)	2·76
	Si(5)	2·79
	2Si(4)	2·88
	2Sc(2)	3·15
Si(5)—	2Re(2)	2·54
	Re(3)	2·70
	2Si(3)	2·73
	Sc(3)	2·75
	Re(3)	2·75
	Si(4)	2·76
	Si(4)	2·79
	2Sc(2)	2·87
Si(6)—	2Re(1)	2·48
	Si(7)	2·51
	Sc(4)	2·60
	Re(4)	2·71
	2Si(1)	2·77
	2Sc(1)	2·83
	Re(4)	2·85
	Si(7)	3·20
Si(7)—	2Re(1)	2·45
	2Re(1)	2·48
	Re(4)	2·49
	Si(6)	2·51
	2Sc(1)	3·03
	2Si(7)	3·09
	Si(6)	3·20
Si(8)—	Re(5)	2·41
	Re(6)	2·44
	2Re(4)	2·50
	2Si(1)	2·54
	Sc(4)	2·68
	2Sc(1)	2·82
Si(9)—	Re(5)	2·51
	Re(6)	2·52
	2Si(3)	2·54
	2Re(3)	2·55
	Sc(3)	2·69
	2Sc(2)	2·95
	Si(9)	2·98

α trigonal prism; β octahedron; γ square antiprism.

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* A list of structure factors, arranged in a standard crystallographic date file (Brown, 1985), has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43990 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. Atomic positional and displacement parameters are given in Table 1, interatomic distances in Table 2.

The single crystal was isolated from the $Sc_4Re_9Si_{12}$ sample; however, its true composition, as deduced from Table 1, is $Sc_5Re_8Si_{12}$. This composition agrees well with the results obtained from microprobe analysis.

Our structure model is similar to the one proposed by Pecharskii, Bodak & Gladyshevskii (1979) for $ScRe_2Si_3$ – same space group (*Amm*2), similar cell parameters and site occupations – but with four more Sc atoms [Sc(3) and Sc(4)] located on Wyckoff sites 2(*b*) and 2(*a*), respectively. These Sc atoms have similar atom surroundings consisting of a deformed trigonal prism of Si atoms plus extra atoms in the intermediate plane perpendicular to the prism axis. The Sc–Si interatomic distances are short (2·60–2·89 Å) but not unusual for this kind of compound. As can be deduced from Fig. 1, and as already mentioned by Pecharskii *et al.* (1979), the crystal structure of $Sc_5Re_8Si_{12}$ has a symmetry which differs slightly from *Fmm*2. However, deviations from the *F* Bravais lattice cannot be ignored when considering reflections which violate the corresponding systematic absences: for example, the structure factor for reflection 19,0,2 has a value of $F_{\rm obs} = 583$ (8) ($F_{\rm calc} = 506$) which corresponds to $\frac{1}{3}$ of that of the strongest reflection 402 [$F_{\rm obs} = 1796$ (9); $F_{\rm calc} = 1587$]. Contrary to the procedure followed by Pecharskii *et al.* (1979) for $ScRe_2Si_3$, we have used all reflections of this kind in the structure refinement: the proposed structure model for $Sc_5Re_8Si_{12}$ is based on the contribution of 2269 reflections (including antireflections) instead of only 347 reflections in the case of the $ScRe_2Si_3$ study.

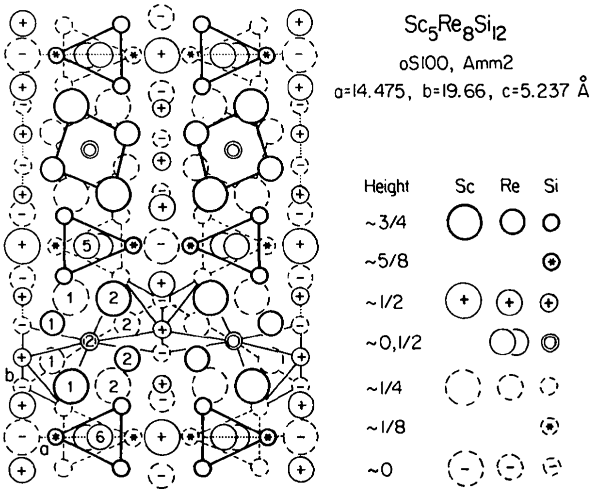

Fig. 1. The $Sc_5Re_8Si_{12}$ structure type in a projection along the short *c* axis. Infinite square antiprism columns and infinite octahedron columns parallel to [001] are indicated with heavy outlines. The numbers correspond to the atom labels used in Tables 1 and 2. The octahedra around Re atoms (only those with a same *z*) which participate in the square antiprism are indicated with thin outlines. The exact heights of the atoms are as follows: $\sim\frac{3}{4}$ at 0·77 and 0·78; $\sim\frac{5}{8}$ at 0·64; $\sim\frac{1}{2}$ at 0·51, 0·53, 0·54, 0·56, 0·60 and 0·63; $\sim 0,\frac{1}{2}$ at 0·02, 0·49, 0·52 and 0·99; $\sim\frac{1}{4}$ at 0·27 and 0·28; $\sim\frac{1}{8}$ at 0·14; ~0 at 0·01, 0·03, 0·04, 0·06, 0·10 and 0·13.

Comparison of the $Sc_5Re_8Si_{12}$ structure (Fig. 1) with that of $Sc_3Re_2Si_4$ (Fig. 3 in Chabot & Parthé, 1985) and $Hf_2Ru_3Si_4$ ($Zr_2Ru_3Si_4$) (Fig. 1 in Chabot, Parthé & Braun, 1985) shows that they all contain similar parallel structural slabs formed from alternating columns of face-joined Si-centered deformed square antiprisms and face-joined Re(Ru)-centered deformed Si octahedra. The structural slabs differ in the atom composition of the square antiprisms: in $Hf_2Ru_3Si_4$ and $Sc_5Re_8Si_{12}$ they have the composition Hf_4Ru_4 and Sc_4Re_4 respectively [square antiprisms of type III′ in the structural classification of Pecharskii *et al.* (1979)] instead of Sc_6Re_2 (antiprism of type II) in $Sc_3Re_2Si_4$. The structures of $Hf_2Ru_3Si_4$ and $Sc_3Re_2Si_4$ are in fact two substitution variants built up with only two structural slabs which are in both cases symmetry related by a *c*-glide plane perpendicular to the prism columns (they differ only in the composition of the square antiprisms). $Sc_5Re_8Si_{12}$ also contains two such slabs (with the same atom ordering as in $Hf_2Ru_3Si_4$ and not as in $Sc_3Re_2Si_4$) but in this case one is the mirror image of the other, and they are separated by additional atoms arranged in two planes: (200) containing the atoms Sc(3), Re(3), Si(4,5) and (100) containing Sc(4), Re(4), Si(6,7), both with composition $ScRe_2Si_4$. The Si atoms of the additional layers participate in the octahedral Si-atom surrounding of the four Re atoms [2Re(1) and 2Re(2)] of the face-joined square antiprisms (see Fig. 1 and Table 2).

In the particular case of $Hf_2Ru_3Si_4$ and $Sc_3Re_2Si_4$, in which the intermediate layers do not exist, part of the atoms of the square antiprisms [2Ru(3) and 2Sc(3), respectively] are also octahedrally surrounded by Si atoms. The Si atoms belonging to the columns of face-joined Si octahedra of the adjacent structural slabs (see Chabot *et al.*, 1985) play the same role as, in $Sc_5Re_8Si_{12}$, the Si atoms of the intermediate layers.

The arrangement of the four deformed octahedra surrounding the four Re atoms belonging to one square antiprism can be deduced from the drawing of $Sc_5Re_8Si_{12}$ (Fig. 1). Each of the four octahedra has common edges with three of its neighbors: one edge, formed by 2Si(2) (perpendicular to the plane of projection), is common to octahedra centered at the same *z* value and two edges are common with the octahedra centered at ($z \pm \frac{1}{2}$). Furthermore, the four octahedra have a common vertex [either Si(3) or Si(1)] with the octahedra of a face-joined Si-octahedron column belonging to the same structural slab and a common face with an octahedron of the adjacent structural slab (related by the mirror plane). In this latter case, the Si atoms forming the common face belong to one of the two intermediate layers. It is interesting to note that the interatomic distances between the Re atoms centering these face-joined octahedra [Re(1)–Re(1) at 3·12 and Re(2)–Re(2) at 3·61 Å] are notably different. They are also notably longer than the interatomic distances between the Re atoms centering the face-joined octahedron columns [2·66 and 2·75 Å].

$Sc_5Re_8Si_{12}$ belongs to the category of structures built up with columns of square antiprisms and octahedra which has been discussed recently by Chabot & Parthé (1985). It has been shown above that the $Sc_5Re_8Si_{12}$ structure can be described as an arrangement of $Hf_2Ru_3Si_4$-type slabs with interspersed monoatomic layers. Similarly, $ZrMnSi_2$ (Venturini, Steinmetz & Roques, 1982) can be described as an arrangement of deformed $Sc_3Re_2Si_4$-type slabs [parallel to $(1\bar{1}0)$ in $ZrMnSi_2$] with another kind of interspersed monoatomic layer.

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Orthorhombic Perovskite $CaTiO_3$ and $CdTiO_3$: Structure and Space Group

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Abstract. Structural aspects and physical properties strongly indicate that the $CdTiO_3$ perovskite has a centrosymmetric structure with space group *Pbnm*. Single-crystal X-ray studies have revealed that both $CaTiO_3$ and $CdTiO_3$ can be described well as $GdFeO_3$-type perovskites in terms of the size ratio of two kinds of cation occupying *A* and *B* sites. Distortions and tiltings of polyhedra are systematically related to the *observed tolerance factor*. The crystal data for $CaTiO_3$ are: $M_r = 135·98$, *Pbnm*, $a = 5·3796\ (1)$, $b = 5·4423\ (3)$, $c = 7·6401\ (5)$ Å, $V = 223·68\ (1)$ Å^3, $Z = 4$, $D_x = 4·04$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0·7107$ Å, $\mu = 58·0$ cm^{-1}, $F(000) = 264$, $T = 293$ K, $R = 0·023$, 703 unique reflections used for refinements, crystal synthesized at 1470 K and 2·5 GPa. The crystal data for $CdTiO_3$ are: $M_r = 208·30$, *Pbnm*, $a = 5·3053\ (1)$, $b = 5·4215\ (3)$, $c = 7·6176\ (3)$ Å, $V = 219·10\ (1)$ Å^3, $Z = 4$, $D_x = 6·31$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0·7107$ Å, $\mu = 130·6$ cm^{-1}, $F(000) = 376$, $T = 293$ K, $R = 0·019$, 829 unique reflections, crystal synthesized at 1470 K and 1·5 GPa.

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