substance: $CoAs_2$
property: physical properties

energy level scheme: Fig. 1.

energy gap

$E_{g.th}$	≈ 0.15 eV		from log $\rho \propto E_g/2kT$, sintered sample	59H
	≈ 0.35 eV		rom log $\rho \propto E_g/2kT$, T = 450...650 K, single crystal	83S

thermoelectric power

S	– 200 μV K^{-1}	T = 300 K	measured on the sintered, weakly paramagnetic sample of [63H]	80H

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

χ_m	– 4	T = 80...900 K	sample sintered at 1073 K ($\chi_g = 0.02 \cdot 10^{-6}$ cm^3 g^{-1})	71K
	– 16	T = 300...400 K, B = 0.5 T	non-oriented single crystals grown by an iodine transport reaction,	83S
	– 10	T = 600 K	Faraday method	
	0	T = 720 K		
	+ 23	T = 810 K	transition temperature	
	+ 28	T = 920 K	linear increase above T_{tr}	

The weak paramagnetism of sintered samples [63H, 66B] is obviously due to impurity phases.

lattice parameters $a(T)$, $b(T)$, $c(T)$, $\beta(T)$ at T = 300...1270 K [77K].

volume expansion coefficient

β	$4.2 \cdot 10^{-5}$ K^{-1}	T = 300 K	from graphic representation; unit-cell volume linear in T in the range 300...1300 K	77K

structural transition

(monoclinic → orthorhombic (Fig. 2).)

T_{tr}	870 K	second-order transition to the loellingite structure	77K
	810 K	from magnetic susceptibility	83S
	796...800 K	from DTA	83S

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:

59H Hulliger, F.: Helv. Phys. Acta 32 (1959) 615.
63H Hulliger, F.: Phys. Lett. 4 (1963) 282.
66B Bennett, S. L., Heyding, R. D.: Can. J. Chem. 44 (1966) 3017.
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.
80H Hulliger, F.: unpublished results 1980.
83S Siegrist, T., Hulliger, F.: unpublished.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].

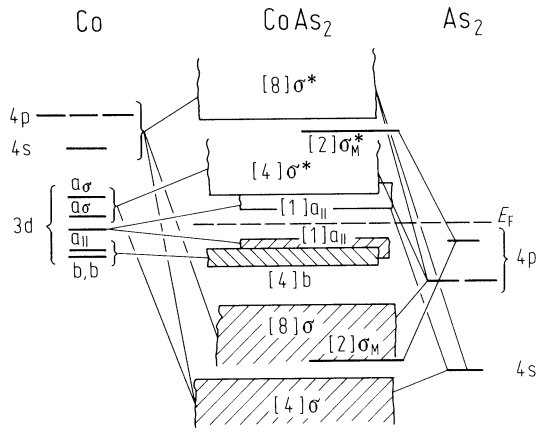

Fig. 2.

$CoAs_2$. Lattice parameters vs. temperature [77K]. Pseudo-marcasite cell *a*', *b*', *c*', β ', with $\boldsymbol{a}' = (\boldsymbol{a} - \boldsymbol{c})/2$, $\boldsymbol{b}' = \boldsymbol{b}$ and $\boldsymbol{c}' = (\boldsymbol{a} + \boldsymbol{c})/2$, where $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$, β refer to the true arsenopyrite-type cell. Linear temperature dependence of the unit cell volume from 300 to 1300 K.