

substance: CoAsSe

property: crystal structure, physical properties

CoAsSe (r) (pararammelsbergite-type modification)

energy gap

$E_{g,th}$	0.2 eV	from $\log \rho \propto E_g/2kT$ up to 670K (refers possibly to the marcasite-type modification)	59H
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transition temperatures

T_{tr}	753 K		79K
	$\approx 753 - 8100$ x	x < 0.02	for Se rich compositions CoAs _{1-x} Se _{1+x}
	$\approx 753 - 8760$ y	y < 0.02	for As rich compositions CoAs _{1+y} Se _{1-y}

A 30 min treatment at $T = 1870$ K, $p = 60$ kbar partially transformed the marcasite phase to the cubic pyrite derivative [75H].

lattice parameters, density

(RT values) (space group $D_{2h}^{15} - Pbca$)

Compound	a [Å]	b [Å]	c [Å]	d_X [g cm ⁻³]	Ref.
CoAsSe (r) ^b	5.7285	5.7741	11.365	7.52	79K

^b) Ordered.

interatomic distances (in Å)

CoAsSe (h):	Co	- 2(As,Se)	2.352	
		4(As,Se)	2.375	
	(As,Se) - (As,Se)		2.485	79K

CoAsSe (marcasite-type modification)

thermoelectric power

S	$- 50 \mu V K^{-1}$	$T = 300$ K	on sintered material (quenched?)	80H
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For structure, chemical bond and comparative tables on crystallographic and physical properties of transition metal-V-VI compounds, see documents , , , .

References:

- 59H Hulliger, F.: *Helv. Phys. Acta* 32 (1959) 615.
- 75H Henry, R., Steger, J., Nahigian, H., Wold, A.: *Inorg. Chem* 14 (1975) 2915.
- 79K Kjekshus, A., Rakke, T.: *Acta Chem. Scand. A*33 (1979) 609.
- 80H Hulliger, F.: unpublished 1980.