

substance: NiAs₂

property: physical properties

NiAs₂ (r) (α -NiAs₂) (pararammelsbergite)

certainly semiconducting.

magnetic susceptibility

(in $10^{-6} \text{ cm}^3 \text{ mol}^{-1}$)

χ_m	– 20	$T = 80 \text{ K}$	χ in CGS-emu, powder sample	66B
	– 10	$T = 530 \text{ K}$		

very narrow homogeneity range [79K].

structural transition temperature

T_{tr}	853 K		77K, 79K 61Y
	863 K	at the Ni-rich side	
	871 K	at the As-rich side	

Ni_{0.94}Co_{0.06}As_{1.86}S_{0.14}

pararammelsbergite type, diamagnetic [72F].

NiAs₂ (β -NiAs₂) (rammelsbergite, marcasite type)

energy gap

$E_{g,th}$	0.05 eV	from $\log \rho \propto E_g/2kT$, $T = 400...500 \text{ K}$, sintered sample	59H
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magnetic susceptibility: constant paramagnetism 373...700 K, weakly T -dependent below; paramagnetic due to impurities [66B].

melting point

T_m	> 1313 K (?)	congruent, from tentative phase diagram (?)	61Y
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peritectic temperature

T_{perit}	1125 K		77K
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range of homogeneity: NiAs_{2-x}, $x \leq 0.01$ [63R, 68D].

lattice parameters $a(T)$, $b(T)$, $c(T)$: above 700 K increase of $a(T)$ and $b(T)$ steeper than linear in T , while $c(T)$ decreases [77K].

volume expansion coefficient

β	$3.0 \cdot 10^{-5} \text{ K}^{-1}$	$T = 300 \text{ K}$	from graphic representation; linear increase of unit-cell volume in the range 300...1100 K	77K
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The metastable marcasite structure persists down to 4 K [77K].

Comparative tables on structural data of transition metal dipnictides:

structure, chemical bond: see document [\[1\]](#) ,

crystallographical data of compounds with octahedrally coordinated cations, see document [\[2\]](#)

interatomic distances in pyrite- and pararammelsbergite-type compounds, see document [\[3\]](#) , in
marcasite- and loellingite-type compounds, see document [\[4\]](#) .

References:

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- 61Y Yund, R. A.: *Econ. Geol.* 56 (1961) 1273.
- 63R Roseboom, E. H.: *Amer. Mineral.* 48 (1963) 271.
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