Journal of Alloys and Compounds, 189 (1992) L11–L13
JALCOM 373

Letter

Crystal structure of the compound $Ce_2Pt_7Ge_4$

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(Received May 12, 1992)

The crystal structure of the compound $Ce_2Pt_7Ge_4$ was determined by X-ray analysis of a single crystal (autodiffractometer DARTCH, Mo Kα radiation, 301 independent reflections, the *R*-factor is 0.0357 in isotropic approximation). This structure was found to belong to a new structural type: space group *Pnma*, $a = 19.866(9)$ Å, $b = 4.089(2)$ Å, $c = 11.439(4)$ Å, $Z = 4$. The coordination polyhedra of cerium atoms have 22 and 21 apexes, those of platinum are distorted cubo-octahedra and those of germanium are trigonal prisms with additional atoms.

The interaction of cerium with platinum and germanium has not been studied over the whole range of concentrations. The literature gives data on some ternary compounds of the Ce–Pt–Ge system: $CePt_2Ge_2$ (structural type $CeGa_2Al_2$) [1], $CePtGe_2$ (structural type $NdIrGe_2$) [2], $CePtGe_3$ (space group *Pnnm*) [3], $Ce_3Pt_4Ge_6$ (space group *Bmmb*) [4].

The present paper presents data on the new ternary compound $Ce_2Pt_7Ge_4$ which has been found in the Ce–Pt–Ge system at 870 K; the determination of its structure is described below.

A single crystal suitable for 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 a DARTCH autodiffractometer (Mo Kα radiation, flat graphite monochromator, θ–2θ scanning, $2\theta_{max} = 60°$). The lattice parameters are as follows: $a = 19.866(9)$ Å, $b = 4.089(2)$ Å, $c = 11.439(4)$ Å. Calculations using 301 independent reflections with $I \geqslant 2\sigma I$ were performed with the CSD-programs [5] on an IBM PC AT/286 computer.

The structure of $Ce_2Pt_7Ge_4$ was determined by direct methods to belong to the space group *Pnma*. The atomic position parameters were refined in isotropic approximation down to $R = 0.0357$ and the corresponding values are listed in Table 1. The interatomic distances are listed in Table 2. The structure is a novel type for ternary intermetallic compounds.

The projection of a unit cell of the $Ce_2Pt_7Ge_4$ structure onto the *XZ*-plane and the coordination polyhedra of the atoms are given in Fig. 1. For cerium atoms, polyhedra with 22 apexes – $Ce1[Ce_3Pt_{12}Ge_7]$ (Fig. 1(a)) – and with 21 apexes – $Ce2[Ce_3Pt_{11}Ge_7]$ (Fig. 1(b)) – are typical. The platinum atom polyhedra are distorted cubo-octahedra: $Pt1[Ce_3Pt_5Ge_4]$ (Fig. 1(c)), $Pt2[Ce_3Pt_6Ge_3]$ (Fig. 1(d)), $Pt3[Ce_3Pt_6Ge_3]$ (Fig. 1(e)), $Pt4[Ce_2Pt_7Ge_4]$ (Fig. 1(f)), $Pt5[Ce_4Pt_4Ge_4]$ (Fig. 1(g)), $Pt6[Ce_3Pt_5Ge_4]$ (Fig. 1(h)) and $Pt7[Ce_5Pt_3Ge_4]$ (Fig. 1(i)). Trigonal prisms with additional atoms are typical for germanium atoms: $Ge1[Ce_2Pt_7]$ (Fig. 1(j)), $Ge2[Ce_3Pt_7]$ (Fig. 1(k)), $Ge3[Ce_4Pt_5]$ (Fig. 1(l)) and $Ge4[Ce_2Pt_7]$ (Fig. 1(m)). The compound $Ce_2Pt_7Ge_4$ was

TABLE 1. The atomic position parameters of $Ce_2Pt_7Ge_4$

Atom	*G* (%)	*x/a*	*y/b*	*z/c*	B_i
Ce1	100	0.2801(3)	1/4	0.0122(4)	0.59(9)
Ce2	100	0.4719(2)	1/4	0.2437(4)	0.47(8)
Pt1	100	0.0351(2)	3/4	0.0604(3)	0.65(7)
Pt2	100	0.2139(2)	3/4	0.1836(3)	0.73(7)
Pt3	100	0.8390(2)	1/4	0.0527(3)	0.54(6)
Pt4	100	0.1293(2)	1/4	0.1198(2)	0.51(7)
Pt5	100	0.5412(2)	3/4	0.0466(2)	0.61(7)
Pt6	100	0.6336(2)	1/4	0.1329(2)	0.58(7)
Pt7	100	0.3465(2)	3/4	0.2449(3)	0.76(6)
Ge1	100	0.5942(5)	3/4	0.2466(8)	0.8(2)
Ge2	100	0.7560(6)	1/4	0.2065(8)	1.0(2)
Ge3	100	0.4123(5)	3/4	0.0631(7)	0.5(2)
Ge4	100	0.9144(6)	3/4	0.0775(7)	0.5(2)

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TABLE 2. Interatomic distances in the structure of $Ce_2Pt_7Ge_4$

Atoms	δ (Å)	Coordination number
Ce1–2Pt2	3.124(6)	22
Ce1–2Pt6	3.142(7)	
Ce1–2Pt3	3.213(9)	
Ce1–Pt4	3.240(11)	
Ce1–Ge2	3.253(11)	
Ce1–2Ge2	3.310(9)	
Ce1–2Ge3	3.379(12)	
Ce1–2Pt7	3.607(7)	
Ce1–Pt5	3.614(11)	
Ce1–Pt2	3.761(7)	
Ce1–Ge1	3.873(12)	
Ce1–Pt7	3.959(9)	
Ce1–Ge4	3.999(15)	
Ce1–2Ce1	4.089(2)	
Ce1–Ce2	4.640(10)	
Ce2–2Ge4	3.109(9)	21
Ce2–2Ge3	3.138(9)	
Ce2–2Ge1	3.176(11)	
Ce2–2Pt7	3.222(8)	
Ce2–2Pt1	3.284(6)	
Ce2–Pt5	3.331(6)	
Ce2–2Pt5	3.340(6)	
Ce2–Pt6	3.454(10)	
Ce2–Pt4	3.495(10)	
Ce2–Pt3	3.522(9)	
Ce2–Pt1	3.625(7)	
Ce2–2Ce2	4.089(2)	
Ce2–Ce3	4.195(12)	
Ce2–Ce1	4.640(10)	
Pt1–Ge4	2.406(15)	12
Pt1–Ge1	2.500(11)	
Pt1–2Ge4	2.770(8)	
Pt1–Pt3	2.816(10)	
Pt1–2Pt1	2.835(6)	
Pt1–2Pt4	2.853(7)	
Pt1–2Ce2	3.284(6)	
Pt1–Ce2	3.625(7)	
Pt2–Ge1	2.508(14)	12
Pt2–2Ge2	2.542(7)	
Pt2–Pt7	2.727(10)	
Pt2–2Pt4	2.746(7)	
Pt2–Pt3	2.899(7)	
Pt2–2Ce1	3.124(6)	
Pt2–2Pt6	3.336(6)	
Pt2–Ce1	3.761(7)	
Pt3–Ge2	2.411(12)	12
Pt3–2Ge4	2.551(9)	
Pt3–Pt1	2.816(10)	
Pt3–Pt2	2.899(7)	
Pt3–2Pt4	2.911(5)	
Pt3–2Pt7	3.093(5)	
Pt3–2Ce1	3.213(9)	
Pt3–Ce2	3.522(9)	
Pt4–Ge4	2.418(10)	13
Pt4–2Ge1	2.645(7)	

Atoms	δ (Å)	Coordination number
Pt4–2Pt2	2.746(7)	13
Pt4–Pt6	2.830(6)	
Pt4–2Pt1	2.853(7)	
Pt4–2Pt3	2.911(5)	
Pt4–Ge2	3.208(13)	
Pt4–Ce1	3.240(11)	
Pt4–Ce2	3.495(10)	
Pt5–Ge1	2.519(11)	12
Pt5–Ge3	2.566(15)	
Pt5–2Ge3	2.570(7)	
Pt5–2Pt5	2.827(7)	
Pt5–2Pt6	2.920(7)	
Pt5–Ce2	3.331(6)	
Pt5–2Ce2	3.340(6)	
Pt5–Ce1	3.614(11)	
Pt6–Ge3	2.420(10)	10
Pt6–2Ge1	2.547(7)	
Pt6–Ge2	2.574(14)	
Pt6–Pt4	2.830(6)	
Pt6–2Pt5	2.920(7)	
Pt6–2Ce1	3.142(7)	
Pt6–Ce2	3.454(10)	
Pt7–Ge4	2.438(11)	12
Pt7–Ge3	2.457(11)	
Pt7–Pt2	2.727(10)	
Pt7–2Ge2	2.778(10)	
Pt7–2Pt3	3.093(5)	
Pt7–2Ce2	3.222(8)	
Pt7–2Ce1	3.607(7)	
Pt7–Ce1	3.959(9)	
Ge1–Pt1	2.500(11)	9
Ge1–Pt2	2.508(14)	
Ge1–Pt5	2.519(11)	
Ge1–2Pt6	2.547(7)	
Ge1–2Pt4	2.645(7)	
Ge1–2Ce2	3.176(11)	
Ge2–Pt3	2.411(12)	10
Ge2–2Pt2	2.542(7)	
Ge2–Pt6	2.574(14)	
Ge2–2Pt7	2.778(10)	
Ge2–Pt4	3.208(13)	
Ge2–Ce1	3.253(11)	
Ge2–2Ce1	3.310(9)	
Ge3–Pt6	2.420(10)	9
Ge3–Pt7	2.457(11)	
Ge3–Pt5	2.566(15)	
Ge3–2Pt5	2.570(7)	
Ge3–2Ce2	3.138(9)	
Ge3–2Ce1	3.379(12)	
Ge4–Pt1	2.406(15)	9
Ge4–Pt4	2.418(10)	
Ge4–Pt7	2.438(11)	
Ge4–2Pt3	2.551(9)	
Ge4–2Pt1	2.770(8)	
Ge4–2Ce2	3.109(9)	

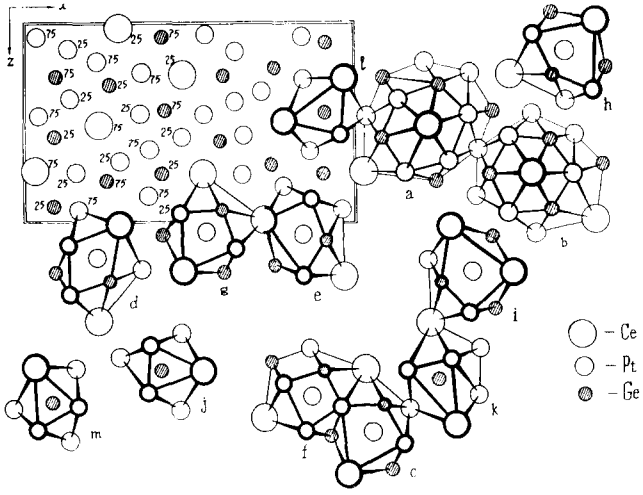

Fig. 1. Projection of a $Ce_2Pt_7Ge_4$ unit cell onto the XZ plane and coordination polyhedra of the cerium (a), (b), platinum (c)–(i) and germanium (j)–(m) atoms.

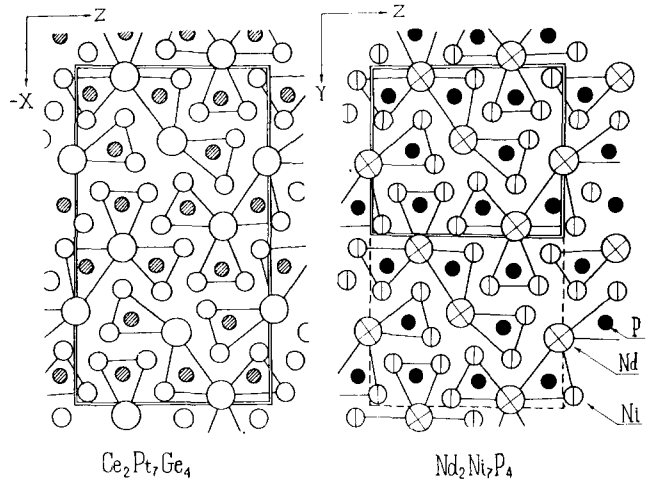

Fig. 2. The interrelation between $Ce_2Pt_7Ge_4$ and $Nd_2Ni_7P_4$ structures.

found to belong to the structural class with trigonal prism coordination of the lesser-volume atoms [6].

The atoms of cerium and platinum produce trigonal prisms in which the germanium atoms are located. Three trigonal prisms combine with each other owing to a common ribbon to give a typical "star". The fourth prism has a common ribbon with one of these prisms. This fragment corresponds to the composition $Ce_2Pt_7Ge_4$. Prisms packing in the $Ce_2Pt_7Ge_4$ structure are shown in Fig. 2. The distance between two similarly oriented "star" fragments is $\frac{1}{2}a$ parameter.

The crystal structure of $Ce_2Pt_7Ge_4$ (I) is similar to that of the compound $Nd_2Ni_7P_4$ (II) (space group $Pmn2_1$) [7] ($a_I \approx 2b_{II}$, $b_I \approx a_{II}$, $c_I \approx c_{II}$), in which packing of the same "stars" is observed.

Interatomic distances in the structure $Ce_2Pt_7Ge_4$ are in the range typical of intermetallic compounds.

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