9b. Structure, Melting Point, Density, and Energy Gap of Simple Inorganic Compounds

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Table 9b-1 lists the following properties of inorganic compounds:
Crystal structure (see also Sec. 9a)
Space group (see also Sec. 9a)
Melting point (see also Secs. 4d and 4j)
Density (see also Secs. 2b, 3f, and 4c)
Energy gap (for definition see Sec. 9c-1)

The compounds are listed not alphabetically but according to the location of the constituent elements in the periodic table (see Sec. 7b). The bulk of the table presents data on binaries; a few ternaries are also listed. Compounds are listed in groups beginning with the constituent elements from the first column and the seventh column and successively progressing toward the middle of the periodic system as follows (Roman numerals refer to columns):

IA-VII	IIB-VI
IA-VI	IIB-V
IA-V	IIIB-VI
IB-VII	IIIB-V
IB-VI	IVB-VII
IB-V	IVB-VI
IB-IV	IVB-V
IIA-VII	IVB-IV
IIA-VI	VB-VI
IIA-V	Transition metal oxides, sulfides, etc.
IIA-IV	Transition metal phosphides, arsenides, etc.
IIB-VII	Ternaries
	Noble gas compounds

With a few exceptions only those compounds have been listed for which at least one of the four properties has been measured. The list of compounds is, of course, far from complete; the cutoff is by necessity somewhat arbitrary.

There is often some disagreement among authors or sources. For an evaluation of the reliability of a particular figure one should go back to the original literature.

For further information the reader is referred to the references at the end of the table.

Abbreviations

cub	cubic	d	decomposes
tetr	tetragonal	b.p.	boiling point
hex	hexagonal	tr	transition (the compound listed is stable *below* the transition temperature)
orth	orthorhombic		
mon	monoclinic	liq	liquid
tricl	triclinic	s	sublimes
rhomb	rhombohedral	ign	ignites
Z	zinc blende	calc	calculated
W	wurzite	met	metallic (conduction)
per	perovskite		

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IA-VII (alkali halides (ref. 7):					
LiF	cub (NaCl)	$Fm3m$	870	2.601	~12
LiCl	cub (NaCl)	$Fm3m$	614	2.06[3]	~10
LiBr	cub (NaCl)	$Fm3m$	547	3.46[4]	~8.5
LiI	cub (NaCl)	$Fm3m$	446	4.06[1]	≥5.9
NaF	cub (NaCl)	$Fm3m$	992	2.79	≥10.5
NaCl	cub	$Fm3m$	800	2.16[4]	8.[illegible]
NaBr	cub (NaCl)	$Fm3m$	755	3.210	7.7
NaI	cub (NaCl)	$Fm3m$	651	3.665	≥5.8
KF	cub (NaCl)	$Fm3m$	880	2.505	10.9
KCl	cub (NaCl)	$Fm3m$	790	1.9917	8.5
KBr	cub (NaCl)	$Fm3m$	730	2.754	7.8
KI	cub (NaCl)	$Fm3m$	723	3.114	≥6.2
RbF	cub (NaCl)	$Fm3m$	760	2.88	10.4
RbCl	cub (NaCl)	$Fm3m$	715	2.76	8.2
RbBr	cub (NaCl)	$Fm3m$	682	3.35	7.7
RbI	cub (NaCl)	$Fm3m$	642	3.55	≥6.1
CsF	cub (NaCl)	$Fm3m$	683	3.58[5]	10.0
CsCl	cub	$Pm3m$	tr 460	3.988	≥8.0
CsCl (β)	cub (NaCl)	$Fm3m$	646	3.54 (calc.)	≥7.5
CsBr	cub (CsCl)	$Pm3m$	636	4.43[1]	7.0–8.0
CsI	cub (CsCl)	$Pm3m$	621	4.51	≥6.3
IA-VI:					
Li_2O	cub (CaF_2)	$Fm3m$	>1700	2.01[1]	
Li_2S	cub (CaF_2)	$Fm3m$	.....	1.66	
Li_2Se	cub (CaF_2)	$Fm3m$	.....	2.91	
Li_2Te	cub (CaF_2)	$Fm3m$	.....	3.24	
Na_2O	cub (CaF_2)	$Fm3m$	s	2.27	
Na_2S	cub (CaF_2)	$Fm3m$	950	1.85[6]	
Na_2Se	cub (CaF_2)	$Fm3m$	>875	2.58	
Na_2Te	cub (CaF_2)	$Fm3m$	.....	2.90	
K_2O	cub (CuF_2)	$Fm3m$	.....	2.32	
K_2S	cub (CaF_2)	$Fm3m$	471	1.80[5]	
IA-V:					
Li_3N	hex	$P6/mmm$	840	.....	2.3
NaN_3	orth (?)	.....	tr 19		
NaN_3	hex	$R32$ or $R\bar{3}m$	d 340	1.853	
KN_3	tetr	$I4/mcm$	350	2.038	
Rb_3N	tetr	$I4/mcm$	.....	2.788	
Li_3P	hex (β Al_2O_3)	$P6_3/mmc$	.....	1.43	
Na_3P	hex	$P6_3/mmc$	d	1.74 (calc)	
Li_3As	hex	$P6_3/mmc$	.....	2.42 (calc)	
Na_3As	hex	$P6_3/mmc$	.....	2.328	
K_3As	hex	$P6_3/mmc$	.....	2.14 (calc)	
Li_3Sb	hex	$P6_3/mmc$	>950	2.96 (calc)	
NaSb	mon	$P2_1/n$	465	4.03 (calc)	~0.8
Na_3Sb	hex (β Al_2O_3)	$P6_3/mmc$	856	2.67 (calc)	
KSb	.....	.....	605	.....	0.9
K_3Sb	hex (β Al_2O_3)	$P6_3/mmc$	812	2.35 (calc)	0.8
Cs_3Sb	cub	$Fd3m$	.....	5.01 (calc)	0.8
Na_3Bi	hex	$P6_3/mmc$	773	3.70 (calc)	
K_3Bi	hex	$P6_3/mmc$	.....	2.98 (calc)	
Cs_3Bi	cub	$Fd3m$	.....	5.01 (calc)	0.5–0.6
IB-VII:					
CuCl (1)	cub (Z)	$F\bar{4}3m$	tr 407	4.136	3.31
CuCl (2)	hex (W)	$P6_3mc$	422		
CuBr (1)	cub (Z)	$F\bar{4}3m$	tr 382	4.72	2.98
CuBr (2)	hex (W)	$P6_3mc$	488		
CuI	cub (Z)	$F\bar{4}3m$	605	5.667	3.06
AgF	cub (NaCl)	$Fm3m$	435	5.85[2]	
AgCl	cub (NaCl)	$Fm3m$	455	.....	3.0
AgBr	cub (NaCl)	$Fm3m$	430	.....	2.9
AgI (1)	cub (Z)	$F\bar{4}3m$	.....	6.0	2.8
AgI (2)	hex (W)	$P6_3mc$	558	5.68	
AgI (α) (146–558°C)	cub				

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IB-VII (*Cont.*):					
AuCl	.....	.....	tr 170 (→ $AuCl_3$)	7.4	
AuBr	.....	.....	d 115	7.9	
AuI	.....	$P4_2/n$	d 120	8.25	
IB-VI:					
CuO	mon	$A2/a$	d	6.40	~1.95
Cu_2O	cub	$Pn3m$	1236	6.0	2.2
CuS	hex	$P6_3/mmc$	tr 103	4.681	
$Cu_{1.8}S$	cub (NaCl?)	$Fm3m$(?)	.....	5.6 (170°C)	
Cu_2S (α)	orth	$Cmma$, $Cm2a$, $C2ma$ (?)	tr 105	5.8	
Cu_2S (β)	cub (CaF_2)	$Fm3m$(?)	1100	5.6	
CuSe	hex	$P6_3/mmc$	.....	5.99	
Cu_2Se (β)	cub (CaF_2)	$Fm3m$	1148	6.75	
Cu_2Te	hex	$P6/mmm$	1125	7.41 (calc)	
AgO	cub	?	d >100	7.44	
Ag_2O	cub (Cu_2O)	$Pn3m$	d 300	7.14_3	
Ag_2S (β)	mon	$P2_1/n$	tr 175	7.32_6	~1.3
Ag_2S (α)	cub (CsCl)	$Pm3m$	825	7.3_7	met
Ag_2Se (β)	mon	$P2_1/n$	.....	.....	~0.075
Ag_2Se (α)	cub (CsCl)	$Pm3m$	897	8.187	met (?)
Ag_2Te (α)	mon	$P2_1/n$	955	8.350	0.17
$AuTe_2$	mon	$C2/m$	464	9.31 (calc)	
IB-V:					
Cu_3N	cub	?	d 300	6.12 (calc)	
Cu_3P	hex	?	.....	7.15	
Cu_3As	hex	$P\bar{3}c$	830	7.85	
Cu_2Sb	tetr	$P4/nmm$	585		
Cu_3Sb	hex	?	687		
Ag_3Sb	orth	?	559(?)	9.74	
$AuSb_2$	cub (FeS_2)	$Pa3$	460(?)	9.98	
Au_2Bi	cub (spinel)	$Fd3m$	373	15.46	
IB-IV:					
AuSn	hex (NiAs)	$P6_3/mmc$	418	11.6	
Au_2Pb	cub	$Fd3m$, $F4_132$?			
IIA-VII:					
BeF_2	tetr	.....	800	2.01	
$BeCl_2$	orth	$Ibam$	s 405	1.90	
$BeBr_2$	.....	.....	s 488	3.46_5	
BeI_2	.....	.....	480	4.36 (calc)	
MgF_2	tetr (SnO_2)	$P4/mnm$	1263	3.148	~11
$MgBr_2$	hex (CdI_2)	$P\bar{3}m1$	711	3.72	
$MgCl_2$	hex (CdI_2)	$P\bar{3}m1$	714	2.32	
MgI_2	hex (CdI_2)	$P\bar{3}m1$	d	4.43	
CaF_2	cub	$Fm3m$	1418	3.18	~10
$CaCl_2$	orth	$Pnnm$	782	2.22	
$CaBr_2$	.....	.....	760	3.35_2	
CaI_2	hex	$P\bar{3}m$	575	3.95_6	
SrF_2	cub (CaF_2)	$Fm3m$	1400	4.18	
$SrCl_2$	cub (CaF_2)	$Fm3m$	875	3.05_2	
$SrBr_2$	orth	$Pbnm$	643	4.21_6	
SrI_2	.....	.....	402	4.54_9	
BaF_2	cub (CaF_2)	$Fm3m$	1320	4.893	
$BaCl_2$ (1)	mon	?	tr 925	3.85_6	
$BaCl_2$ (2)	cub (CaF_2)	$Fm3m$	962		
$BaBr_2$	orth	$Pnam$	850	4.886	
BaI_2	orth	$Pnam$	740	5.236	
IIA-VI:					
BeO	hex (W)	$P6_3mc$	2550	3.01–3.09	
BeS	cub (Z)	$F\bar{4}3m$	.....	2.36	
BeSe	cub (Z)	$F\bar{4}3m$	.....	4.32 (calc)	
BeTe	cub (Z)	$F\bar{4}3m$	.....	5.09 (calc)	
MgO	cub (NaCl)	$Fm3m$	2800	3.65	7.3

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IIA-VI (*Cont.*):					
MgS	cub (NaCl)	$Fm3m$	d	2.82	
MgSe	cub (NaCl)	$Fm3m$			
MgTe	hex (W)	$P6mc$	.....	3.86 (calc)	
CaO	cub (NaCl)	$Fm3m$	2600	2.62	6–7
CaS	cub (NaCl)	$Fm3m$	.....	2.80	
CaSe	cub (NaCl)	$Fm3m$			
CaTe	cub (NaCl)	$Fm3m$	.....	7.59₃	
SrO	cub (NaCl)	$Fm3m$	2415	3.9–4.8	~6
SrS	cub (NaCl)	$Fm3m$	.....	3.7	
SrSe	cub (NaCl)	$Fm3m$	.....	4.53 (calc)	~2
SrTe	cub (NaCl)	$Fm3m$	.....	.....	~2
BaO	cub (NaCl)	$Fm3m$	1923	4.7–5.7	~4.8
BaS	cub (NaCl)	$Fm3m$	.....	4.25	
BaSe	cub (NaCl)	$Fm3m$			
BaTe	cub (NaCl)	$Fm3m$			
IIA-V:					
Be_3N_2	cub (Tl_2O_3)	$Ia3$	~2200	2.70₉	
Be_3P_2	cub (Tl_2O_3)	$Ia3$	.....	2.23₄	
Mg_3N_2	cub (Tl_2O_3)	$Ia3$	d 1500	2.71	
Mg_3P_2	cub (Tl_2O_3)	$Ia3$	.....	2.05₅	
Mg_3As_2	cub (Tl_2O_3)	$Ia3$	800	3.148	
Mg_3Sb_2	hex	$P\bar{3}m$	930	4.09	0.82
Mg_3Bi_2	hex	$P\bar{3}m$	715	5.94	met (?)
Ca_3N_2	cub (Tl_2O_3)	$Ia3$	1195	2.63	
Ca_3P_2	cub (Tl_2O_3) (?)	$Ia3$ (?)	>1600	2.51	
Ca_3As_2	cub (Tl_2O_3) (?)	$Ia3$ (?)	d	2.50	
Ca_3Sb_2	cub (Tl_2O_3) (?)	$Ia3$ (?)			
Ca_3Bi_2	cub (Tl_2O_3) (?)	$Ia3$ (?)	928		
IIA-IV:					
Be_2C	cub (CaF_2)	$Fm3m$	d >2100	1.9	
Mg_2Si	cub (CaF_2)	$Fm3m$	1102	1.88	0.77
Mg_2Ge	cub (CaF_2)	$Fm3m$	1115	3.09	0.6–0.7
Mg_2Sn	cub (CaF_2)	$Fm3m$	778	3.591	0.3
Mg_2Pb	cub (CaF_2)	$Fm3m$	550	3.29	met (?)
Ca_2C	tetr				
Ca_2Si	tetr	.....	920	.....	1.9
$CaSi_2$	hex	$R\bar{3}m$	1220	2.450	
Ca_2Ge	orth	$Pnam$			
Ca_2Sn	tetr	.....	1122	.....	0.9
Ca_2Pb	.....	.....	1150	.....	0.4–0.5
IIB-VII:					
ZnF_2	tetr (SnO_2)	$P4/mnm$	872	4.84	
$ZnCl_2$	hex ($CdCl_2$)	$R\bar{3}m$	262	2.91	
$ZnBr_2$	hex ($CdCl_2$) (?)	$R\bar{3}m$ (?)	394	4.21₉	
ZnI_2	hex ($CdCl_2$)	$R\bar{3}m$	446	4.696	
CdF_2	cub (CaF_2)	$Fm3m$	1110	6.64	>6.0
$CdCl_2$	hex (rhomb)	$R\bar{3}m$	568	4.04₇	
$CdBr_2$	hex (rhomb)	$R\bar{3}m$	568	5.19₂	
CdI_2	hex (W)	$P6mc$	387	5.4–5.6	
HgF_2	cub (FeS_2)	$Pa3$	d 645	8.95	
Hg_2F_2	cub	$I4/mmm$	570	8.73	
$HgCl_2$	orth	$Pmnb$	277	5.6	
Hg_2Cl_2	tetr	$I4/mmm$	s 400	6.47	
$HgBr_2$	orth	$Bb2m$	241	6.05₂	
Hg_2Br_2	tetr	$I4/mmm$	s 345	7.307	
HgI_2	tetr	$P4/nmc$	tr 126	6.28	
HgI_2	orth	.....	259	6.27₁	
Hg_2I_2	tetr	$I4/mmm$	s 140	7.70	
IIB-VI (refs. 11, 12):					
ZnO	hex (W)	$P6mc$	1975	5.7	3.436
ZnS (β)	cub (Z)	$F\bar{4}3m$	tr 1020	4.10₂	3.84
ZnS (α)	hex (W)	$P6mc$	1850 (150 atm)	4.08	3.91
ZnSe	cub (Z)	$F\bar{4}3m$	~1500	5.65	2.83
ZnTe	cub (Z)	$F\bar{4}3m$	1238	5.54–6.39	2.39

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IIB-VI (refs. 11, 12) (*Cont.*):					
CdO	cub (NaCl)	$Fm3m$	s 1559	8.15	2.2(?)
CdS (β)	cub (Z)	$F\bar{4}3m$	s 685	4.87	2.5
CdS (α)	hex (W)	$P6mc$	1750 (100 atm)	4.82	2.582
CdSe	hex (W)	$P6mc$	>1258	5.81	1.84
CdTe	cub (Z)	$F\bar{4}3m$	1098	6.20	1.607
HgO	orth	$Pmnn$	d 100	11.23	
HgS (α)	hex	$P3_121$	tr 386	8.176	
HgS (β)	cub (Z)	$F\bar{4}3m$	s 583	7.65	2.5
HgSe	cub (Z)	$F\bar{4}3m$	798	8.24 (calc)	met
HgTe	cub (Z)	$F\bar{4}3m$	670	8.12 (calc)	met
IIB-V (ref. 13):					
Zn_3N_2	cub	$Ia3$	.....	6.4 (calc)	
Zn_3P_2 (1)	cub	$Pn3m$	>420	4.678 (calc)	
Zn_3P_2 (2)	tetr	$P4_2nmc$	.....	4.54 (calc)	
Zn_3As_2 (1)	cub	$Pn3m$	1015	5.578	1.0
Zn_3As_2 (2)	tetr	$P4_2nmc$	.....	4.21–4.76	
ZnSb	orth	$Pbcn$	544	6.383	0.56
Cd_3N_2	cub	$Ia3$			
Cd_3P_2 (1)	cub	$Pn3m$	.....	5.95_6 (calc)	0.6
Cd_3P_2 (2)	tetr	$P4_2nmc$	.....	5.956	
Cd_3As_2 (1)	cub	$Pn3m$	.....	6.21	
Cd_3As_2 (2)	tetr	$P4_2/nmc$	721	4.25	0.13
Cd_3Sb_2	mon	.....	421		
CdSb	orth	$Pbcn$	456	6.02	0.48
IIIB-VII:					
B_2F_4	mon	$P2_1/n$	− 56	1.92 (calc)	
BCl_3	hex	$P6_3$	−107	1.80 (calc)	
BBr_3	hex	?	− 46	3.41 (calc)	
BI_3	hex	$P6_3$	43		
AlF_3	hex	$R32$	1040	3.197 (calc)	
$AlCl_3$	mon	$A2/m$	s 178	2.48 (calc)	
$AlBr_3$	mon	$P2_1/a$	97.5	3.205	
GaF_3	hex	$R\bar{3}c$	>1000		
$GaCl_3$	orth	$Pcnn$	170.5	2.74 ?	
GaI_3	orth	$Amma$	212		
InF_3	hex	$R\bar{3}c$	1170		
$InCl_2$	orth	?	235	3.64	
$InCl_3$	mon	$C2/m$	s 400		
InBr	orth	$Amam$	220	4.96	
InI	orth	$Amam$	351	5.39 (calc)	
TlF	orth	$Fmmm$	b.p. 300	8.23	
TlCl	cub	$Pm3m$	430	7.02	3.41
$TlCl_3$	mon	$C2/m$	25		
TlBr	cub	$Pm3m$	460	7.54	3.02
TlI	orth	$Amam$	tr 175		
TlI	cub	$Pm3m$	440	7.45 (calc)	
IIIB-VI)ref. 8):					
B_2O_3	cub or hex (?)	$P3_1$	294	2.44	
B_2S_3	cub or hex (?)	.....	390	1.85	
B_2S_3	cub or hex (?)	.....	310	1.55	
B_2Se_3	cub or hex (?)	.....	d		
Al_2O_3 (α)	hex (Fe_2O_3)	$R\bar{3}c$	2050	3.99	8.3
Al_2O_3 (β)	hex (NiAs)	$P6_3/mmc$	2040	3.30	
Al_2O_3 (γ)	cub (spinel)	$P4_132$	tr to α	3.619	
Al_2S_3	hex	.....	1118	2.32	4.1
Al_2Se_3	hex	$P6mc$	.....	3.21	3.1
Al_2Te_3	hex	$P6mc$	900	4.54	2.5
Ga_2O_3	hex (Fe_2O_3)	$R3c$	1740	6.44 (calc)	4.4
Ga_2O	.....	.....	>660	4.77	
Ga_2S_3 (β)	hex (W)	$P6mc$	1255	3.67 (calc)	~2.5
Ga_2S_3 (α)	cub (Z)	$F\bar{4}3m$	tr 550	3.63	2.85
GaS	hex	$P6/mmc$	965	3.86	~2.9
Ga_2S	.....	.....	>800	4.18	
Ga_2Se_3 (β)	hex (W)	$P6mc$	1020	4.92	

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IIIB-VI (ref. 8) (*Cont.*):					
Ga_2Se_3 (α)	cub (Z)	$F\bar{4}3m$	.....	.....	~1.9
GaSe	hex	$P6_3/mmc$	960	5.03	2.04
Ga_2Se	.....	.....	.....	5.02	
Ga_2Te_3 (β)	hex (W)	$P6mc$	790		
Ga_2Te_3 (α)	cub (Z)	$F\bar{4}3m$	tr 670	5.57	1.2 or 1.5
GaTe	.....	.....	824	5.44	1.7
In_2O_3	cub (Tl_2O_3)	$Ia3$	d 850	7.18	~2.8
InO					
In_2O	.....	.....	2 650–700 (in vac)	6.99	
In_2S_3	cub	$Fd3m$	1050	4.63	~2.0
InS	.....	.....	692	5.18	
In_2S	.....	.....	653	5.87	
In_2Se_3 (β)	.....	.....	890		
In_2Se (α)	.....	.....	tr 196	5.48	1.2
InSe	hex	$P6_3/mmc$	660	5.55	1.05
In_2Se	.....	.....	.....	6.17	
In_2Te_3 (α)	cub (Z)	$F\bar{4}3m$	667	5.75	~1.0
InTe	tetr	$I4/mcm$	696	6.29	
In_2Te	.....	.....	460	6.47	
Tl_2O_3	cub	$Ia3$	717	10.19	
Tl_2O	.....	.....	300		
Tl_2S_3	.....	.....	260		
TlS	tetr	$I4/mcm$	.....	7.62	
Tl_2S	hex	$R\bar{3}$ or $R3$	448	8.0	~1.0
Tl_2Se_3					
TlSe	tetr	$I4/mcm$	.....	5.175	0.57
Tl_2Se	.....	.....	398		
Tl_2Te_3	.....	.....	428		
IIIB-V (refs. 9, 10):					
BN	cub (Z)	$F\bar{4}3m$	s 3000	2.20	4.6
BP	cub (Z)	$F\bar{4}3m$	ign 200		
AlN	hex (W)	$P6_3mc$	>2200	3.26	~3.3
AlP	cub (Z)	$F\bar{4}3m$	.....	2.424 (calc)	2.5
AlAs	cub (Z)	$F\bar{4}3m$	1600	3.598	2.3
AlSb	cub (Z)	$F\bar{4}3m$	1060	4.34	1.55
GaN	hex (W)	$P6mc$	.....	6.10	
GaP	cub (Z)	$F\bar{4}3m$	~1350	.....	2.35
GaAs	cub (Z)	$F\bar{4}3m$	1280	.....	1.35
GaSb	cub (Z)	$F\bar{4}3m$	728	.....	0.7
InN	hex (W)	$P6mc$	.....	6.88	2.1
InP	cub (Z)	$F\bar{4}3m$	1055	.....	1.3
InAs	cub (Z)	$F\bar{4}3m$	942	.....	0.35
InSb	cub (Z)	$F\bar{4}3m$	525	.....	0.17
InBi	tetr	.....	110	.....	met
TlSb	cub (CsCl)	$Pm3m$			
TlBi	cub (CsCl)	$Pm3m$	230		
IVB-VII:					
CBr_4 (α)	mon	.....	tr 47	3.42	
CBr_4 (β)	cub	$P\bar{4}3m$	90		
CI_4	cub	$P\bar{4}3m$	d 171	4.32	
$SiBr_4$	.....	.....	5	2.81_4	
SiI_4	cub (FeS_2?)	$Pa3$	120.5		
$GeBr_2$	.....	.....	122		
$GeBr_4$	.....	.....	26.1	3.13_2	
GeI_4	cub (FeS_2)	$Pa3$	144.0	4.32_2	
$SnCl_2$	orth	.....	247	3.9	
$SnCl_4$	.....	.....	−33	2.23 (liq)	
$SnBr_2$	orth	.....	232	5.12	
$SnBr_4$	orth	.....	31	3.34 (liq)	
SnI_2	mon	.....	320	5.21	
SnI_4	cub (FeS_2)	$Pa3$	145	4.46	

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
IVB-VII (*Cont.*):					
PbF_2	orth	*Pnam*	tr 200	8.37	
PbF_2	cub (CaF_2)	*Fm3m*	822	7.66	~5.0
$PbCl_2$	orth	?	501	5.85	
$PbCl_4$	.....	.....	−15	3.18	
$PbBr_2$	orth	*Pnam*	373	6.71 (calc)	
PbI	.....	.....	d 300		
PbI_2	hex	$P\bar{3}m1$	402	6.18	2.57
IVB-VI:					
SiO_2:					
α-Cristobalite	pseudocub.	$P2_12_12_1$	.....	2.30	
β-Cristobalite	cub	$P2_13$	1728	2.32	
α-Quartz	hex	$P3_121$ or $P3_221$	tr 600	2.66	
β-Quartz	hex	$P6_122$ or $P6_422$			
α-Tridymite	orth	.....	1680	2.3	
β-Tridymite	hex	$P6_3/mmc$			
Fused silica	tetr				
SiS_2	orth	*Ibam*	1090	2.02	
SiS	.....	.....	.....	1.85	
GeO_2	hex	$P3_121$	1115	4.7	
GeS_2	orth	*Fdd2*	~800	3.01	
GeS	orth	*P6nm*	625	4.01	1.8
GeSe	orth	*P6nm*	780	.....	1.0
$GeSe_2$	orth	.....	707	4.50	
GeTe	cub (NaCl)	*Fm3m*	725		
SnO_2	tetr	*P4/mnm*	d 1127	7.0	
SnO	tetr (PbO)	*P4/nmm*	d 700–950	6.45	
SnS_2	hex (W)	*P6mc* (?)	d	4.5	2.3
SnS	orth	*P6nm*	880	5.08	~1.1
$SnSe_2$	.....	.....	650	5.0	~1.0
SnSe	orth	.....	860	6.18	1.3
SnTe	cub (NaCl)	*Fm3m*	800	6.48	0.3
PbO_2	tetr (SnO_2)	*P4/mnm*	d 290	9.33–9.44	
PbO (red)	tetr	*P4/nmm*	888	9.13	~2.6
PbO (yellow)	orth	*Pca2*	.....	9.52	
Pb_2O	cub (Cu_2O)	*Pn3m*	d	8.35	
PbS	cub (NaCl)	*Fm3m*	1114	7.5	0.37
PbSe	cub (NaCl)	*Fm3m*	1065	8.1–8.2	0.27
PbTe	cub (NaCl)	*Fm3m*	905	8.16	0.33
IVB-V:					
SnAs	cub (NaCl)	*Fm3m*	600		
Sn_2As_2	orth	.....	585		
SnSb	cub (NaCl)	*Fm3m*	425		
IVB-IV:					
SiC	hex (W)	Pb_3mc	~2700	3.17–3.22	3.1
SiC (carborundum)	cub (Z)	$F\bar{4}3m$	.....	3.21₈	2.86
VB-VI (ref. 8):					
As_2O_3 (1)	mon	$P2_1n$	315	4.14	
As_2O_3 (2)	cub	*Fd3m*	s 193	3.874	
As_2S_3	mon	$P2_1n$	300	3.43	
As_2Se_3	hex (rhomb)	$R\bar{3}m$ (?)	360	4.75	1.3
As_2Te_3	mon	$P2_1n$ (?)	362	.....	1.0–1.2
Sb_2O_3 (1)	cub	*Fd3m*	656	5.1–5.8	
Sb_2O_3 (2)	orth	*Pnaa*	656	~5.7	
Sb_2S_3	orth	*Pbnm*	550	4.64	1.7
Sb_2Se_3	orth	*Pbnm*	611	5.8	1.2–1.35
Sb_2Te_3	hex (rhomb)	$R\bar{3}m$ (?)	629	.....	0.3
Bi_2O_3 (1)	orth	.....	820	8.9	
Bi_2O_3 (α)	cub	*Pn3m*	tr 704	8.2	
Bi_2O_3 (β)	tetr	$P\bar{4}b2$	.....	9.14	
Bi_2S_3	orth	*Pbnm*	850 (?)	7.39	1.1–1.3
Bi_2Se_3	hex (rhomb)	$R\bar{3}m$ (?)	710	6.82	0.35
Bi_2Te_3	hex (rhomb)	$R\bar{3}m$	580	7.65	0.15

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
Transition Metal Oxides, Sulfides, Selenides, and Tellurides					
Sc_2O_3	cub (Tl_2O_3)	$Ia3$	.....	3.86[1]	
TiO_2 (rutile)	tetr (SnO_2)	$P4/mnm$	1835	4.283	3.05
Ti_2O_3	hex (Fe_2O_3)	$R\bar{3}c$	2130	4.6	
TiO	cub (NaCl)	$Fm3m$	1750	4.93	met
V_2O_3	orth	$Pnm2$	700–800	3.57[7]	
V_2O_4	tetr (SnO_2)	$P4/mnm$	1967	4.4	
V_2O_5	hex (Fe_2O_3)	$R\bar{3}c$	1970	4.78	
Cr_2O_3	hex (Fe_2O_3)	$R\bar{3}c$	1990	5.215	
MnO_2	tetr (SnO_2)	$P4/mnm$	d 535	5.02[6]	
Mn_2O_3	cub (Tl_2O_3)	$Ia3$	d 1080	4.5 or 4.8	
MnO	cub (NaCl)	$Fm3m$	1650	5.4	
Mn_3O_4	tetr	$I4/amd$	1705	4.8	
MnS_2	cub (FeS_2)	$Pa3$	d	3.40	
MnS	cub (NaCl)	$Fm3m$	d	3.95	
$MnSe_2$	cub (FeS_2)	$Pa3$	.....	.....	0.15
MnSe	cub (NaCl)	$Fm3m$	.....	5.59	2.5
$MnTe_2$	cub (FeS_2)	$Pa3$	.....	6.15 (calc)	
MnTe	hex (NiAs)	$P6_3/mmc$			
Fe_2O_3 (hematite)	hex	$R\bar{3}c$	1565	5.24	
Fe_2O_3 (γ)	cub	$P4_132$ or $P2_13$	.....	4.59	
FeO	cub (NaCl)	$Fm3m$	1420	5.7	
Fe_3O_4 (magnetite)	cub (spinel)	$Fd3m$	d 1538	5.17	
FeS	hex (NiAs)	$P6_3/mmc$	1193	4.84	
FeS_2 (1) (pyrite)	cub	$Pa3$	1171	5.005	1.2
S_2 (2)	orth	$Pnnm$	tr 450	4.92	
Se	hex (NiAs)	$P6_3/mmc$			
$FeSe_2$	cub (FeS_2)	$Pa3$	.....	5.0	
CoO	cub (NaCl)	$Fm3m$	1935	5.7–6.7	
CoS	hex (NiAs)	$P6_3/mmc$	>1116	5.45	
CoS_2	cub (FeS_2)	$Pa3$	.....	4.27	
Co_3S_4	cub (spinel)	$Fd3m$	.....	4.86	
CoSe	hex (NiAs)	$P6_3/mmc$	.....	7.65	
CoTe	hex (NiAs)	$P6_3/mmc$			
NiO	cub (NaCl)	$Fm3m$	2090	6.7–6.9	~4.0
NiS (millerite)	hex	.....	797	5.41	
NiS (β)	hex (NiAs)	$P6_3/mmc$	797	4.6	
NiS_2	cub (FeS_2)	$Pa3$	.....	4.3 (calc)	
NiSe	hex (NiAs)	$P6_3/mmc$	.....	8.46	
NiTe	hex (NiAs)	$P6_3/mmc$			
ZrO_2 (1)	cub (CaF_2)	$Fm3m$	2715	5.35	
ZrO_2 (2)	mon	$P2_1/a$	2700	5.82	
Nb_2O_5	orth	.....	1520	4.5–4.6	
Nb_2O_5	.....	.....	1772		
MoO_2	tetr (SnO_2)	$P4/mnm$	.....	6.44–6.47	
MoO_3	orth	$Pbnm$	795	4.5	
MoS_2 (molybdenite)	hex (NiAs)	$P6_3/mmc$	1185	4.92	~1.0
Ta_2O_5	orth	.....	d 1470	8.73[5]	
WO_2	tetr (SnO_2)	$P4/mnm$	ign	12.11	
WO_3	tricl	.....	1470	7.16	
ThO_2	cub (CaF_2)	$Fm3m$	3050	9.87	
UO_2	cub (CaF_2)	$Fm3m$	2227	10.9	
Transition Metal Phosphides, Arsenides, etc.					
CrAs	hex	.....	.....	6.35	
CrSb	hex (NiAs)	$P6_3/mmc$	1100		
MnP	orth	$Pnam$	1190	5.49	
MnAs	orth	$Pnam$	d 400	~6.2	
MnSb	hex (NiAs)	$P6_3/mmc$	809		
Mn_2Sb	tetr	$P4/nmm$	948		
MnBi	hex (NiAs)	$P6_3/mmc$			
MnSi	cub (FeSi)	$P2_13$	1280	5.9	
FeP	orth	$Pnam$	>1000	5.2 or 6.07	
FeAs (η)	hex (NiAs)	$P6_3/mmc$	1020	7.83	

TABLE 9b-1. CLASSIFICATION AND PROPERTIES OF INORGANIC COMPOUNDS (*Continued*)

Compound	Structure	Space group	Melting point, °C	Density, g/cm³	Energy gap, eV
Transition Metal Phosphides, Arsenides, etc. (*Cont.*):					
FeSb	hex (NiAs)	$P6_3/mmc$	~1000		
FeSi	cub	$P2_13$	1410	6.21	
NiAs	hex	$P6_3/mmc$	968	7.72	
NiSb	hex	$P6_3/mmc$	1158	7.54	
NiSi	cub (FeSi)	$P2_13$	1000		
Ternaries (refs. 17, 18)					
$CuFeS_2$ (chalcopyrite)	tetr	$I\bar{4}2d$	1085	4.1–4.3	0.53
$CuAlS_2$	tetr	$I\bar{4}2d$	.....	3.45	2.5
$CuInS_2$	tetr	$I\bar{4}2d$	950	4.71	1.2
$CuInSe_2$	tetr	$I\bar{4}2d$	990	5.65	0.92
$CuInTe_2$	tetr	$I\bar{4}2d$	790	6.00	0.95
$CuTlS_2$	tetr	$I\bar{4}2d$	.....	6.07	
$AgInS_2$	tetr	$I\bar{4}2d$	850	4.97	1.9
$AgInSe_2$	tetr	$I\bar{4}2d$	.....	5.80	1.18
$AgInTe_2$	tetr	$I\bar{4}2d$	.....	6.08	0.96
$ZnSiAs_2$	tetr	$I\bar{4}2d$	.....	.....	2.1
$ZnGeP_2$	tetr	$I\bar{4}2d$	.....	4.04	2.2
$CdGeP_2$	tetr	$I\bar{4}2d$	.....	.....	1.8
$ZnGeAs_2$	tetr	$I\bar{4}2d$	.....	5.26	>0.6
Cu_3SbS_3	cub	$I\bar{4}3m$	550	4.4–5.1	~1.0
Cu_3AsS_3	cub	$I\bar{4}3m$	640	~4.5	~1.0
Ag_3SbS_3	hex	$R3c$	.....	5.85	~1.9
Ag_3AsS_3	hex	$R3c$	.....	5.69 (calc)	~2.0
$AgSbS_2$	mon	$A2/a$	.....	5.2–5.3	
$AgSbSe_2$	cub	.....	611	6.64	~0.7
$AgSbTe_2$	cub	.....	555	7.12	~0.6
$MgAl_2O_4$ (spinel)	cub	$Fd3m$	2135	3.57	
$ZnFe_2O_4$	cub (spinel)	$Fd3m$	1590	5.29	
$CuFe_2O_4$	cub (spinel)	$Fd3m$	.....	5.42	
$NiFe_2O_4$	cub (spinel)	$Fd3m$	.....	5.268	
$MnFe_2O_4$	cub (spinel)	$Fd3m$	.....	4.52	
$ZnAl_2S_4$	cub (spinel)	$Fd3m$	.....	3.30	
$CaIn_2S_4$	cub (spinel)	$Fd3m$	.....	4.10	
$HgIn_2S_4$	cub (spinel)	$Fd3m$	.....	5.79	
$CaTiO_3$ (perovskite)	cub	$Pm3m$	1915	~4.0	3.7
$BaTiO_3$ (1)	cub (per)	$Pm3m$	1618	~6.0	
$BaTiO_3$ (2)	tetr	$P4/mmm$	tr 120	6.02 (calc)	3.5
$SrTiO_3$	cub (per)	$Pm3m$	1910	5.11 (calc)	3.4
$PbTiO_3$ (2)	tetr	$P4/mmm$	tr 490	7.94 (calc)	
$FeTiO_3$	hex	$R\bar{3}$	1470	4.4–4.9	
$PbZrO_3$ (2)	tetr	$P4/mmm$	tr 233	8.10 (calc)	
$KNbO_3$ (1)	cub (per)	$Pm3m$	1039	4.634 (calc)	
$KNbO_3$ (2)	orth	.....	tr 434		
$KTaO_3$ (1)	cub (per)	$Pm3m$	1357	7.022 (calc)	3.5
$NaNbO_3$ (1)	cub (per)	$Pm3m$	1450	4.609 (calc)	
$LaMnO_3$	pseudo cub (distorted per)	.....	.....	6.89 (calc)	
$NaClO_3$	cub (FeSi)	$P2_13$	248	2.49	
$NaBrO_3$	cub (FeSi)	$P2_13$	381	3.254	
$NaIO_3$	orth	$Pnma$	.....	~4.26	
$KClO_3$	mon	$P2_1/m$	368	2.32	
Noble gas compounds (ref. 19):					
XeF_2	tetr	$I4/mmm$	140	4.32 (calc)	
XeF_4	mon	$P2_1/n$	~114	4.04 (calc)	
XeF_6	.....	.....	46		
XeO_3	orth	$P2_12_12_1$	.....	4.55	

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