substance: $CoSb_2$
property: crystal structure, physical properties

Energy level scheme is similar to that shown in Fig. 1 for $CoAs_2$.

energy gap

$E_{g,th}$	0.2 eV (?)	polycrystal	from log $\rho \propto E_g/2kT$, T = 550...800 K, measured across the arsenopyrite → marcasite transition	56D, 57D
	0.17 eV	single crystal	from log $\rho \propto E_g/2kT$, T = 450...600 K, semiconducting also in the marcasite modification (?)	83S

resistivity

ρ	$2.5 \cdot 10^{-3}$ Ω cm	$T \approx 550$ K	polycrystalline material	56D

thermoelectric power

S	40 μV K^{-1}	T = 300 K		80H
	54 μV K^{-1}	T = 400 K	polycrystalline material	56D
	75 μV K^{-1}	T = 600 K		
	60 μV K^{-1}	T = 700 K		
	70 μV K^{-1}	T = 800 K		

magnetic susceptibility
(in 10^{-6} cm^3 mol^{-1}, χ in CGS units)

χ_m	0.0	T = 80...900 K, B = 0.8 T	samples sintered at 1073 K, Faraday method	71K
	– 4	T = 300 K, B =0.5 T	non-oriented single crystals grown	83S
	0	T = 465 K	by an iodine transport reaction;	
	+ 10	T = 585 K	Faraday method	
	+ 22	T = 640 K	transition temperature (monoclinic → orthorhombic)	
	+ 36	T = 900 K	linear increase above Ttr	

lattice parameters $a(T)$, $b(T)$, $c(T)$, $\beta(T)$ at T = 300...1200 K: Fig. 2.

volume expansion coefficient

β	$6.8 \cdot 10^{-5}$ K^{-1}	T = 300 K	from graphical representation, T = 300...400 K	77K
	$4.2 \cdot 10^{-5}$ K^{-1}	T = 500 K	unit-cell volume linear in T, T = 450...1200 K	

structural transition

(monoclinic → orthorhombic (Fig. 2))

T_{tr}	650 K	second-order transition to the loellingite structure	77K
	640 K	from magnetic susceptibility	83S
	643...646 K	from DTA	83S

peritectic (decomposition) temperature

T_{perit}	1192 K	56D, 60Z, 78A
	1204 K	77K

Comparative tables on structural data of transition metal dipnictides:

structure, chemical bond:, see document ,

crystallographical data of compounds with octahedrally coordinated cations, see document ,

interatomic distances in arsenopyrite-type phases, see document .

References:

56D Dudkin, L. D., Abrikosov, N. Kh.: Zhur. Neorg. Khim. 1 (1956) 2096.

57D Dudkin, L. D., Abrikosov, N. Kh.: Zhur. Neorg. Khim. 2 (1957) 212; translation: Russ. J. Inorg. Chem. 2 (1957) 325.

60Z Zhuravlev, N. N., Zhdanov, G. S., Kuz'min, RN.: Kristallografiya 5 (1960) 553; translation: Sov. Phys. Cryst. 5 (1961) 532.

71K Kjekshus, A.: Acta Chem. Scand. 25 (1971) 411.

72G Goodenough, J. B.: J. Solid State Chem. 5 (1972) 144.

77K Kjekshus, A., Rakke, T.: Acta Chem. Scand. A31 (1977) 517.

78A Abrikosov, N. Kh., Petrova, L. I.: Izv. Akad. Nauk SSSR, Neorg. Mater. 14 (1978) 457; translation: Inorg. Mater. 14 (1978) 346.

80H Hulliger, F.: unpublished results 1980.

83S Siegrist, T., Hulliger, F.: unpublished.

Fig. 1.

$CoAs_2$. Energy-level scheme for the valence electrons in the arsenopyrite-type phase with formal d^5 configuration [72G].

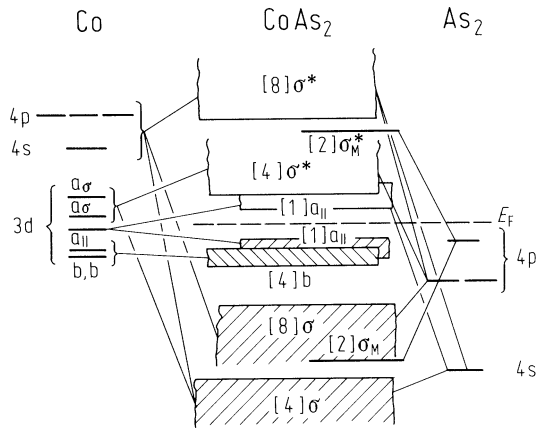

Fig. 2.

$CoSb_2$. Lattice parameters vs. temperature [77K]. Pseudo-marcasite cell. $CoSb_2$ decomposes at 1204 K.