Sc₂Pt with orthorhombic Ni₂Si structure type.

By B. Chabot and E. Parthé, *Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*

Abstract

Sc_2Pt crystallizes with the Ni_2Si structure type; space group $Pnma$, $a = 6.592$ (3), $b = 4.491$ (2), $c = 8.206$ (5) Å, $Z = 4$, $D_x = 7.79$ Mg m^{-3}, $M_r = 285$, $F(000) = 480$, μ(Mo $K\alpha$) = 65.6 mm^{-1}, $\sum |\Delta F|/\sum |F_o| = 10.9$ for 320 reflexions with $|F_o| > 3\sigma(F_o)$. Atomic parameters were refined from single-crystal intensities. Sc_2Pt is compared with the rare-earth–Pt compounds having the same structure type.

Introduction

In the course of a structural study of intermetallic compounds in the Sc–transition-metal phase diagrams, samples of different compositions have been prepared in the system Sc–Pt by arc melting under an argon atmosphere.

Only two phases are known in the Sc–Pt phase diagram. These are ScPt₃, which has the Cu₃Au type (Dwight, Downey & Conner, 1961), and ScPt which crystallizes with the CsCl type (Aldred, 1962). Examination of the X-ray

Table 1. *Atomic parameters for* Sc₂Pt *crystallizing in the* Ni₂Si *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 (Å²)
Sc(1)	4(c)	0.852 (2)	¼	0.074 (1)	1.3 (2)
Sc(2)	4(c)	0.983 (2)	¼	0.675 (1)	1.4 (2)
Pt	4(c)	0.257 (1)	¼	0.103 (1)	1.5 (1)

Table 2. *Interatomic distances in* Sc₂Pt *up to* 3.93 Å

The Sc atoms forming the surrounding trigonal prism are marked with asterisks.

Sc(1)–Pt	2.680 (14)	Sc(2)–Pt	2.724 (12)
–Pt	2.723 (11)	–2Pt	2.886 (09)
–2Pt	2.769 (07)	–Sc(1)	3.176 (16)
–Sc(2)	3.176 (16)	–2Sc(1)	3.235 (09)
–Sc(1)	3.213 (12)	–2Sc(1)	3.256 (13)
–2Sc(2)	3.235 (09)	–2Pt	3.296 (09)
–2Sc(2)	3.256 (13)	–Sc(1)	3.386 (12)
–Sc(2)	3.386 (12)	–2Sc(2)	3.518 (18)
–Pt	3.929 (14)	–2Sc(2)	3.652 (09)
Pt–Sc(1)	2.680 (14)		
–Sc(1)	2.723 (11)		
–Sc(2)	2.724 (12)		
–2Sc(1)*	2.769 (07)		
–2Sc(2)*	2.886 (09)		
–2Sc(2)*	3.296 (09)		
–Sc(1)	3.929 (14)		

powder pattern of a sample prepared with the starting composition Sc₂Pt showed the existence of a new phase.

However, at the time, the structure was not recognized as being isotypic with Ni₂Si and for this reason a single crystal of irregular size (mean diameter 80 µm) was isolated from the crushed sample and analysed on an automatic four-circle diffractometer. The refined orthorhombic lattice parameters are given in the *Abstract*. Systematic absences (0*kl* only with $k + l = 2n$, $hk0$ only with $h = 2n$) indicate $Pn2_1a$ and $Pnma$ as possible space groups. Scans in the θ–2θ mode were used out to a limit of $\sin\theta/\lambda = 0.7$ Å^{-1} to collect 433 intensities with monochromated Mo $K\alpha$ radiation. Intensities were corrected for absorption for a spherical crystal [μ(Mo $K\alpha$) = 65.6 mm^{-1}]. The structure was solved by direct methods, with *SINGEN* and *TANGEN* (XRAY system, 1976), in the space group $Pnma$. Positional and isotropic thermal parameters refined satisfactorily with *CRYLSQ* (XRAY system, 1976). The final R for 320 independent reflexions with $|F_o| > 3\sigma(F_o)$ is 10.9. A refinement in $Pn2_1a$ did not give any significant improvement in R.*

The final positional and isotropic thermal parameters are listed in Table 1, bond lengths in Table 2.

Discussion

The structure of Sc₂Pt, isotypic with Ni₂Si (Toman, 1952), is built up of linked Sc₆Pt trigonal prisms. A drawing of this structure type together with a detailed crystallochemical discussion has been given in a paper describing the isotypic phases found in rare-earth (and yttrium)–Pt phase diagrams (Le Roy, Moreau, Paccard & Parthé, 1978). A simple

---

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34382 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
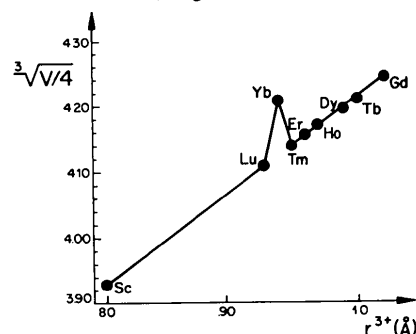

Fig. 1. Cube root of the volume associated with the formula unit *versus* trivalent ionic radii for Sc₂Pt and R₂Pt (R = rare earth) with Ni₂Si structure type.

method for finding out if the rare-earth elements (and Sc) in these compounds contribute an equal number of electrons to the bonding is to compare the volumes of the unit cells of the isotypic compounds. In Fig. 1 is plotted the cube root of the volume associated with the formula unit $[\equiv$ (volume of cell/4)$^{1/3}]$ *versus* the trivalent ionic radii of the rare-earth (or Sc) ions (Parthé, 1967). One can conclude that all rare-earth elements (and Sc) with the exception of Yb exhibit the same behaviour. The deviation for Yb_2Pt is probably correlated with the divalent character of Yb in this compound.

References

ALDRED, A. T. (1962). *Trans. Metall. Soc. AIME*, **224**, 1082–1083.

DWIGHT, A. E., DOWNEY, J. W. & CONNER, R. A. (1961). *Acta Cryst.* **14**, 75–76.

LE ROY, J., MOREAU, J. M., PACCARD, D. & PARTHÉ, E. (1978). *Acta Cryst.* **B34**, 9–13.

PARTHÉ, E. (1967). *Colloq. Int. CNRS*, **157**, 195–205.

TOMAN, K. (1952). *Acta Cryst.* **5**, 329–331.

XRAY system (1976). Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1979). B**35**, 1746

Synthesis and properties of low-dimensional materials. Edited by JOEL S. MILLER and ARTHUR J. EPSTEIN. Pp. 828, *Ann. NY Acad. Sci.* **313**. The New York Academy of Sciences, 1978. Price US$80.00.

This book contains the series of papers presented at a conference entitled *Synthesis and Properties of Low-Dimensional Materials*, held by The New York Academy of Sciences, June 13–16, 1977.

Besides an introduction by one of the editors, containing a valuable bibliography on the development of the subject, and appendices (common abbreviations, constants, author index), the book is divided into four sections: Part I: General Papers (16 papers), Part II: Organic Materials (17 papers), Part III: Inorganic Materials (17 papers), Part IV: Covalent Materials (10 papers).

The general papers of Part I present a very good introduction to some of the main topics of the subject from the chemical and the physical points of view, while the more specialized contributions of Parts II–IV, reporting mostly experimental work, give insight into recent research ac-

tivities. Altogether this volume contains abundant and very interesting chemical and physical information.

Materials of so-called low dimensionality are actually three-dimensional substances which are highly anisotropic with respect to some physical properties. Some of these have been known to chemists for a long time. In the last two decades, however, physicists have evaluated the unique properties arising from cooperative interactions within linear chains or layers. Thus theoretical and experimental work on physical properties, especially those associated with cooperative phenomena of highly anisotropic conducting materials, has mushroomed in the last few years, stimulating also the efforts of inorganic and organic chemists to synthesize new substances of this class. Therefore the whole spectrum of research in this field has become very interdisciplinary, rendering it more and more difficult to survey it. Certainly this book, which is very well equipped from the technical point of view, can help to remedy these difficulties.

H. BOLLER
Institut für Physikalische Chemie der Universität Wien
Währingerstrasse 42
A-1090 Wien
Austria