

Table 2. *Interatomic distances* (Å)

Pt—Si	2.456	(3 ×)	Mg—Mg	2.796	(4) (3 ×)
—Mg	2.803	(6) (2 ×)	—Pt	2.803	(6)
—Mg	2.861	(3) (6 ×)	—Pt	2.861	(3) (3 ×)
Si—Pt	2.456	(3 ×)	—Si	2.861	(3) (3 ×)
—Mg	2.861	(3) (6 ×)	—Mg	2.935	(9)
	3.727	(5) (6 ×)			

The structure of Mg<sub>2</sub>PtSi is an ordered ternary variant of the Na<sub>3</sub>As structure (Brauer & Zintl, 1937). The lateral Pt—Si distance (2.456 Å) is significantly shorter than the Pt—Mg distances (mean value 2.846 Å). As a consequence, the axial ratio ( $c/a = 2.0122$ ) is definitely higher than that for the binary compounds with Na<sub>3</sub>As structure, which is remarkably constant at  $1.769 \pm 0.03$  (Pearson, 1972).

**Related literature.** No structural details for ternary Mg—Pt—Si compounds could be found in the literature. For the parent compound Mg<sub>3</sub>Pt see Ferro & Rambaldi (1960). The geometrical features of the

Na<sub>3</sub>As structure have been discussed by Pearson (1972).

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## ErVO<sub>4</sub>-II, a Scheelite-Type High-Pressure Modification of Erbium Orthovanadate

BY KLAUS-JÜRGEN RANGE\* AND HELMUT MEISTER

*Institut für Anorganische Chemie der Universität, Universitätstr. 31, D-8400 Regensburg,  
Federal Republic of Germany*

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**Abstract.**  $M_r = 282.20$ , tetragonal,  $I4_1/a$ ,  $a = 5.003$  (1),  $c = 11.143$  (2) Å,  $V = 278.91$  Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 6.72$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 1.58$  mm<sup>-1</sup>,  $F(000) = 492$ ,  $T = 298$  K. The structure was refined to  $R = 0.035$ ,  $wR = 0.037$  for 478 absorption-corrected observed reflections. The high-pressure modification ErVO<sub>4</sub>-II, prepared at 40 kbar and 1525 K, crystallizes with the scheelite-type structure and comprises VO<sub>4</sub> tetrahedra [V—O = 1.722 (3) Å] and ErO<sub>8</sub> dodecahedra [Er—O = 2.333 (3) (4 ×), 2.368 (3) Å (4 ×)].

**Experimental.** The normal-pressure-phase ErVO<sub>4</sub>-I used as starting material was synthesized from a stoichiometric mixture of Er<sub>2</sub>O<sub>3</sub> and V<sub>2</sub>O<sub>5</sub> in an argon-flushed, evacuated, sealed quartz ampoule (1250 K, 12 h). Guinier patterns showed the product to be single-phase ErVO<sub>4</sub>-I with zircon-type structure. High-pressure experiments were carried out in a modified Belt-type apparatus (Range & Leeb, 1975),

using platinum or pyrophyllite as crucible material. At 35 kbar, 1000–1500 K, ErVO<sub>4</sub>-I transforms completely into a quenchable high-pressure modification (ErVO<sub>4</sub>-II). Single crystals could be isolated after reaction of a 1:1 mixture of ErVO<sub>4</sub> and V<sub>2</sub>O<sub>5</sub> (acting as flux material) at 40 kbar, 1575 K.

An irregularly shaped crystal fragment (approximate dimensions 0.06 × 0.08 × 0.08 mm) was used for data collection on an Enraf–Nonius CAD-4 diffractometer (Mo  $K\alpha$ , graphite monochromator in incident beam). Lattice parameters have been refined from  $2\theta$  values of 25 reflections in the range  $9.3 \leq \theta \leq 17.2^\circ$ . Intensities were measured for  $2 \leq \theta \leq 45^\circ$ ;  $\omega$ - $2\theta$  scan technique, scan width  $(2.0 + 0.4 \tan \theta)^\circ$ . Three standard reflections indicated no loss of intensity throughout data collection. An experimental correction for absorption was applied, based on  $\psi$  scans; transmission factors varied between 85.5 and 99.4%. Merging of the 680 collected intensities  $[(\sin \theta)_{\max} / \lambda = 0.995 \text{ \AA}^{-1}; 0 \leq h \leq 9, 0 \leq k \leq 9, 0 \leq l \leq 22]$  gave 519 unique reflections ( $R_{\text{int}} = 0.018$ ), of which 478 with  $I > 1.0\sigma(I)$  were considered as

\* To whom correspondence should be addressed.

observed and used for all calculations (program system *SHELX76*; Sheldrick, 1976).

The structure was solved by routine direct methods. In the least-squares refinement  $|F|$  magnitudes were used to refine an overall scale factor, atomic coordinates and anisotropic temperature factors. Final  $R = 0.035$ ,  $wR = 0.037$ ,  $w^{-1} = \sigma^2(F) + 0.0075|F|^2$  and  $(\Delta/\sigma)_{\max} < 0.001$  for 14 variables. Max. features in the final  $\Delta\rho$  map ( $\pm 2 e \text{ \AA}^{-3}$ ) near the heavy atoms, obviously resulting from insufficient absorption correction by  $\psi$  scans. Atomic scattering factors and  $f'$ ,  $f''$  values were taken from *International Tables for X-ray Crystallography* (1974). Bond distances and angles were calculated using the program *SADIAN* (Baur & Wenninger, 1969). Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1, derived bond distances in Table 2.\* ErVO<sub>4</sub>-II crystallizes with the scheelite (CaWO<sub>4</sub>) structure (Dickinson, 1920; Zalkin & Templeton, 1964). The structure comprises VO<sub>4</sub> tetrahedra [V—O = 1.722 (3) Å] and ErO<sub>8</sub> dodecahedra [Er—O = 2.333 (3) (4 ×), 2.368 (3) Å (4 ×)].

**Related literature.** The zircon-type structure of the normal-pressure-phase ErVO<sub>4</sub>-I has been refined by Patscheke, Fuess & Will (1968). The *P,T*-phase diagrams for rare-earth orthovanadates obtained by Stubican & Roy (1963*a,b*) using an opposed-anvil high-pressure apparatus are definitely wrong, most probably due to kinetic problems at the rather low temperatures investigated (Range & Meister, 1990).

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\* Lists of structure factors, anisotropic temperature factors and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52562 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and equivalent isotropic temperature factors (Å<sup>2</sup>)*

$U_{\text{eq}}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U_{\text{eq}}$
Er	0	$\frac{1}{2}$	$\frac{1}{2}$	0.0030 (1)
V	0	$\frac{1}{2}$	$\frac{1}{2}$	0.0035 (5)
O	0.1460 (6)	0.5050 (6)	0.2054 (3)	0.0051 (9)

Origin at centre ( $\bar{1}$ ).

Table 2. *Interatomic distances (Å)*

VO <sub>4</sub> tetrahedron		ErO <sub>8</sub> dodecahedron	
V—O	1.722 (3) 4 ×	Er—O	2.333 (3) 4 ×
O—O	2.745 (5) 4 ×		2.368 (3) 4 ×
	2.940 (4) 2 ×	O—O	2.692 (4) 4 ×
			2.843 (4) 4 ×
			2.854 (4) 2 ×
			2.881 (5) 2 ×
			2.882 (5) 2 ×
			3.534 (4) 4 ×

the Fonds der Chemischen Industrie is gratefully acknowledged.

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## Structure of Bis( $\eta^6$ -*N,N*-dimethylaniline)chromium(0)

BY V. M. LYNCH, M. O. YOON, J. J. LAGOWSKI AND B. E. DAVIS

*Department of Chemistry, University of Texas at Austin, Austin, TX 78712, USA*

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**Abstract.** [Cr(C<sub>6</sub>H<sub>11</sub>N)<sub>2</sub>],  $M_r = 294.36$ , orthorhombic, *Pbca*,  $a = 16.871$  (8),  $b = 10.194$  (2),  $c = 8.185$  (3) Å,  $V = 1407.7$  (9) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.39$  g cm<sup>-3</sup>,  $\mu = 0108-2701/90/061094-03\$03.00$

7.806 cm<sup>-1</sup>, Mo  $K\alpha$  radiation,  $\lambda = 0.7107$  Å,  $F(000) = 624$ ,  $T = 163$  K,  $R = 0.0546$  for 831 reflections [ $F_o \geq 4\sigma(F_o)$ ]. The Cr atom lies on an inversion center.

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