New Scandium Platinum Silicides: ScPt_2Si with ‘Inverse’ MgCuAl_2 Structure, and $\text{Sc}_5\text{Pt}_9\text{Si}_7$, a Variant of the $\text{Zr}_2\text{Fe}_{12}\text{P}_7$ -Type

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New Scandium Platinum Silicides:

ScPt₂Si with ‘Inverse’ MgCuAl₂ Structure, and Sc₅Pt₉Si₇, a Variant of the Zr₂Fe₁₂P₇-Type

Peter Lorenz and Walter Jung*

Dedicated to Professor Gerd Meyer on the Occasion of his 60th Birthday

Keywords: scandium platinum silicide; crystal structure

Abstract. Two new scandium platinum silicides, ScPt₂Si (orthorhombic, *Cmcm*, *a* = 3.6653(6) Å, *b* = 9.831(1) Å, *c* = 5.757(1) Å, *Z* = 4) and Sc₅Pt₉Si₇ (hexagonal, *P*6̄, *a* = 9.9418(5) Å, *c* = 3.8832(2) Å, *Z* = 1) were prepared by reaction of the elements in an electric arc furnace and subsequent annealing. The crystal structures were solved and refined from single crystal diffraction data. ScPt₂Si crystallizes with an ‘inverse’ MgCuAl₂ structure while Sc₅Pt₉Si₇ forms a variant of the Zr₂Fe₁₂P₇ type.

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Results and Discussion

ScPt₂Si

ScPt₂Si crystallizes in space group *Cmcm* and may be formally assigned to the MgCuAl₂ type of structure [9], an ordered variant of the Re₃B type [11]. This structure type is frequently observed, especially with alkaline earth or rare earth transition metal gallides, indides, and stannides like CaPtGa₂ [12], CePdIn₂ [13], or EuIrSn₂ [14]. In these compounds transition metal and post-transition metal atoms occupy the sitesets 4*c* and 8*f*, respectively. In ScPt₂Si, however, these sitesets are interchanged. Platinum atoms are now the majority component and reside on 8*f*, while silicon atoms are found on 4*c*. Therefore, the ScPt₂Si structure may be called an ‘inverse’ MgCuAl₂ type.

The MgCuAl₂ structure has been described in a somewhat formal way [13], aiming at rows of trigonal prisms running along the *a* axis and shifted against each other by *a*/2. In the case of ScPt₂Si the prisms are formed by platinum and scandium atoms and they are centered by silicon atoms. In Figure 1a, a projection of the structure along [100], these prisms are emphasized by bold lines. In Figure 1b they are compared to corresponding prisms in the structure of

Introduction

While ternary silicides of the platinum metals with a havier rare earth metal (Y, La-Lu) as a third component have been studied to a larger extent [1], less is known about corresponding compounds with scandium. Former phase analytical work done by Braun et al. [2] in the system Sc-Rh-Si revealed the existence of 9 ternary phases. However, later on only ScRhSi [3], ScRhSi₂ [4], ScRh₃Si₇ [5] and Sc₅Rh₄Si₁₀ [6] were structurally characterized, the latter only from powder data. Four ternary phases have been reported in the System Sc-Ir-Si, but only the structures of ScIr₃Si₇ [5] and Sc₅Ir₄Si₁₀ [6] are known from single crystal work. The structures of ScIrSi [3] and Sc₄Ir₇Si₆ [7] were assigned on the basis of powder patterns. This holds also for the structures of ScPdSi and ScRuSi [3]. The structure of Sc₃Os₂Si₆ is not yet known [6]. In the system Sc-Pt-Si for a long time only ScPtSi with TiNiSi type structure was known [3], until recently Sc₃PtSi₃ together with Sc₂RuSi₂ was presented by Harmering et al. at a conference [8]. Here we report on ScPt₂Si and Sc₅Pt₉Si₇ crystallizing with variants of the MgCuAl₂ [9] and the Zr₂Fe₁₂P₇ type [10], respectively.

CaPtGa₂. This view of the structure originates from the archetype Re₃B, because trigonal transition metal prisms centered by boron atoms are typical building elements of metal rich borides. To ScPt₂Si a different description is more adequate. According to the differences between the electronegativities of scandium on one side and platinum and silicon on the other side, the commonly accepted bonding model regards positively charged scandium atoms and a polyanion built of platinum and silicon atoms. In Figure 2 showing perspective views of the structure, this polyanion is emphasized by drawing Pt-Pt and Pt-Si bonds. It contains channels with pentagonal and with hexagonal cross sections running along the a- and the c-axis, respectively. The scandium atoms are located at the points of intersection inside of these channels. Their environment is shown in Figure 3a. It consists of three silicon atoms (*d*(Sc-Si): 1x2.766(5) Å, 2x2.825(4) Å) and 10 platinum atoms (*d*(Sc-Pt): 4x2.913(1) Å, 4x2.937(2) Å, 2x3.402(3) Å). From the latter only 8 are close enough for bonding interactions. Their distances correspond to the sum of the metallic radii for coordination number (CN) 12 [15]. The silicon atoms are surrounded by 6 platinum atoms (*d*(Si-Pt): 2x2.430(2) Å, 4x2.496(2) Å) forming a distorted trigonal prism and three scandium atoms capping the side-faces of the prism (Figure 3b). The coordination polyhedron around the platinum atom is quite irregular. It is built up by four scandium, four platinum, and three silicon atoms. The shortest interatomic distances in the structure are those between platinum and silicon atoms with a mean value of 2.474 Å which is nearly the same as the sum of *Pauling's* single bond radii for platinum and silicon of 2.468 Å [15]. Strong bonding interactions may thus be assumed, supporting the model of a Pt-Si-polyanion. All the interatomic distances considered above compare well with those found in ScPtSi [3].

ScPt₂Si is the first silicide crystallizing with an ordered variant of the Re₃B type. The structure of Re₃B is closely related to that of Fe₃C [16]. An ordered variant of the latter is already known with the YPd₂Si structure adopted by two series of ternary rare earth silicides of palladium and platinum [17]. Therefore the existence of a ternary silicide with Re₃B derived structure was formerly predicted by *Parthé and Chabot* [1b].

Sc₅Pt₉Si₇

The crystal structure of Sc₅Pt₉Si₇, shown as a projection along the c-axis in Figure 4, is a substitution variant of the Zr₂Fe₁₂P₇ structure [10], a well known structure type, which is adopted by numerous ternary transition metal phosphides preferentially with a rare earth metal as the third component. Sc₅Pt₉Si₇ and Zr₂Fe₁₂P₇ both crystallize in space group *P*6̄ with similar lattice constants and positional parameters. The phosphorus positions are taken by the silicon atoms. Three of the four iron sitesets (2x3j + 3k) are occupied by platinum

atoms, while the remaining one (3k) is occupied by scandium atoms. The other scandium atoms reside on the zirconium positions. Sc₅Pt₉Si₇ is not the first compound, in which a substitution of transition metal atoms on this special 3k site by the more electropositive component is observed, but it is the first example of a complete substitution, and it is the first silicide with a Zr₂Fe₁₂P₇ derivative structure. Examples of substitution to a small extent are the compounds Mg_{2.5}Ni_{11.5}P₇, Ca_{2.1}Ni_{11.9}P₇, and Ca_{2.3}Ni_{11.7}As₇ [18], while in Yb_{2+3-x}Pd_{12-3+x}P₇ with (x=0.40) the substitution is nearly complete [19]. With regard to these examples, a statistical distribution of scandium and platinum atoms on the 3k site of Sc₅Pt₉Si₇ could also be possible. However, in samples with different compositions no significant deviations of the lattice parameters were observed. Therefore a constant composition is assumed.

As stated above for ScPt₂Si, the structure of Sc₅Pt₉Si₇ is best discussed considering a 3D-polyanion built from platinum and silicon atoms in which positively charged scandium atoms are inserted (Figure 4). This view is again supported by the short distances between platinum and silicon atoms (Table 4) indicating strong bonding interactions. The three kinds of platinum atoms are tetrahedrally coordinated by four silicon atoms. The Pt-Si distances range from 2.336(6) to 2.761(5) Å with a mean value of 2.486 Å which again is nearly equal to the sum of *Pauling's* single bond radii [15]. Moreover three platinum atoms (*d*(Pt-Pt): 2.815(1) Å – 2.900(1) Å) and four scandium atoms (*d*(Pt-Sc): 2.913(4) Å – 3.402(1) Å) contribute to the first coordination spheres of the platinum atoms. The silicon atoms Si1, Si2, and Si3 are connected to three, five, and six platinum atoms, respectively.

The three crystallographically distinct scandium atoms are located in channels with pentagonal and hexagonal cross-sections running in the direction of the c-axis (Figure 4). Their environments are shown in Figure 5. The pentagonal channels containing the Sc1 atoms are arranged in groups of three. This results in a clustering of the Sc1 atoms (Figure 5a) and Sc1-Sc1 distances of 3.396(8) Å, which are the shortest distances between scandium atoms in the structure. They are, however, still larger than those observed in *hcp* scandium (3.254 and 3.309 Å [20]). All other Sc-Sc distances are larger than 3.78 Å indicating the absence of bonding interactions. Depending on the cross-sections of the channels, the first coordination spheres of the scandium atoms are either pentagonal or hexagonal prisms. They are completed by additional atoms in front of the rectangular side-faces. The prisms, highlighted by bold lines in Figure 5, are composed of six platinum and four silicon atoms in the case of Sc1 and of six platinum and six silicon atoms in the case of Sc2 and Sc3. Atoms capping the side-faces are 1Pt+1Si for Sc1, 3Pt for Sc2, and 6Pt for Sc3. The Sc-Pt distances range from 2.913(4) to 3.200(1) Å, the Sc-Si

distances from 2.759(3) to 2.990(5) Å. The former are thus close to, the latter smaller than the sum of the metallic radii for CN 12 [15].

Figure 1. Projections along [100] of the structures of a) ScPt₂Si ('inverse' MgCuAl₂ type) and b) CaPtGa₂ (MgCuAl₂ type) (Pt: black; Si, Ga: gray; Sc, Ca: white; this holds for all drawings; numbers indicate x parameters of the atoms; unit cells outlined). The lines emphasizing the trigonal prisms do not all represent chemical bonds.

Figure 2. Perspective views of the ScPt₂Si structure approximately along [100] and [001].

Figure 3. Environments of a) Sc- and b) Si-atoms in the structure of ScPt₂Si.

Figure 4. Projection of the Sc₅Pt₉Si₇ structure along [001].

Figure 5. Environments of the scandium atoms in the structure of Sc₅Pt₉Si₇.

Table 1. Crystallographic data and structure refinement of ScPt₂Si and Sc₅Pt₉Si₇

Formula	ScPt ₂ Si	Sc ₅ Pt ₉ Si ₇
Crystal system	orthorhombic	hexagonal
Space group	<i>Cmcm</i>	<i>P</i> $\bar{6}$
Lattice parameters (powder data)	<i>a</i> = 3.665(6) Å <i>b</i> = 9.831(1) Å <i>c</i> = 6.967(1) Å <i>V</i> = 251.05 Å ³	<i>a</i> = 9.9418(5) Å <i>c</i> = 3.8832(2) Å <i>V</i> = 332.39 Å ³
Fomula units/cell, <i>Z</i>	4	1
Calculated density	12.256 g/cm ³	10.877 g/cm ³
Absorption coefficient	113.9 mm ⁻¹	97.23 mm ⁻¹
Crystal size	20x40x50 μm ³	30x40x50 μm ³
Transmission ratio (max/min)	2.72	4.31
Diffractometer	STOE IPDS	STOE IPDS
Radiation	MoKα	MoKα
φ Range, increment	0–200°, 2.0°	0–200°, 2.0°
Exposure time	9 min	10 min
θ _{max} for data collection	33°	33°
Ranges for <i>h</i> , <i>k</i> , <i>l</i>	±5, ±13, ±10	±15, ±15, ±5
Reflections measured	1805	4787
unique	281	922
<i>I</i> > 2σ(<i>I</i>)	258	829
<i>R</i> _{int}	0.0566	0.1165

R_{σ}	0.0289	0.0631
Refined parameters	16	44
$R1$	0.0255	0.0381
$wR2$	0.0543	0.0840
Goodness-of-fit	1.126	1.094
Extinction coefficient	0.0030(3)	0.0025(3)
Flack parameter	-	0.01(3)
Max/min residual density	3.14/-2.65 e/Å ³	3.98/-3.34 e/Å ³

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (pm²) for ScPt₂Si (space group *Cmcm*) and Sc₅Pt₉Si₇ (space group *P6*). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	Wyckoff position	x	y	z	U_{eq}
<i>ScPt₂Si</i> :					
Sc	4c	0	0.0469(3)	1/4	64(6)
Pt	8f	0	0.36214(4)	0.04860(6)	62(2)
Si	4c	0	0.7656(4)	1/4	58(8)
<i>Sc₅Pt₉Si₇</i> :					
Sc1	3k	0.2274(5)	0.1244(6)	1/2	76(7)
Sc2	1f	2/3	1/3	1/2	85(14)
Sc3	1c	1/3	2/3	0	107(23)
Pt1	3j	0.1229(1)	0.2854(1)	0	68(2)
Pt2	3j	0.4338(1)	0.3531(1)	0	77(2)
Pt3	3k	0.0517(1)	0.4487(1)	1/2	71(2)
Si1	1a	0	0	0	76(7)
Si2	3j	0.4298(1)	0.1148(7)	0	47(11)
Si3	3k	0.2844(7)	0.4275(8)	1/2	58(12)

Table 3. Anisotropic displacement parameters (pm²) for ScPt₂Si and Sc₅Pt₉Si₇.

Atom	Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{12}
<i>ScPt₂Si</i>						
Sc	4c	48(11)	30(11)	112(15)	0	0
Pt	8f	81(2)	46(2)	57(3)	-2(1)	0
Si	4c	82(1)	36(17)	54(21)	0	0
<i>Sc₅Pt₉Si₇</i>						
Sc1	3k	43(18)	114(20)	60(19)	0	32(16)
Sc2	1f	99(21)	U_{11}	56(35)	0	49(10)
Sc3	1c	101(23)	U_{11}	127(40)	0	51(12)
Pt1	3j	68(4)	73(4)	63(4)	0	35(3)
Pt2	3j	54(4)	67(4)	100(4)	0	23(3)
Pt3	3k	87(4)	73(4)	60(4)	0	46(4)
Si1	1a	85(33)	U_{11}	151(60)	0	42(17)
Si2	3j	37(25)	19(24)	70(30)	0	3(21)
Si3	3k	47(26)	65(29)	49(30)	0	19(24)

Table 4. Selected interatomic distances (Å) for ScPt₂Si and Sc₅Pt₉Si₇

Atoms	d	Atoms	d
<i>ScPt₂Si</i>			
Sc – 1Si	2.766(5)	Pt – 1Si	2.430(2)
2Si	2.825(4)	2Si	2.496(2)
4Pt	2.913(1)	1Pt	2.794(1)
4 Pt	2.937(2)	1Pt	2.806(1)
Si – 2Pt	2.430(2)	2Sc	2.913(1)
4Pt	2.496(2)	2Sc	2.937(2)
1Sc	2.766(5)	2Pt	2.946(1)
2Sc	2.826(4)		
<i>Sc₅Pt₉Si₇</i>			
Sc1 – 2Si1	2.759(3)	Pt3 – 1Si3	2.336(6)
1Si3	2.774(9)	1Si3	2.426(7)
2Si2	2.827(6)	2Si2	2.466(4)
2Pt2	2.913(4)	2Pt1	2.839(1)
2Pt1	2.940(4)	2Pt2	2.900(1)
1Pt3	2.976(5)	1Sc1	2.976(5)
2Pt1	3.012(4)	2Sc3	3.200(1)
Sc2 – 6Si2	2.990(5)	1Sc2	3.402(1)
6Pt2	3.102(1)	Si1 – 3Pt1	2.465(1)
1Pt3	3.402(1)	6Sc1	2.759(3)
Sc3 – 6Si3	2.916(5)	Si2 – 1Pt2	2.346(6)
6Pt3	3.200(1)	1Pt2	2.353(7)
Pt1 – 2Si3	2.465(4)	2Pt3	2.466(4)
1Si1	2.465(1)	1Pt1	2.520(6)
1Si2	2.520(6)	2Sc1	2.827(6)
1Pt2	2.815(1)	2Sc2	2.990(5)
2Pt3	2.839(1)	Si3 – 1Pt3	2.336(6)
2Sc1	2.940(4)	1Pt3	2.426(7)
2Sc1	3.012(4)	2Pt1	2.465(4)
Pt2 – 1Si2	2.346(6)	2Pt2	2.761(5)
1Si2	2.353(7)	1Sc1	2.774(9)
2Si3	2.761(5)	2Sc3	2.916(5)
1Pt1	2.815(1)		
2Pt3	2.900(1)		
2Sc1	2.913(4)		
2Sc2	3.102(1)		

Experimental Section

Synthesis

Starting materials for the preparation of the title compounds were the elements: scandium metal, cut into small pieces (99.9% Johnson Matthey), platinum powder (99.9%, Degussa), and silicon pieces (m8N, Johnson Matthey). Mixtures of the elements in the atomic ratios according to the formulas were pressed into pellets of about 700 mg weight and arc melted under purified argon. To achieve homogeneity, the buttons were turned around and remelted two times. Weight loss during the melting process was negligible. Subsequently the buttons were placed in alumina crucibles, sealed in silica tubes under argon atmosphere and annealed four days at 1200 °C. Finally they were cooled to room temperature at a rate of 20 °C/h. From the crushed samples single crystals of irregular shape were isolated. They are stable to moist air for long periods of time. Semi-quantitative EDX measurements (Philips XL40 scanning electron microscope with EDAX detector) confirmed the compositions of the crystals as obtained from the structure analysis and excluded the presence of other elements.

X-ray diffraction and crystal structure

X-ray powder data were taken with a Guinier diffractometer (Huber G645, CuK α_1 , Si as external standard). For correct indexing of the patterns they were compared to theoretical ones calculated on the basis of the structure refinements. While ScPt₂Si was single phase according to the accuracy of the method, the Sc₅Pt₉Si₇ samples contained ScPtSi as a by-product.

The quality of the single crystals was checked by means of Laue photographs taken on a Buerger precession camera. Single crystal intensity data were collected at room temperature on a STADI-I diffractometer. Numerical absorption corrections were performed after optimizing the crystal faces with the program X-SHAPE [21]. The structures were solved by means of direct methods with SHELXS-97 [22] and refined on F^2 values using SHELXL-97 [23] with anisotropic displacement parameters for all atoms. No significant peaks were found in the difference Fourier syntheses. Crystallographic data and details of the data collection and the structure refinement are listed in Table 1. Table 2 contains the positional parameters and the equivalent isotropic displacement parameters, Table 3 the anisotropic displacement parameters. Selected interatomic distances are listed in Table 4.

Further details of the structure determinations may be obtained from: Fachinformationszentrum Karlsruhe, D-76344 Eggenstein-Leopoldshafen (Germany) by quoting the Registry No's. CSD-420355 (ScPt₂Si) and CSD-420356 (Sc₅Pt₉Si₇).

Acknowledgments

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Figure 1. Projections along [100] of the structures of a) ScPt₂Si ('inverse' MgCuAl₂ type) and b) CaPtGa₂ (MgCuAl₂ type) (Pt: black; Si, Ga: gray; Sc, Ca: white; this holds for all drawings; numbers indicate *x* parameters of the atoms; unit cells outlined). The lines emphasizing the trigonal prisms do not all represent chemical bonds.
162x104mm (600 x 600 DPI)

Figure 2. Perspective views of the ScPt₂Si structure approximately along [100] and [001].
175x137mm (600 x 600 DPI)

Figure 3. Environments of a) Sc- and b) Si-atoms in the structure of ScPt₂Si.
201x109mm (600 x 600 DPI)

Figure 4. Projection of the $\text{Sc}_5\text{Pt}_9\text{Si}_7$ structure along $[001]$.
1963x1029mm (96 x 96 DPI)

Figure 5. Environments of the scandium atoms in the structure of Sc₅Pt₉Si₇
184x65mm (600 x 600 DPI)