substance: (transition metal)$(V)_2$ compounds
property: crystallographic data of transition-element dipnictides with octahedrally coordinated cations

Abbreviations: r: room temperature modification, h: high-temperature modification, l: low-temperature modification, p: high-pressure phase.

See also documents , , .
(RT values)

Cation configu-ration	Compound (Space group, coordination number)	*a* [Å]	*b* [Å]	*c* [Å]	*β* [°]	*d* [g cm^{-3}]	Ref.
d^6	Pyrites (T_h^6 – Pa3; *Z* = 4)						
	NiP_2(p)*)	5.4831				4.86	68D
	$NiAs_2$(p)*)	5.7634				7.24	68D
	$Ni_{0.5}Pd_{0.5}As_2$*)	5.877				7.60	66B
	$PdAs_2$*)	5.9845				7.94	66B
		5.9855				7.935	65F
	$PdSb_2$*)	6.459				8.625	63M
		6.4584					65F
	PtP_2	5.6956				9.238	60K1, 65F, 69D, 74B
	PtPAs	5.842					63H2
	$PtAs_2$	5.968					65M, 66B, 68S
		5.9665				10.79	65F, 60K1
	$PtSb_2$	6.428				10.964	65D
		6.4400					60K1, 65F
	PtSbBi	6.570					63H2
	$PtBi_2(h_l)$*)	6.7022				13.526	60K1, 65F
d^6	Marcasites (D_{2h}^{12} – Pnnm; *Z* = 2)						
	$NiAs_2$(h)^{b,d}) (β-$NiAs_2$)	4.759	5.797	3.539		7.09	60S
		4.757	5.793	3.544			61Y, 66B
		4.7583	5.7954	3,5449		7.088	68H2, 74K, 79K
	$NiSb_2$^{b,d})	5.178	6.319	3.832		8.01	70C
		5.1823	6.3168	3.8403		7.984	74K
		5.1837	6.3184	3.8408		7.979	68H2, 79K
d^6	Pararammelsbergites (D_{2h}^{15} – Pbca; *Z* = 8)						
	$NiAs_2$(r) (α-$NiAs_2$)	5.75	5.82	11.43			60H
		5.770	5.838	11.419		7.20	66B, 68S
		5.772	5.834	11.420			77K3, 68H2
	$Ni_{0.94}Co_{0.06}As_{1.86}S_{0.14}$	5.753	5.799	11.407			72F2
	$PtBi_2$(r)	6.732	6.794	13.346		13.34	80B

d^5	Arsenopyrites (C_{2h}^5 – $P2_1/c$; $Z = 4$)						
	CoP_2	5.610	5.591	5.643	116.82	5.08	72D
	$CoAs_2$[b])	5.918	5.876	5.964	116.45		62Q, 67P, 66B
		5.916	5.872	5.960	116.45	7.480	66S
		5.9106	5.8680	5.9587	116.432	7.49	71K
	$CoSb_2$[b,c])	6.52	6.38	6.55	118.2	8.37	61Z
		6.5077	6.3879	6.5430	117.660	8.34	71K
	RhP_2	5.7429	5.7942	5.8370	112.92	6.053	61R
		5.7417	5.7951	5.8389	112.911	6.12	71K
	$RhAs_2$[b,c])	6.041	6.082	6.126	114.33	8.127	62Q, 66B
		6.0629	6.0816	6.1498	114.707	8.15	71K
	RhAsSb[a])	6.36	6.28	6.41	115.4	8.55	63H1
	$RhSb_2$[b,c])	6.604	6.557	6.668	116.63	8.867	62Q, 61Z
		6.6156	6.5596	6.6858	116.821	8.89	71K
	$RhBi_2$(r)[b]) (α-$RhBi_2$)	6.96	6.83	7.01	118.2	11.79	61K, 61Z
		6.9207	6.7945	6.9613	117.735	11.86	71K
	IrP_2	5.746	5.791	5.851	111.60	9.32	77K1
		5.7453	5.7915	5.8494	111.575	9.25	71K
		5.7457	5.7906	5.8500	111.60	9.33	61R
	$IrAs_2$[b])	6.060	6.071	6.158	113.27	10.92	62Q, 66B
		6.0549	6.0717	6.1587	113.197	10.83	71K
	IrAsSb[a])	6.35	6.30	6.41	114.2	11.04	63H1
	$IrSb_2$[b])	6.58	6.53	6.68	115.5	11.17	61Z, 65Z
		6.5945	6.5492	6.6951	115.158	10.98	71K
	$IrBi_2$(?)	7.0	6.9	7.1	117	13.3	65Z
d^4	Loellingites (D_{2h}^{12} – Pnnm; $Z = 2$)						
	FeP_2	4.9732	5.6570	2.7235		5.11	68H2, 68H1
		4.9729	5.6568	2.7230		5.107	69D
	$FeAs_2$[b])	5.3007	5.9792	2.8816			63R
		5.3013	5.9859	2.8822		7.47	68H2, 74K, 79K
		5.291	5.981	2.880			68R
		5.300	5.984	2.881		7.48	72R, 60S, 60H
	$FeSb_2$[b,d])	5.830	6.535	3.197		8.16	72R, 72F1
		5.8328	6.5376	3.1973		8.154	68H2, 68H1
		5.819	6.520	3.189			53R
		5.830	6.534	3.195			77G
	RuP_2	5.1169	5.8915	2.8709		6.256	77K2
		5.1173	5.8932	2.8711			68H2, 68H1
		5.115	5.888	2.870		6.26	77K2
	RuPAs	5.26	6.04	2.92		7.41	63H2
	$RuAs_2$	5.4279	6.1834	2.9685		8.364	77K2
		5.4302	6.1834	2.9714			68H2, 68H1
	RuAsSb	5.76	6.48	3.10		8.45	63H2

	$RuSb_2$	5.9514	6.6743	3.1790	9.063	77K2
		5.9524	6.6737	3.1803		68H2, 68H1
		5.930	6.637	3.168	9.18	60K2
	OsP_2	5.1012	5.9022	2.9183	9.531	77K2
		5.1001	5.9012	2.9182		68H2, 68H1
	$OsAs_2$	5.4115	6.1900	3.0127	11.191	77K2
		5.4129	6.1910	3.0126		68H2, 68H1
	$OsSb_2$	5.937	6.684	3.210	11.31	61J
		5.9409	6.6880	3.2112		68H2, 68H1
		5.9411	6.6873	3.2109	11.291	77K2
		5.912	6.653	3.196	11.45	60K2
d^2	$CrSb_2$	6.020	6.877	3.275	7.24	67P
		6.025	6.873	3.266		78A
		6.0275	6.8738	3.2715	7.24	70H, 68H2
	at 80 K	6.0183	6.8736	3.2704	7.25	70H
d^4, d^6	$Fe_{0.5}Ni_{0.5}As_2$[b])	5.1377	5.9205	3.1077	7.28	79K
	$Fe_{0.5}Ni_{0.5}Sb_2$[b])	5.6417	6.4402	3.3855	8.12	79K
d^3, d^5(?)	$Mn_{0.5}Co_{0.5}P_2$*) (?)	4.996	5.685	2.745	5.06	72D

*) Metallic.

[a]) Anions probably disordered.

[b]) Temperature dependence of the lattice parameters: [77K3] and Figs. 1...4.

[c]) Arsenopyrite → loellingite transformation at high temperatures [77K3].

[d]) Marcasite structure persists down to 4 K [70H].

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Fig. 1.

$CoAs_2$. Lattice parameters vs. temperature [77K3]. 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.

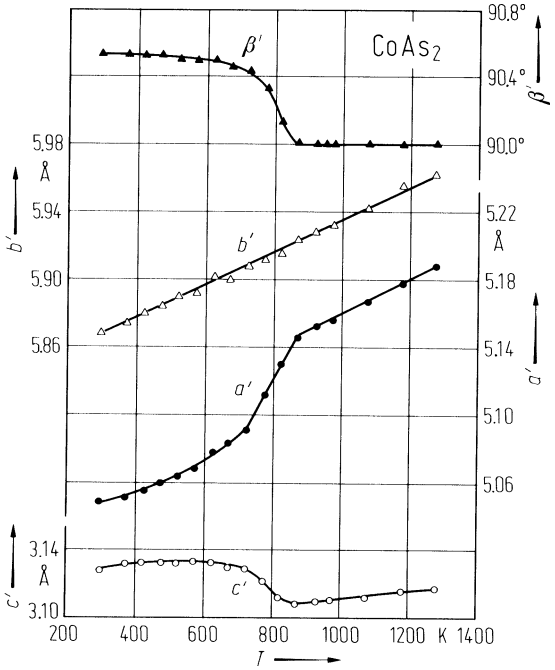

Fig. 2.

$CoSb_2$. Lattice parameters vs. temperature [77K3]. Pseudo-marcasite cell (cf. caption of Fig. 1). $CoSb_2$ decomposes at 1204 K.

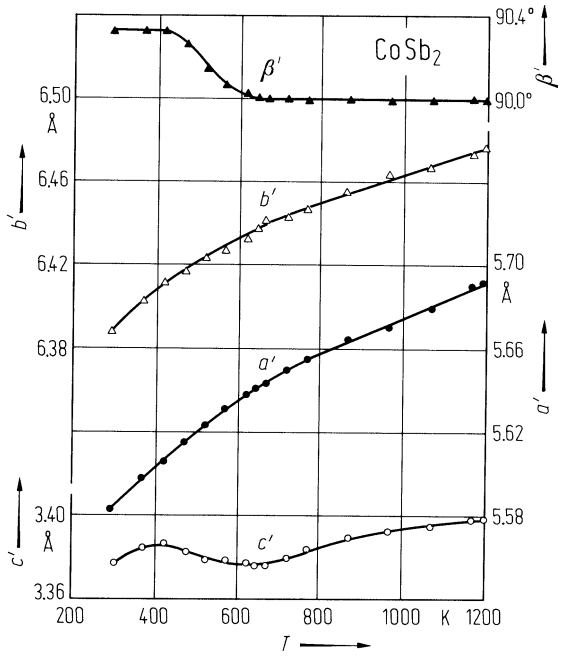

Fig. 3.

$RhSb_2$. Lattice parameters vs. temperature [77K3]. The unit-cell volume varies linearly with temperature. Cf. caption of Fig. 3 for parameters a',b', c', β'.

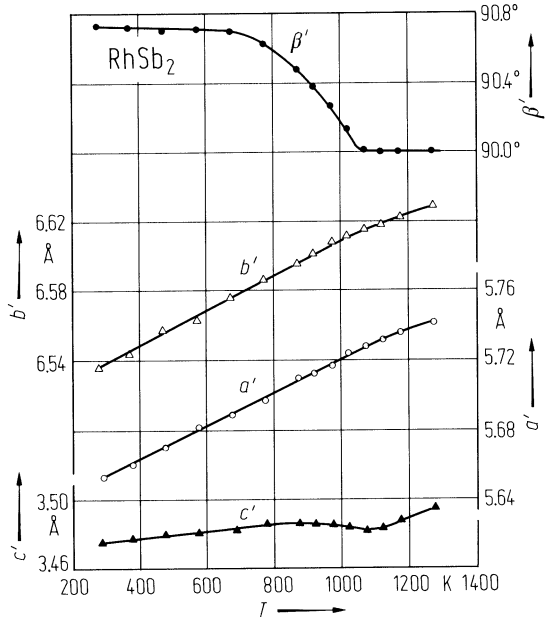

Fig. 4.

$IrSb_2$. Lattice parameters vs. temperature [77K3]. Cf. caption of Fig. 1 for parameters *a*', *b*', *c*', β'.