

## Synthesis, crystal structure and magnetic properties of the new ternary indide $\text{SmPd}_2\text{In}_4$

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The crystal structure of the novel compound  $\text{SmPd}_2\text{In}_4$  was determined from single-crystal X-ray diffraction data. The indide crystallizes in a new structure type; Pearson symbol  $oP112$ , space group  $Pnma$ ,  $a = 52.597(9)$  Å,  $b = 4.5074(8)$  Å,  $c = 9.8875(19)$  Å,  $Z = 16$ . It orders antiferromagnetically near 10 K possibly with a complex magnetic structure that involves as many as four crystallographically independent sites of Sm atoms.

Rare-earth / X-ray diffraction / Crystal structure / Magnetic properties / Intermetallic compounds

### Introduction

The ternary Sm–Pd–In system is not yet fully characterized. Five ternary compounds have been reported up to now:  $\text{Sm}_4\text{Pd}_{10}\text{In}_{21}$  ( $\text{Ho}_4\text{Ni}_{10}\text{Ga}_{21}$  structure type, space group  $C2/m$ ,  $a = 22.956$ ,  $b = 4.4707$ ,  $c = 19.357$  Å,  $\beta = 133.16^\circ$  [1]),  $\text{SmPdIn}_2$  (structure type  $\text{HfNiGa}_2$ , space group  $I4mm$ ,  $a = 13.883$ ,  $c = 9.186$  Å [2]),  $\text{SmPdIn}$  ( $\text{ZrNiAl}$  structure type, space group  $P-62m$ ,  $a = 7.656$ ,  $c = 3.934$  Å [3]),  $\text{Sm}_2\text{Pd}_2\text{In}$  ( $\text{Mo}_2\text{FeB}_2$  structure type, space group  $P4/mbm$ ,  $a = 7.7098$ ,  $c = 3.8044$  Å [4];  $a = 7.7009$ ,  $c = 3.8085$  Å [5]), and  $\text{Sm}_2\text{PdIn}_8$  ( $\text{Ho}_2\text{CoGa}_8$  structure type, space group  $P4/mmm$ ,  $a = 4.6510(2)$ ,  $c = 12.0644(8)$  Å [6]).

Our recent investigation of the Ce–Pd(Pt)–In systems resulted in the synthesis of the new compounds  $\text{CePd}_2\text{In}_4$  and  $\text{CePt}_2\text{In}_4$  [7] crystallizing in the  $\text{NdRh}_2\text{Sn}_4$  structure type [8]. The synthesis of isotypic indides with other light rare-earths (RE) was complicated due to the easy formation and high stability of the  $\text{RE}_4\text{Pd}_{10}\text{In}_{21}$  compounds. Our search for further isostoichiometric indides led to the formation of the new compound  $\text{SmPd}_2\text{In}_4$  with similar composition but different structure.

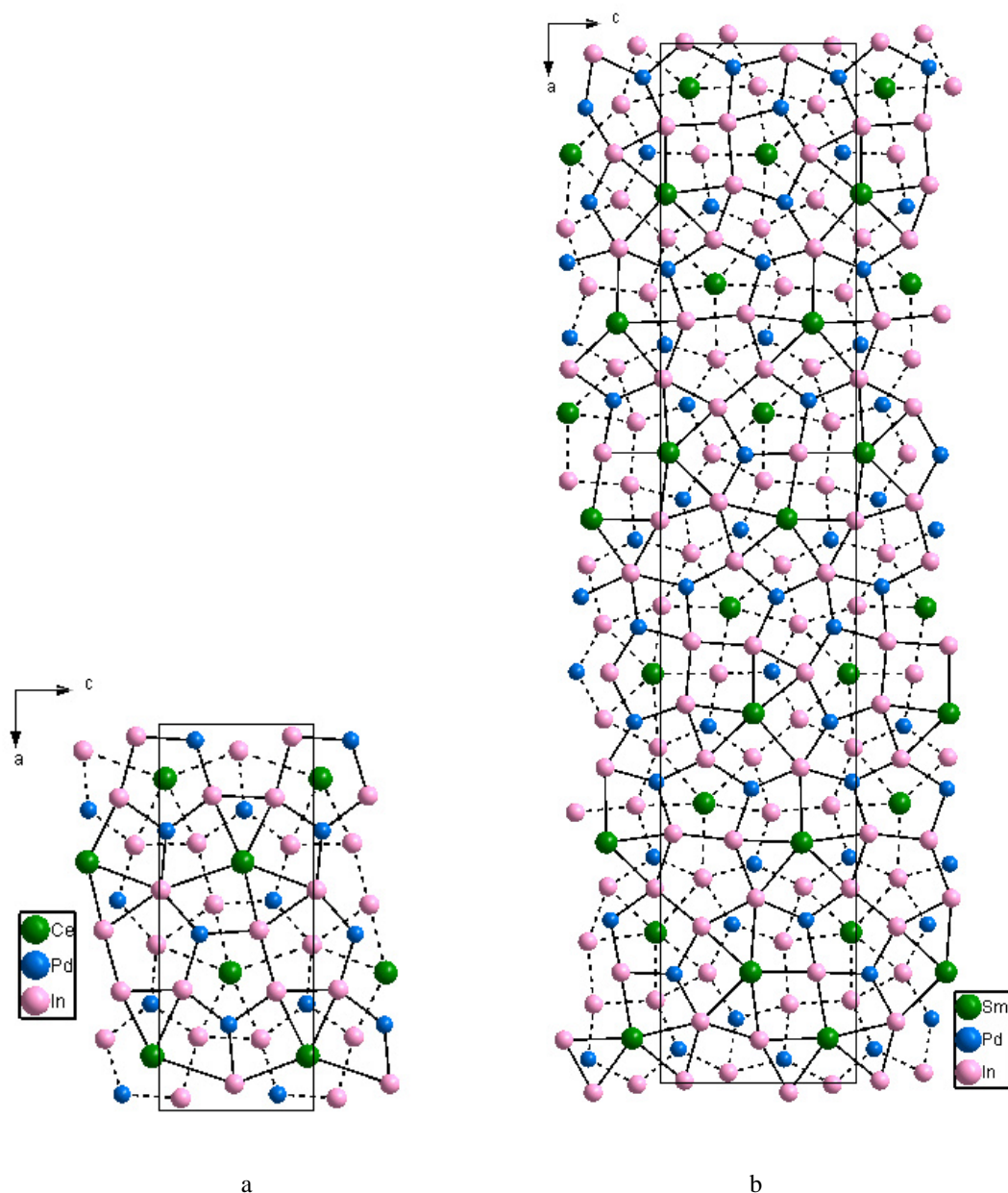
$\text{SmPd}_2\text{In}_4$  has many common features with the  $\text{CePd}_2\text{In}_4$  compound investigated earlier. Both compounds crystallize in space group  $Pnma$  with the  $b$  cell parameter approximately equal to 4.5 Å. In both structures, all the atoms are located in the mirror

planes ( $4c$  crystallographic sites) with full occupancy. Each crystallographic site is occupied by a single type of atom. The structures can be considered as built of two identical atom layers composed of five-, four-, and three-membered rings at heights  $y = 1/4$  and  $y = 3/4$ , related by an inversion center at  $y = 1/2$  (Fig. 1). The structures are well described by a covalently bonded  $[\text{PdIn}_2]$  network in which the RE atoms fill distorted pentagonal channels. The coordination polyhedra in the structures are of the same types: the RE atoms are situated in pentagonal prisms, the palladium atoms are arranged in trigonal prisms, the indium atoms are located in either tetragonal or pentagonal prisms.

### Experimental

Starting materials for the preparation of the  $\text{SmPd}_2\text{In}_4$  indide were ingots of samarium (99.95 %) and indium (99.999 %), and palladium plate (99.99 %). The elemental components were taken in the ideal 1:2:4 atomic ratio and arc-melted in an argon atmosphere. The sample was remelted to ensure good homogeneity. The weight loss was smaller than 1 wt.%. The melted button was subsequently sealed in an evacuated silica tube and annealed at 1053 K for one month.

A single crystal of  $\text{SmPd}_2\text{In}_4$  was selected from the surface of the arc-melted alloy. X-ray single crystal intensity data were collected on a Nonius Kappa CCD



**Fig. 1** Projection of the atomic networks of the  $\text{CePd}_2\text{In}_4$  (a) and  $\text{SmPd}_2\text{In}_4$  (b) structures along the  $b$ -axis.

diffractometer (Mo  $K\alpha$  radiation,  $\varphi$ - and  $\omega$ -scan). An empirical absorption correction was applied using the program SADABS [9].

The starting atomic parameters were deduced from an automatic interpretation of direct methods with SHELXS97 [10] and the structure was refined using SHELXL97 [10] (full-matrix least-squares on  $F^2$ ) with anisotropic displacement parameters for all the atoms. Data collection and refinement details are given in Table 1. Atomic coordinates and equivalent isotropic displacement parameters can be found in Table 2. Interatomic distances are presented in Table 3.

In order to estimate the purity, the annealed polycrystalline sample was analyzed by

EDX measurements using a Jeol JSM 6400 scanning electron microscope with a Si/Li energy-dispersive analyzer, and by powder X-ray diffraction (HUBER Imaging Plate Guinier Camera G670). With EDX, a small amount of a secondary phase of approximate composition  $\text{Sm}_{11}(\pm 2)\text{Pd}_{32}(\pm 2)\text{In}_{57}(\pm 2)$  was detected. From the powder pattern, the secondary phase was identified as the  $\text{Sm}_4\text{Pd}_{10}\text{In}_{21}$  compound [1] with a volume fraction of  $7(\pm 2)\%$ .

Magnetic measurements were performed in the temperature interval 1.71–300 K and in magnetic fields up to 5 T, using a Quantum Design MPMS-5 SQUID magnetometer.

**Table 1** Crystallographic data for SmPd<sub>2</sub>In<sub>4</sub> and experimental details of the structure determination and refinement.

Formula weight (g/mol)	822.43
Space group	<i>Pnma</i> (62)
Pearson symbol	<i>oP112</i>
Crystal dimensions (mm <sup>3</sup> )	0.04×0.06×0.08
Unit cell dimensions (Å)	52.597(9) 4.5074(8) 9.8875(19)
Unit cell volume (Å <sup>3</sup> )	2344.1(7)
Number of formula units, <i>Z</i>	16
Calculated density, <i>D<sub>x</sub></i> (g/cm <sup>3</sup> )	9.322
Absorption coefficient, $\mu$ (mm <sup>-1</sup> )	31.152
Scan mode	$\varphi$ and $\omega$
Theta range for data collection (deg.)	3.72-27.50
<i>F</i> (000)	5600
Range in <i>h k l</i>	-68 ≤ <i>h</i> ≤ 68, -5 ≤ <i>k</i> ≤ 5, -12 ≤ <i>l</i> ≤ 12
Total number of reflections	19894
Independent reflections	3010 ( <i>R</i> <sub>int</sub> = 0.0425)
Reflections with <i>I</i> > 2σ( <i>I</i> )	2529 ( <i>R</i> <sub>sigma</sub> = 0.0299)
Weighting scheme	[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0178 <i>P</i> ) <sup>2</sup> + 116.1596 <i>P</i> ] <sup>-1</sup> , where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
Data/parameters	2529/170
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0384, <i>wR</i> 2 = 0.0732
Final <i>R</i> indices [all data]	<i>R</i> 1 = 0.0511, <i>wR</i> 2 = 0.0770
Largest electron density peak and hole (e/Å <sup>3</sup> )	5.64 and -3.25

**Table 2** Atomic coordinates<sup>a</sup> and equivalent isotropic displacement parameters.

Atom	<i>x</i>	<i>z</i>	<i>U</i> <sub>eq</sub> , Å <sup>2</sup>	Atom	<i>x</i>	<i>z</i>	<i>U</i> <sub>eq</sub> , Å <sup>2</sup>
Sm1	0.144526(17)	0.02635(9)	0.01022(19)	In3	0.07937(2)	0.02672(13)	0.0105(3)
Sm2	0.268807(17)	0.77750(9)	0.0107(2)	In4	0.10549(2)	0.76259(12)	0.0107(3)
Sm3	0.393514(18)	0.04010(9)	0.0113(2)	In5	0.13571(2)	0.37314(13)	0.0104(3)
Sm4	0.457264(17)	0.64556(9)	0.0103(2)	In6	0.18852(2)	0.27114(12)	0.0093(3)
Pd1	0.02253(3)	0.37000(15)	0.0148(3)	In7	0.19679(2)	0.78562(13)	0.0126(3)
Pd2	0.06154(3)	0.61407(15)	0.0133(3)	In8	0.26011(2)	0.43681(13)	0.0110(3)
Pd3	0.15256(3)	0.63482(14)	0.0122(3)	In9	0.26651(2)	0.12777(13)	0.0108(3)
Pd4	0.21043(3)	0.52223(14)	0.0125(3)	In10	0.31299(2)	0.53153(13)	0.0103(3)
Pd5	0.21706(3)	0.03600(14)	0.0102(3)	In11	0.32253(2)	0.01297(12)	0.0097(3)
Pd6	0.34334(3)	0.75691(15)	0.0127(3)	In12	0.34976(2)	0.29232(12)	0.0113(3)
Pd7	0.39561(3)	0.43036(14)	0.0120(3)	In13	0.39376(2)	0.70423(13)	0.0122(3)
Pd8	0.53225(3)	0.59151(14)	0.0130(3)	In14	0.44135(2)	0.29633(12)	0.0099(3)
In1	0.00955(2)	0.65484(13)	0.0114(3)	In15	0.49815(2)	0.37898(13)	0.0107(3)
In2	0.07543(2)	0.34242(13)	0.0128(3)	In16	0.95886(3)	0.50449(13)	0.0142(3)

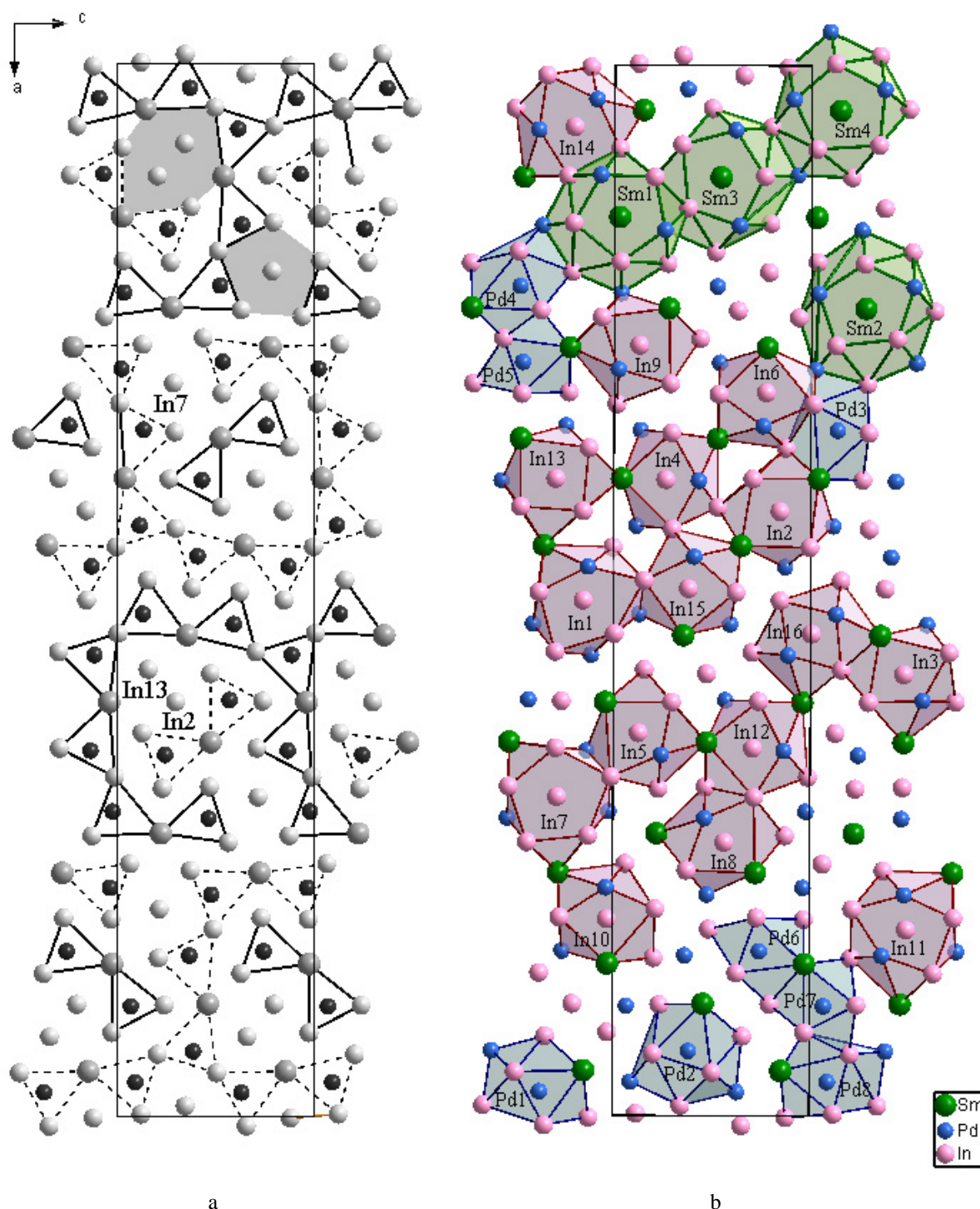
<sup>a</sup> *y* is equal to ¼ for all the atoms

## Results and discussion

### Crystal structure

According to our knowledge, the compound SmPd<sub>2</sub>In<sub>4</sub> represents a novel structure type (Pearson symbol *oP112*, space group *Pnma*, *a* = 52.597(9), *b* = 4.5074(8), *c* = 9.8875(19) Å, *Z* = 16). The SmPd<sub>2</sub>In<sub>4</sub> structure appears to be relatively complex with 28 crystallographically independent sites and 112 atoms within the unit cell. All the atoms have distorted coordination polyhedra. From a geometrical point of

view, the structure contains three types of building block, *i.e.* palladium-centered trigonal prisms with the side faces capped by three, four or five additional atoms (Fig. 2a). As emphasized in Fig. 2a, the trigonal prisms are condensed *via* common edges. The trigonal prisms of the Pd3, Pd4, and Pd5 atoms are condensed with the pentagonal prisms that are formed around the In7 atoms (shaded in Fig. 2a). The trigonal prisms of the Pd1, Pd2, Pd6, and Pd7 atoms are condensed with the interpenetrating cuboctahedra of the In2 and In13 atoms (shaded area in Fig. 2a), which form infinite



**Fig. 2** Projections of the structure of  $\text{SmPd}_2\text{In}_4$  along the  $b$ -axis, emphasizing the trigonal prismatic coordination of the palladium atoms (a) and the coordination polyhedra of the atoms (b).

zigzag chains in hexagonal channels along the  $b$ -axis with In2-In13 distances of 3.3093(13) Å.

Each of the four samarium sites have eleven indium neighbors and six (Sm1, Sm3, Sm4) or seven (Sm2) palladium neighbors. The coordination polyhedra of the samarium atoms can be considered as pentagonal prisms with seven or eight

additional atoms centering side faces and side edges of the prisms (Fig. 2b). Due to the high palladium and indium content, the samarium atoms are well separated. The shortest Sm-Sm contacts for all four samarium sites are 4.5074(8) Å, which corresponds to the lattice parameter  $b$ . The Sm-In (3.1423(11)–3.7885(17) Å) and Sm-Pd

**Table 3** Interatomic distances (*d*) and coordination numbers (CN) of the atoms in the structure of SmPd<sub>2</sub>In<sub>4</sub>.

Atom CN	To atom	<i>d</i> (Å)	Atom CN	To atom	<i>d</i> (Å)	Atom CN	To atom	<i>d</i> (Å)			
Sm1 17	2 In10	3.1742(11)	Pd6 9	In13	2.7029(19)	In7 15	Pd5	2.6952(19)			
	2 Pd7	3.2305(12)		In10	2.7412(19)		Pd4	2.7013(19)			
	2 In12	3.2440(12)		In11	2.7582(19)		Pd3	2.7636(19)			
	2 Pd6	3.2686(13)		2 In5	2.7594(11)		2 In12	3.3285(14)			
	In4	3.3192(16)		2 In6	2.8121(12)		2 In9	3.3527(14)			
	In6	3.3488(16)		2 Sm1	3.2686(13)		2 In10	3.3549(14)			
	In3	3.4270(16)		Pd7 9	In13		2.7096(19)	2 In8	3.5286(14)		
	In5	3.4601(17)			In14		2.7466(19)	Sm1	3.6363(16)		
	2 In13	3.4969(13)			In12		2.7711(19)	2 In11	3.6578(14)		
	In7	3.6364(16)	2 In3		2.7783(11)		Sm2	3.7885(17)			
	Pd5	3.8161(18)	2 In4		2.7991(12)		2 Pd5	3.7355(11)			
	Pd3	3.8942(18)	2 Sm1		3.2304(12)		Pd4	2.7462(19)			
	Sm2 18	2 In8	3.1423(11)		Pd8 10		In3	2.7405(19)	In8 12	In10	2.9345(18)
		2 In6	3.1812(11)				In15	2.763(2)		In9	3.0741(19)
		2 In9	3.2744(12)	In1			2.777(2)	2 Sm2		3.1423(11)	
		In10	3.3637(16)	2 In15			2.7785(11)	2 In9		3.2565(14)	
		2 Pd5	3.3666(13)	2 In14			2.8702(12)	Sm2		3.3995(17)	
In8		3.3994(17)	Pd2	3.294(2)		2 In7	3.5286(14)				
In9		3.4654(17)	2 Sm4	3.2982(13)		Pd5	2.7549(19)				
2 Pd4		3.4824(13)	In1 15	Pd2		2.7639(19)	2 Pd4	2.7639(11)			
In11		3.6611(16)		Pd8		2.777(2)	In8	3.0741(19)			
Pd5		3.7339(17)		2 Pd1		2.8260(12)	In11	3.1573(18)			
In7		3.7885(17)		Pd1	2.899(2)	2 In8	3.2565(14)				
Pd6		3.9254(18)		In16	3.0527(18)	2 Sm2	3.2743(12)				
Pd4		3.9746(17)		2 In15	3.1865(13)	2 In7	3.3527(14)				
Sm3 17		2 In4		3.1498(11)	2 In16	3.2127(14)	In10 12	Sm2		3.4655(17)	
		2 In5	3.1886(11)	Sm4	3.3850(16)	Pd6		2.7412(19)			
		In13	3.3209(17)	2 In14	3.7021(15)	2 Pd5		2.7529(11)			
		2 Pd2	3.3471(13)	2 In1	3.934(2)	In8		2.9345(18)			
	In12	3.3935(16)	Pd2	2.783(2)	In12	3.0551(18)					
	2 In2	3.4012(12)	Pd1	2.796(2)	2 Sm1	3.1741(11)					
	2 Pd3	3.4392(13)	2 In13	3.0939(13)	2 In6	3.2709(13)					
	In16	3.4652(17)	In3	3.1283(19)	2 In7	3.3549(14)					
	In14	3.5705(16)	In5	3.1854(19)	Sm2	3.3638(16)					
	In11	3.7435(17)	2 In16	3.2592(14)	In11 15	Pd6		2.7582(19)			
	Pd6	3.8478(18)	2 Sm3	3.4012(12)		2 Pd4		2.8448(12)			
	Pd7	3.8603(18)	2 Sm4	3.4387(12)		2 Pd3		2.8720(12)			
	Sm4 17	2 In3	3.1894(11)	In3 12		Pd8		2.7405(19)	In12	3.1116(18)	
		2 In15	3.2616(11)			2 Pd7		2.7783(11)	In9	3.1573(18)	
		2 Pd8	3.2982(13)			In4		2.9508(19)	2 In6	3.3367(13)	
		2 Pd1	3.3368(13)			In2		3.1283(19)	2 In5	3.4375(14)	
		In1	3.3851(16)			2 In13		3.1869(13)	2 In7	3.6578(14)	
In13		3.3901(17)	2 Sm4			3.1895(11)	Sm2	3.6611(16)			
In15		3.4018(16)	2 In14			3.3847(14)	Sm3	3.7435(17)			
2 In2		3.4387(12)	Sm1		3.4270(16)						
In16		3.4612(17)									
In14		3.5531(17)									
Pd7		3.8786(17)									
Pd8		3.9799(18)									

**Table 3** Interatomic distances (*d*) and coordination numbers (CN) of the atoms in the structure of SmPd<sub>2</sub>In<sub>4</sub> (continued).

Atom CN	To atom	<i>d</i> (Å)	Atom CN	To atom	<i>d</i> (Å)	Atom CN	To atom	<i>d</i> (Å)
Pd1 10	2 In16	2.7527(12)	In4 12	Pd2	2.7385(19)	In12 12	2 Pd3	2.7422(11)
	In15	2.7756(19)		Pd3	2.7795(19)		Pd7	2.7711(19)
	In2	2.796(2)		2 Pd7	2.7990(12)		In10	3.0551(18)
	2 In1	2.8260(12)		In3	2.9508(18)		In11	3.1116(18)
	In1	2.899(2)		2 Sm3	3.1497(12)		2 Sm1	3.2439(12)
	Pd2	3.168(2)		2 In12	3.2722(14)		2 In4	3.2722(14)
	2 Sm4	3.3367(13)		Sm1	3.3192(16)		2 In7	3.3285(14)
	Pd2	2.7385(19)		2 In14	3.3553(14)		Sm3	3.3935(16)
	2 In16	2.7577(11)		Pd3	2.7348(19)		Pd6	2.7029(19)
	In1	2.7639(19)		2 Pd6	2.7594(11)		Pd7	2.7096(19)
Pd2 11	In2	2.783(2)	In5 12	In6	2.9553(18)	In13 12	2 In2	3.0939(13)
	2 In14	2.8896(12)		In2	3.1854(18)		2 In3	3.1869(13)
	Pd1	3.168(2)		2 Sm3	3.1887(11)		2 In5	3.2049(13)
	Pd8	3.294(2)		2 In13	3.2049(13)		Sm3	3.3209(17)
	2 Sm3	3.3470(13)		2 In11	3.4375(14)		Sm4	3.3900(17)
	Pd3	2.7348(19)		Sm1	3.4602(17)		2 Sm1	3.4969(13)
	2 In12	2.7422(11)		Pd4	2.7369(19)		Pd7	2.7466(19)
	In7	2.7636(19)		Pd5	2.7673(19)		2 Pd8	2.8702(12)
	In4	2.7795(19)		2 Pd6	2.8121(12)		2 Pd2	2.8896(12)
	2 In11	2.8720(12)		In5	2.9553(18)		In15	3.0978(18)
Pd3 10	Pd4	3.241(2)	In6 12	2 Sm2	3.1811(11)	In14 15	In16	3.1137(19)
	2 Sm3	3.4302(13)		2 In10	3.2709(13)		2 In4	3.3553(14)
	In7	2.7013(19)		2 In11	3.3367(13)		2 In3	3.3847(14)
	In6	2.7369(19)		Sm1	3.3488(16)		Sm4	3.5530(17)
	In8	2.7462(19)					Sm3	3.5705(16)
	2 In9	2.7639(11)					2 In1	3.7021(15)
	2 In11	2.8448(12)					Pd8	2.763(2)
	Pd3	3.241(2)					Pd1	2.7756(19)
	2 Sm2	3.4823(13)					2 Pd8	2.7785(11)
	In7	2.6952(19)					In14	3.0973(18)
Pd4 10	2 In8	2.7355(11)			In15 12	2 In1	3.1865(13)	
	2 In10	2.7529(11)				2 Sm4	3.2616(12)	
	In9	2.7549(19)				2 In15	3.2933(19)	
	In6	2.7673(19)				Sm4	3.4018(16)	
	2 Sm2	3.3666(13)				2 Pd1	2.7527(12)	
						2 Pd2	2.7577(11)	
						In1	3.0527(18)	
						In14	3.1137(19)	
						2 In1	3.2127(14)	
						2 In2	3.2592(14)	
Pd5 9					In16 12	Sm4	3.4611(17)	
						Sm3	3.4652(17)	

(3.2305(12)–3.9799(18) Å) distances are quite similar for the four samarium sites.

The smallest coordination numbers (CN) are observed for the palladium atoms, which have trigonal-prismatic coordination, typical for lowest size atoms. Each of the eight crystallographically different palladium atoms forms seven bonds to surrounding indium atoms, with Pd-In distances ranging from 2.6953(19) Å to 2.899(2) Å, which is close to the sum of the covalent radii [11] (2.78 Å). In addition, each Pd atom forms two bonds with Sm atoms, defining a

nine-coordinate site. However the bonding geometries of the eight crystallographically unique Pd sites are not identical due to Pd-Pd contacts (to be discussed below).

In the structure of CePd<sub>2</sub>In<sub>4</sub> [7], the palladium atoms are isolated from one another, forming bonds only with Ce and In atoms. The shortest Pd-Pd distances in CePd<sub>2</sub>In<sub>4</sub> (4.4655(11) Å) are comparable with the *b*-axis lattice parameter (4.5647(9) Å). Unlike CePd<sub>2</sub>In<sub>4</sub>, in the structure of SmPd<sub>2</sub>In<sub>4</sub> three Pd-Pd contacts are observed: Pd1-Pd2 3.168(2) Å, Pd2-Pd8

3.294(2) Å, and Pd3-Pd4 3.241(2) Å. As a result, the CNs of the atoms Pd1, Pd3, and Pd4 increase by one and the CN of the Pd2 atom increases by two (Table 3).

Four of the 14 crystallographically unique indium sites (In1, In7, In11, In14) have pentagonal prismatic (CN = 15) coordination. The pentagonal prisms of In1, In7, In11, and In14 have additional atoms at the centers of all the side faces. Unlike the In1, In11, and In14 atoms having strongly distorted pentagonal prismatic polyhedra, the In7 atom is situated in a slightly distorted pentagonal prism. All the other indium sites have cuboctahedral (CN = 12) coordination. The latter have five or six indium neighbors. The latter have five or six indium neighbors at In-In distances covering the large range from 2.9345(18) Å to 3.5286(14) Å. The next nearest In-In contacts within the coordination cuboctahedra occur between In6 and In8 atoms at the distance 4.1063(18) Å. The range of In-In distances within the pentagonal prisms of the In1, In7, In11, and In14 atoms (from 3.0527(18) Å to 3.934(2) Å) is much larger than in the cuboctahedra. Most of the In-In distances in the structure of SmPd<sub>2</sub>In<sub>4</sub> are shorter than in elemental indium where each indium atom has four neighbours at 3.25 Å and eight further neighbors at 3.38 Å [12].

The number of palladium neighbors of the indium atoms ranges from three to five, with the exception of the In2 and In13 atoms, which have only two contacts with palladium atoms. It is precisely these two In atoms that occupy distorted hexagonal channels forming zigzag chains along the *b*-axis (see above).

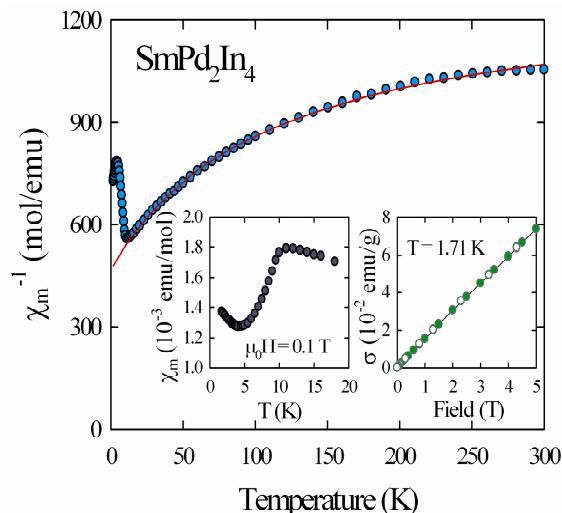
Taking into consideration Pd-In and In-In bonding, the SmPd<sub>2</sub>In<sub>4</sub> structure can be best described by a covalently bonded [PdIn<sub>2</sub>] network in which the samarium atoms occupy distorted pentagonal channels (Fig. 1b).

Additional Pd-Pd contacts of 3.168–3.241 Å in the SmPd<sub>2</sub>In<sub>4</sub> structure, as well as considerable distortion of the coordination polyhedra (when compared with the parent CePd<sub>2</sub>In<sub>4</sub> structure), correlate well with close packing. Actually, the calculated density of the SmPd<sub>2</sub>In<sub>4</sub> (9.32 g/cm<sup>3</sup>) is significantly greater than that of the CePd<sub>2</sub>In<sub>4</sub> compound (8.64 g/cm<sup>3</sup>), even taking into consideration the lanthanide contraction.

#### Magnetic behavior

The magnetic properties of SmPd<sub>2</sub>In<sub>4</sub> are summarized in Fig. 3. As usually observed for samarium compounds, the inverse magnetic susceptibility is strongly curvilinear over an extended temperature range. This feature results from the closeness in energy of the terms <sup>6</sup>H<sub>5/2</sub> and <sup>6</sup>H<sub>7/2</sub> that both originate from the Sm<sup>3+</sup> ground multiplet [13]. Above 10 K, the molar magnetic susceptibility of SmPd<sub>2</sub>In<sub>4</sub> may be described by a modified Curie-Weiss law,

$$\chi_m = \chi_0 + \frac{C}{T - \theta_p},$$



**Fig. 3** Temperature dependence of the inverse molar magnetic susceptibility of SmPd<sub>2</sub>In<sub>4</sub>. The solid line is a modified Curie-Weiss fit with the parameters given in the text. The two insets present the low-temperature molar magnetic susceptibility measured in 0.5 T, and the field variation of the magnetization, taken at *T* = 1.71 K with increasing (full circles) and decreasing (open circles) magnetic field.

with the effective magnetic moment  $\mu_{\text{eff}} = \sqrt{8C} = 0.66(4) \mu_B$ , the paramagnetic Weiss temperature  $\theta_p = -40(1) \text{ K}$  and the Van Vleck contribution  $\chi_0 = 7.7(1) \cdot 10^{-4} \text{ emu/mol}$ . It is worth noting that the experimental value of  $\mu_{\text{eff}}$  is somewhat smaller than the effective magnetic moment predicted for a free Sm<sup>3+</sup> ion in the framework of the LS approach ( $g\sqrt{J(J+1)} = 0.84$ ). The negative and relatively large value of  $\theta_p$  suggests considerable antiferromagnetic exchange correlations. Indeed, as apparent from Fig. 3 (see also the inset), near 10 K the compound undergoes a phase transition into a magnetically ordered state. The overall shape of the observed anomaly in  $\chi_m(T)$ , as well as the linear-in-field character of the magnetization isotherm taken deep in the ordered region (at 1.71 K; see the inset), indicate that the electronic ground state in SmPd<sub>2</sub>In<sub>4</sub> is antiferromagnetic. However, below 5 K, the magnetic susceptibility exhibits an upturn that is at odds with the regular behavior of simple collinear antiferromagnets. This feature hints at a more complex arrangement of the magnetic moments, which might be rationalized considering that the Sm atoms in SmPd<sub>2</sub>In<sub>4</sub> occupy as many as four independent sites. To determine the magnetic structure of the compound, neutron diffraction studies are necessary.

## Conclusions

The novel compound  $\text{SmPd}_2\text{In}_4$  is the first representative of a new structure type that is closely related to the crystal structure of  $\text{CePd}_2\text{In}_4$  ( $\text{NdRh}_2\text{Sn}_4$  type). Although the forms of the coordination polyhedra in the two structures are quite similar, strong distortion of the polyhedra in the  $\text{SmPd}_2\text{In}_4$  structure type leads to a significant enlargement of the unit cell.

$\text{SmPd}_2\text{In}_4$  becomes antiferromagnetic below 10 K. Its magnetic structure is probably complex due to the presence of four crystallographically independent sites of magnetic Sm atoms.

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