

substance: (transition metal)-V-VI compounds
property: crystallographic data for the arsenopyrite-type compounds

(RT values) (space group $C_{2h}^5 - P2_1/c$)

Compound	<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β [°]	d_X [g cm ⁻³]	Ref.
FePS	5.63	5.54	5.66	112.5	4.84	65H
	5.617	5.534	5.637	112.2		83L
FeAsS	5.828	5.720	5.792	113.20	6.09	61M
	5.749	5.724	5.812	113.20	6.15	65H
	5.750	5.702	5.787	112.3		83L
	6.02	5.93	6.02	112.13	6.95	39B
FeSbS*)	5.76	5.74	5.81	112.3	6.20	65H
FePSe	5.768	5.707	5.832	112.9		83L
	5.95	5.89	5.95	112.7	7.24	65H
FeAsSe	5.877	5.871	5.974	113.4		83L
	6.24	6.18	6.27	113.0	7.65	65H
FeAsTe	6.19	6.10	6.21	113.6	7.98	65H
FeSbTe	6.56	6.45	6.58	114.1	7.97	65H
	6.543	6.439	6.578	113.8		83L
RuPS	5.77	5.77	5.81	111.2	6.04	63H
	5.762	5.766	5.819	111.1		83L
RuAsS	5.95	5.92	6.02	113.1	7.08	63H
	5.945	5.920	6.025	112.92		72S
	5.934	5.913	6.016	112.9		83L
RuSbS	6.18	6.14	6.19	111.7	7.76	63H
	6.183	6.144	6.198	111.7		83L
RuPSe	5.97	5.92	5.98	111.8	7.14	63H
	5.969	5.919	5.989	111.6		83L
RuAsSe	6.08	6.06	6.14	112.7	8.11	63H
	6.089	6.067	6.165	112.5		83L
RuSbSe	6.351	6.299	6.396	113.39	8.54	80H
	6.358	6.307	6.404	113.3		83L
RuAsTe	6.36	6.30	6.40	113.6	8.58	63H
	6.361	6.302	6.410	113.5		83L
RuSbTe	6.603	6.538	6.687	114.57	8.87	80H
	6.543	6.601	6.651	114.1		83L
RuBiSe						66B
Ru _{0.5} Os _{0.5} AsS	5.992	5.944	6.044	113.08	8.47	72S
OsPS	5.78	5.78	5.83	110.9	9.24	63H
	5.771	5.779	5.846	110.8		83L
OsAsS	5.94	5.92	6.01	111.9	10.07	63H
	5.964	5.925	6.006	112.03	10.03	72S
	5.933	5.919	6.017	112.1		83L
OsSbS	6.21	6.15	6.22	111.7	10.35	63H
	6.210	6.151	6.227	111.7		83L
OsPSe	5.98	5.94	6.00	111.4	10.05	63H
	5.965	5.938	6.001	111.3		83L

OsAsSe	6.10	6.09	6.19	112.6	10.77	63H
	6.099	6.082	6.199	112.5		83L
OsSbSe	6.38	6.34	6.42	113.4	10.89	66B
	6.391	6.333	6.437	112.3		83L
OsBiSe	6.52	6.46	6.57	113.8	12.54	66B
OsAsTe	6.37	6.31	6.42	113.1	10.99	63H
	6.358	6.313	6.415	113.1		83L
OsSbTe	6.57	6.62	6.66	113.1	10.96	66B

*) See also document

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