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Crystal structure of $Sr₂CdPt₂$ containing linear platinum chains

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The ternary intermetallic title phase, distrontium cadmium diplatinum, was prepared from stoichiometric amounts of the elements at 1123 K for one day. The crystal structure adopts the orthorhombic $Ca₂GaCu₂$ structure type in space group *Immm*. Its main features are characterized by linear $(Pt-Pt\cdots Pt-Pt)_n$ chains that are aligned along [010] and condensed through cadmium atoms forming Cd-centred Pt₂Cd_{2/2} rectangles to build up sheets parallel to (001). These sheets are connected to each other via alternating (001) sheets of strontium atoms along [001]. The strontium sheets consists of corrugated S_{T_4} units that are condensed to each other through edge-sharing parallel to [100].

1. Chemical context

A large number of transition metal-based ternary intermetallic phases have been studied in terms of metal–metal interactions and structure–property relationships (Corbett, 2010). Exploratory synthetic approaches in systems A/Cd/Pt $(A = \text{alkaline earth metal})$ have revealed a great compositional and structural diversity. The calcium phase $Ca_6Cd_{16}Pt_8$ contains a three-dimensional array of isolated $Cd₈$ tetrahedral stars (TS) and a face-centred cube of $Pt@Ca₆$ octahedra (Samal et al., 2013) whilst the structure of $Ca_6Cd_{11}Pt$ crystallizes in its own structure type consisting of apically interbonded $Cd₇$ pentagonal bipyramids and five-membered rings of Ca atoms (Gulo et al., 2013). The strontium phase $SrCd_4Pt_2$ is made up of chains of edge-sharing $Cd₄$ tetrahedra bridged by four-bonded Sr atoms (Samal et al., 2013) and SrCdPt presents six-membered rings of Sr atoms in a chair conformation (Gulo & Köhler, 2014). The barium phase $BaCd₂Pt$ exhibits zigzag chains of Ba atoms and Pt-centred boat and anti-boat conformations formed by six-membered rings of Cd atoms (Gulo & Köhler, 2015). The Pt-based ternary intermetallic compounds with general formula $A_2X\text{Pt}_2$ ($A = \text{alka}$ line-earth or rare-earth metal; $X =$ diel, triel, or tetrel element) adopt five different structure types. $Sr₂InPt₂ (Muts *et al.*, 2007)$ crystallizes in the monoclinic Ca₂Ir₂S type (Schoolaert & Jung, 2002), Pu_2SnPt_2 (Pereira et al., 1997) in the tetragonal $Mo₂FeB₂$ type (Gladyshevskii et al., 1996) while $U₂CdPt₂$ has its own structure type (Gravereau et al., 1994). $Ce₂CdPt₂$ (Pöttgen *et al.*, 2000) adopts the tetragonal U_3Si_2 type (Zachariasen, 1948), and Ca₂CdPt₂ (Samal & Corbett, 2012) the orthorhombic $Ca₂GaCu₂$ type (Fornasini & Merlo, 1988).

In this article we present the crystal structure of the novel intermetallic phase Sr_2CdPt_2 containing linear (Pt-Pt \cdots Pt- $Pt)$ _n chains as a principal structural motif.

Figure 1

Coordination of strontium, cadmium, and platinum atoms in $Sr₂CdPt₂$. Displacement ellipsoids are displayed at the 90% probability level.

2. Structural commentary

The ternary intermetallic title phase adopts the orthorhombic $Ca₂GaCu₂$ structure type (Fornasini & Merlo, 1988) with the Ca, Ga, and Cu sites replaced by Sr, Cd, and Pt sites, respectively. The three atoms occupy three independent sites in the unit cell. The Sr atom resides on a special position with site symmetry $mm2$ (Wyckoff site 4 j), the Cd atom occupies a special positions with site symmetry mmm (2 a) and the Pt atom is on a special positions with site symmetry $m2m$ (4 h). In the two structures, the transition metals (platinum and copper, respectively) occupy the same positions. In contrast, in the structure of $SrCd₄Pt₂$ (Samal et al., 2013) which is isotypic with $ZrFe₄Si₂$ (Yarmolyuk et al., 1975), the transition metals (platinum and iron, respectively) occupy different positions and the Pt atoms reside on the respective Si sites because silicon and platinum atoms are the most electronegative atoms in the two systems. The new phase $Sr₂CdPt₂$ contains 26 valence electrons and, as already mentioned, is isotypic with

Figure 2 Projection of the crystal structure of Sr_2CdPt_2 approximately along the b axis.

 $Ca₂GaCu₂$. However, in comparison the structure of $Sr₂CdPt₂$ is appreciably distorted along the platinum chains, presumably because $Ca₂GaCu₂$ contains much smaller Cu atoms and a larger valence electron count of 29. Coordination spheres of each atomic site in the title structure are illustrated in Fig. 1. The Sr atom is coordinated by five other Sr, four Cd, and four Pt atoms. The $Sr-Sr$ bond lengths vary from 3.674 (3) to 3.854 (1) \AA , the Sr-Cd distances range from 3.490 (1) to 3.577 (1) \AA , whereas the Sr-Pt values vary only slightly, from 3.188 (1) to 3.231 (1) \AA . Six Sr atoms construct a squareplanar pyramid, $Sr@Sr₅$. The existence of $Sr-Sr$ strong bonds is observable in SrCdPt (Gulo & Köhler, 2014) but not in $SrCd₄Pt₂$ (Samal *et al.*, 2013). The Cd atom exhibits a coordination number of twelve and has eight Sr and four Pt atoms in its environment with $Cd-Pt$ distances of 2.785 (1) Å. The Pt atom is surrounded by six Sr, two Cd and one Pt atoms with a Pt—Pt distance of 2.734 (1) A. This distance is slightly longer than those found in Ca₂CdPt₂ (2.659 Å; Samal & Corbett, 2012) or Sr_2InPt_2 (2.707 A; Muts *et al.*, 2007) but shorter than those in Pu₂SnPt₂ (Pereira et al., 1997), U₂CdPt₂ (Gravereau et al., 1994) or $Ce₂CdPt₂$ (Pöttgen et al., 2000). All other interatomic distances (Sr—Cd, Sr—Pt, and Cd—Pt) are in agreement with those found in some ternary compounds in $A/Cd/Pt$ systems $(A = \text{alkaline earth metal}).$

3. Packing features

Sr atoms are bound together into corrugated sheets consisting of edge-sharing Sr_4 -units. These sheets spread parallel to (001) and are linked by another $Sr-Sr$ bond of 3.674 (3) \AA along [001]. (Fig. 2). The crystal structure is also characterized by the existence of linear $(Pt-Pt\cdots Pt-Pt)_n$ chains along [010] with longer distances of $3.2010(14)$ Å between pairs of tightly

Figure 3

Projection of linear platinum chains that are aligned along the b axis and condensed *via* cadmium atoms forming $Pt_2Cd_{2/2}$ -rectangles in the *ab*plane

research communications

Table 1 Experimental details.

Computer programs: XSCANS (Bruker, 2001), SHELXS97 and SHELXL97 (Sheldrick, 2008) and DIAMOND (Brandenburg, 2010).

bound Pt—Pt dumbbells, a significant distortion in the direction of dimerization. The platinum chains are condensed into (001) sheets through Cd atoms, forming Cd-centred rectangles with composition $Pt_2Cd_{2/2}$ (Fig. 3). The $Pt_2Cd_{2/2}$ layers are stacked along [001] and are linked through the corrugated sheets of Sr atoms.

4. Database survey

A search of the Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds (Villars & Cenzual, 2015) for the Sr/Cd/Pt family of compounds returned two compounds only: $SrCd_4Pt_2$ (Samal et al., 2013) and $SrCdPt$ (Gulo & Köhler, 2014).

5. Synthesis and crystallization

The title compound was synthesized from starting materials of Sr granules (99.9+%, Alfa Aesar), Cd powder (99.9+%, Alfa Aesar) and Pt powder (99.95%, Chempur). A stoichiometric mixture of these elements was loaded into a Nb ampoule in an Ar-filled dry box. The Nb ampoule was then weld-sealed under an Ar atmosphere and subsequently enclosed in an evacuated silica jacket. The sample was then heated to 1123 K for 15 h, equilibrated at 923 K for 4 days, and followed by slow cooling to room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The maximum and minimum remaining electron densities are located 1.66 and 0.81 Å , respectively, from the Pt site.

Acknowledgements

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supporting information

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Computing details

Data collection: *XSCANS* (Bruker, 2001); cell refinement: *XSCANS* (Bruker, 2001); data reduction: *XSCANS* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

Distrontium cadmium diplatinum

Crystal data

 $CdPt₂Sr₂$ *Mr* = 677.82 Orthorhombic, *Immm* Hall symbol: -I 2 2 $a = 4.5596(9)$ Å $b = 5.9351(12)$ Å $c = 9.1874(18)$ Å $V = 248.63$ (9) \AA ³ $Z = 2$

Data collection

Refinement

Refinement on *F*² Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.022$ $wR(F^2) = 0.058$ $S = 1.16$ 190 reflections 13 parameters 0 restraints Primary atom site location: structure-invariant direct methods

 $F(000) = 560$ D_x = 9.054 Mg m⁻³ Mo *Kα* radiation, *λ* = 0.71073 Å Cell parameters from 25 reflections θ = 12–18° μ = 81.39 mm⁻¹ *T* = 293 K Block, brown $0.08 \times 0.06 \times 0.05$ mm

1069 measured reflections 190 independent reflections 172 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$ $\theta_{\text{max}} = 28.3^{\circ}, \theta_{\text{min}} = 4.1^{\circ}$ *h* = −5→6 $k = -7 \rightarrow 7$ *l* = −11→11

Secondary atom site location: difference Fourier man $w = 1/[\sigma^2(F_0^2) + (0.0337P)^2 + 3.9776P]$ where $P = (F_0^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}}$ < 0.001 Δ*ρ*max = 1.84 e Å−3 $\Delta\rho_{\text{min}} = -2.51$ e Å⁻³ Extinction correction: *SHELXL*, Fc* =kFc[1+0.001xFc2 *λ*3 /sin(2*θ*)]-1/4 Extinction coefficient: 0.0024 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on *F*² are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å2)

Geometric parameters (Å, º)

Symmetry codes: (i) $-x$, $-y$, $-z+1$; (ii) $x+1$, y , z ; (iii) $-x$, $-y+1$, $-z+1$; (iv) $-x-1/2$, $-y+1/2$, $-z+1/2$; (v) $x+1/2$, $-y+1/2$, $-z+1/2$; (vi) $x+1/2$, $y-1/2$, $z+1/2$; (vii) x-1/2, y-1/2, z+1/2; (viii) x-1, y, z; (ix) -x-1, -y+1, -z+1; (x) x-1/2, y+1/2, z+1/2; (xi) -x-1/2, -z+1/2; (xii) x-1/2, y+1/2, z-1/2; (xiii) *x*+1/2, *y*+1/2, *z*−1/2; (xiv) *x*+1/2, *y*−1/2, *z*−1/2; (xv) −*x*, −*y*+1, −*z*; (xvi) −*x*+1/2, −*y*+3/2, −*z*+1/2.