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Letter

Crystal structure of the compound $Ce_3Pt_4Ge_6$

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Abstract

The crystal structure of the compound $Ce_3Pt_4Ge_6$ has been determined by X-ray analysis of a single crystal (Enraf–Nonius CAD-4 autodiffractometer, Mo Kα radiation, 208 independent reflections, $R=0.033$ in the anisotropic approximation). This structure has been found to belong to a new structural type: space group *Bmmb*, $a=4.419(1)$ Å, $b=4.422(1)$ Å, $c=26.222(5)$ Å, $Z=2$. The coordination polyhedra of cerium atoms have 19 and 21 apexes; those of platinum are tetragonal antiprisms with two additional atoms and trigonal prisms with four additional atoms; those of germanium are trigonal prisms with three additional atoms and distorted cubo-octahedra.

The interaction of cerium with platinum and germanium has not been studied systematically. In the literature the data on some ternary compounds of the Ce–Pt–Ge system are given: $CePt_2Ge_2$ (the structural type $CeGa_2Al_2$) [1], $CePtGe_2$ (the structural type $NdIrGe_2$) [2] and $CePtGe_3$ (space group *Pnnm*) [3].

In the present paper the Ce–Pt–Ge system is studied at 870 K. A new ternary compound $Ce_3Pt_4Ge_6$ has been found; the determination of its structure is described below.

TABLE 1

Atomic position parameters of $Ce_3Pt_4Ge_6$

Atom	*G* (%)	*x/a*	*y/b*	*z/c*	B_i
Ce1	100	0	3/4	0.3425(1)	0.40(7)
Ce2	52(3)	0	1/4	0.0292(2)	0.23(9)
Pt1	100	0	1/4	0.43714(9)	0.24(5)
Pt2	100	0	3/4	0.20423(9)	0.76(6)
Ge1	100	0	1/4	0.2505(2)	0.44(14)
Ge2	100	0	3/4	0.1102(2)	0.9(2)
Ge3	51(3)	0.201(2)	1/4	0.5356(3)	0.60(13)

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TABLE 2

Anisotropic parameters for $Ce_3Pt_4Ge_6$[a]

Atom	B_{11}	B_{22}	B_{33}
Ce1	0.59(12)	0.26(14)	0.34(10)
Pt1	0.18(10)	0.23(10)	0.32(7)
Pt2	0.74(11)	0.87(12)	0.67(9)
Ge1	0.3(2)	0.6(3)	0.5(2)
Ge2	0.7(2)	1.5(3)	0.4(2)

[a]$B_{12}=B_{13}=B_{23}=0$.

TABLE 3

Interatomic distances in the structure of $Ce_3Pt_4Ge_6$[a]

Atom	δ (Å)	Coordination number	Atom	δ (Å)	Coordination number
Ce1–2 Ce1	4.422(1)	21	Pt2–2 Ge1	2.509(3)	11
2 Ce1	4.419(1)		2 Ge2	2.464(7)	
Ce2	4.025(6)				
Pt2	3.625(4)		Ge1–2 Ce1	3.273(5)	12
4 Ge2	3.363(3)		4 Ge1	3.126	
4 Pt2	3.357(2)		2 Ce1	3.289(5)	
2 Pt1	3.324(3)		2 Pt2	2.522(3)	
Ge3	3.318(8)		2 Pt2	2.509(3)	
2 Ge1	3.289(5)				
2 Ge1	3.273(5)		Ge2–4 Ce1	3.363(3)	9
			2 Ce2	3.067(6)	
Ce2–2 Ce2	4.422(1)	19	2 Pt1	2.535(3)	
2 Ce1	4.025(6)		Pt2	2.464(7)	
Ge2	3.657(9)				
2 Pt1	3.273(5)		Ge2–Ce2	3.657(9)	12
4 Pt1	3.248(2)		4 Ce1	3.363(3)	
2 Ge3	3.104(9)		4 Ge3	3.234(7)	
4 Ge3	3.086(6)		2 Pt1	2.535(3)	
2 Ge2	3.067(6)		Pt2	2.464(7)	
Pt1–2 Ce1	3.324(3)	10	Ge3–Ce1	3.318(8)	12
Ce2	3.273(5)		2 Ge2	3.234(7)	
Ge3	2.732(8)		Ce2	3.104(9)	
2 Ge2	2.535(3)		2 Ce2	3.086(6)	
2 Ge3	2.488(4)		2 Ge3	2.895(7)	
2 Ce2	3.248(2)		Pt1	2.732(8)	
			Ge3	2.64(1)	
Pt2–Ce1	3.625(4)		2 Pt1	2.488(4)	
4 Ce1	3.357(2)				
2 Ge1	2.522(3)				

[a]The difference in the coordination numbers of the Ge2 atoms is connected with the Ce2 and Ge3 structure defectiveness.

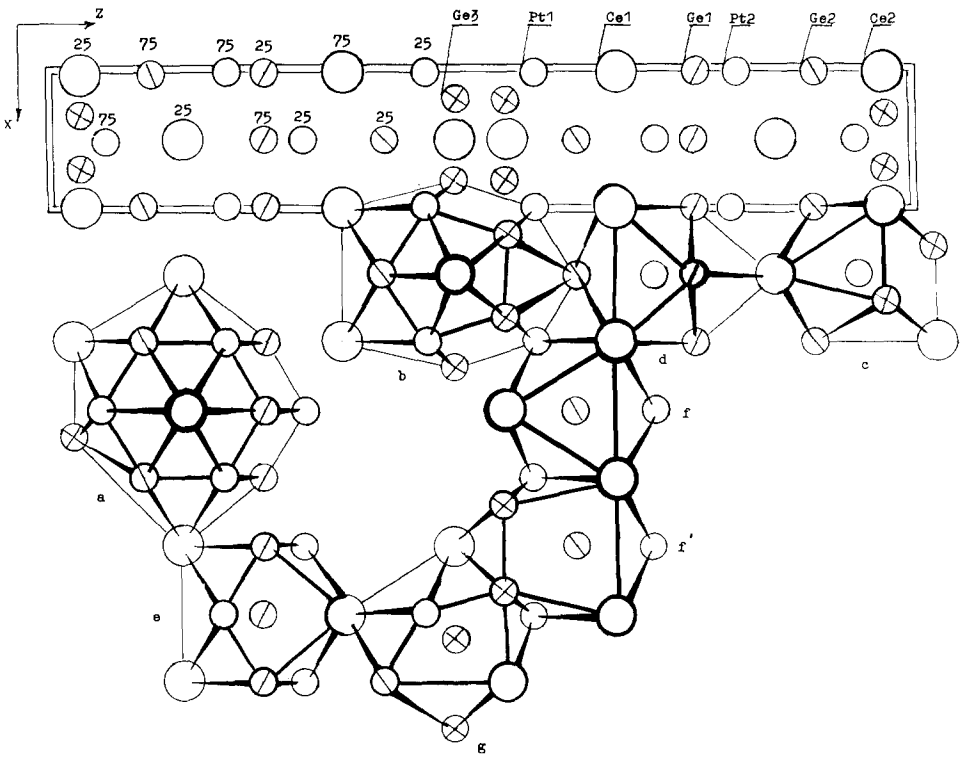

Fig. 1. Projection of a $Ce_3Pt_4Ge_6$ unit cell on the *XZ* plane and coordination polyhedra of the cerium (a,b), platinum (c,d) and germanium (e–g) atoms.

A single crystal in the form of a plate suitable for the X-ray analysis was taken from an ingot of 1 g prepared by melting the starting mixture in an arc furnace in an argon atmosphere followed by annealing at 870 K for 600 h. The purity of the starting metals was better than 99.9%.

A single crystal was examined photographically (RKV-86 and RGNS-2 cameras, Mo Kα and Cu Kα radiation) and then using an Enraf–Nonius CAD-4 autodiffractometer (Mo Kα radiation, flat graphite monochromator, θ–2θ scanning, $2\theta_{max} = 70°$). The lattice parameters are as follows: $a = 4.419(1)$ Å, $b = 4.422(1)$ Å, $c = 26.222(5)$ Å. The calculations, using 208 independent reflections with $I \geqslant 2\sigma I$, were performed with CSD programmes [4] on an 'Elektronica MC 0585' computer.

The structure of $Ce_3Pt_4Ge_6$ was determined by direct methods in the space group *Bmmb*. The atomic position parameters were refined in the anisotropic approximation down to $R = 0.033$ and the corresponding values are listed in Tables 1 and 2. The interatomic distances are listed in Table 3. The structure is a novel type of structure for ternary intermetallic compounds. It is characterized by partial occupation of sites by cerium and germanium atoms, *i.e.* two atoms Ce2 and four atoms Ge3 could be simultaneously placed in one unit cell.

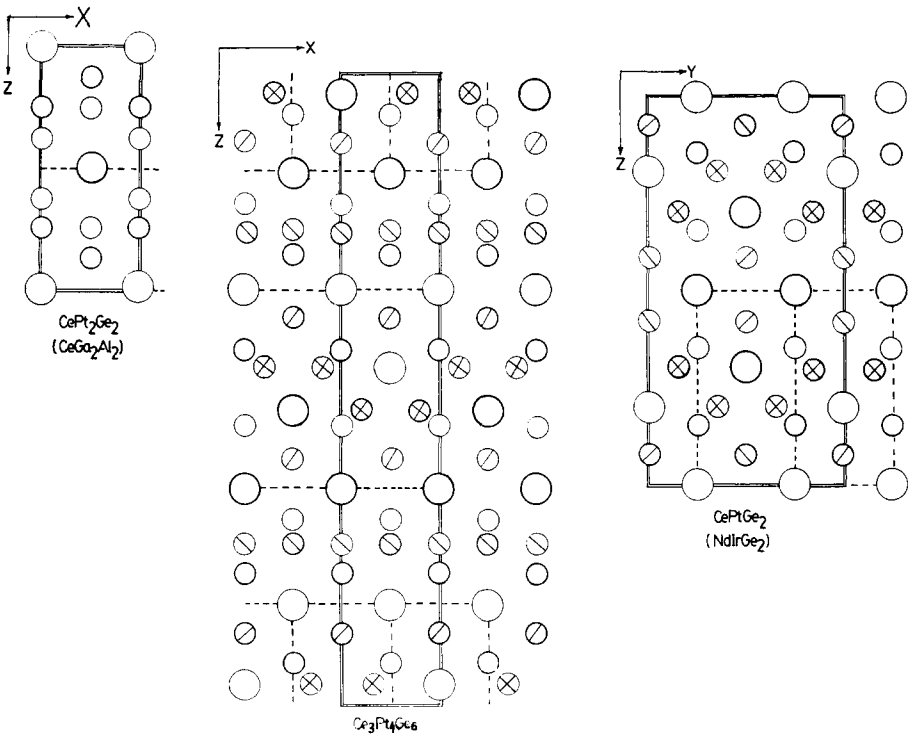

Fig. 2. Interrelation between $CePt_2Ge_2$, $Ce_3Pt_4Ge_6$ and $CePtGe_2$ structures.

The projection of a unit cell of the $Ce_3Pt_4Ge_6$ structure on the *XZ* plane and the coordination polyhedra of the atoms are given in Fig. 1. For the cerium atoms, polyhedra with 21 apexes, Ce1[$Ce_5Pt_7Ge_9$] (Fig. 1a), and 19 apexes, Ce2[$Ce_4Pt_6Ge_9$] (Fig. 1b), are typical. The platinum atom polyhedra are trigonal prisms with four additional atoms, Pt1[Ce_5Ge_5] (Fig. 1c), and tetragonal antiprisms with two additional atoms, Pt2[Ce_5Ge_5] (Fig. 1d). The germanium coordination polyhedra are deformed cubo-octahedra, Ge1[$Ce_4Pt_4Ge_4$] (Fig. 1e), Ge2[$Ce_5Pt_3Ge_4$ (Fig. 1f') and Ge3[$Ce_4Pt_3Ge_5$] (Fig. 1g), and trigonal prisms with three additional atoms, Ge2[Ce_6Pt_3] (Fig. 1f).

In the concentration triangle of the Ce–Pt–Ge system the compound $Ce_3Pt_4Ge_6$ is located between $CePt_2Ge_2$ and $CePtGe_2$. Analysis of the determined structure shows $Ce_3Pt_4Ge_6$ to be a combination of these two structures. The relationship between the $CePt_2Ge_2$, $Ce_3Pt_4Ge_6$ and $CePtGe_2$ structures is shown in Fig. 2. The marked fragment in the $CePtGe_2$ (structural type $NdIrGe_2$ [5]) has the composition $Ce_2Pt_2Ge_4$. The composition $2Ce_3Pt_4Ge_6$ is the result of the next fragment packing: $\frac{1}{2}Ce_2Pt_2Ge_4 + CePt_2Ge_2 + Ce_2Pt_2Ge_4 + CePt_2Ge_2 + \frac{1}{2}Ce_2Pt_2Ge_4$. Interatomic distances in the structure $Ce_3Pt_4Ge_6$ are in the range typical of intermetallic compounds.

The new structural type $Y_3Pt_4Ge_6$ (m) described earlier in ref. 6 is monoclinically deformed $Ce_3Pt_4Ge_6$ (p) with $a(m) \approx 2a(p)$, $b(m) \approx b(p)$ and $c(m) \approx \frac{1}{2} c(p)$. Both structural types $Y_3Pt_4Ge_6$ and $Ce_3Pt_4Ge_6$ consist of identical fragments of the $CeAl_2Ga_2$ and $NdIrGe_2$ structures.

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