











































Crystal structure	Element
Hexagonal close-packed (hcp)	Be, Ca, Co, Mg, Ti, Zn
Cubic close-packed (ccp)	Ag, Al, Au, Cd, Cu, Ni, Pb, Pt
Body-centred cubic (bcc)	Ba, Cr, Fe, W, alkali metals
Primitive cubic (cubic-P)	Ро









Radius ratio ( $\gamma$ )	CN for 1:1 and 1:2 stoichiometries	Binary AB structure type	Binary AB <sub>2</sub> structure type
1	12	None known	None known
0.732-1	8:8 and 8:4	CsCl	CaF <sub>2</sub>
0.414-0.732	6:6 and 6:3	NaCl (ccp), NiAs (hcp)	TiO <sub>2</sub>
0.225-0. 414	4:4	ZnS (ccp and hcp)	

Lattice Type	$R.R. = r_+/r$	1/R.R. 4
1:1 Stoichiometry		
Zinc blende	0.225	4.44
Rock salt	0.414	2.41
Cesium chloride	0.732	1.37
1:2 Stoichiometry		ă.
Rutile	0.414	2.41
Fluorite	0.732	1.37







		Lattic	е Туре			Lattic	е Туре
Compound	R.R.	Predicted	Observed	Compound	R.R.	Predicted	Observed
lie	0.76	CsCl	NaCl	CsF	(0.66)	NaCl	NaCl
	0.70	NaCl	NaCl	CsCl	(0.93)	CsCl	CsCl
LiBr	0.24	NaCl	NaC1	CsBr	0.99	CsCl	CsCl
Libi	0.42	NaCl	NaCl	Csl	0.88	CsCl	CsCl
NaF	0.47	CsCl	NaCl	BeO	0.47	NaCl	ZnS
NaCi	0.57	NaCl	NaCl	BeS	0.35	ZnS	ZnS
NaD-	0.03	NaCl	NaCl	MgO	0.68	NaCl	NaCl
Nal	0.56	NaCl	NaCl	MgS	0.51	NaCl	NaCl
KE	(0.79)	CrCl	NaCl	CaO	0.90	CsCl	NaCl
KC	(0.70)	CaCl	NaCl	CaS	0.67	NaCl	NaCl
KU.	0.91	CsCl	NaCl	AIP	0.32	ZnS	ZnS
KBI	0.84	CsCl	NaCl	TICI	0.98	CsCl	CsCl
	0.74		NaCl	ZnS	0.52	NaCl	ZnS
RDF	(0.72)	NaCl	NaCl	CdS	0.64	NaCl	ZnS
RDCI DLD	0.99	CsCl	NaCl	Has	0.68	NaCl	ZnS
RDBr	0.91	CsCl	NaCl	iigo			
RbCl RbBr RbJ	0.99 0.91	CsCl CsCl	NaCl NaCl NaCl	HgS	0.68	NaCl	Zr













	i stracture to the hinning of h	
Close-packing type	Hole filling	Structure type (exemplar)
Cubic (ccp)	All octahedral	Rock salt (NaCl)
	All tetrahedral	Fluorite (CaF <sub>2</sub> )
	Half octahedral	CdCl <sub>2</sub>
	Half tetrahedral	Sphalerite (ZnS)
Hexagonal (hcp)	All octahedral	Nickel arsenide (NiAs); with some distortion from perfect hcp CdI <sub>2</sub>
	Half octahedral	Rutile (TiO <sub>2</sub> ); with some distortion from perfect hcp
	All tetrahedral	No structure exists: tetrahedral holes share faces
	Half tetrahedral	Wurtzite (ZnS)

Table 3.4         The crystal structure	s of compounds
Crystal structure	Example*
Antifluorite	K <sub>2</sub> O, K <sub>2</sub> S, Li <sub>2</sub> O, Na <sub>2</sub> O, Na <sub>2</sub> Se, Na <sub>2</sub> S
Caesium chloride	CsCl, TII, CsAu, CsCN, CuZn , NbO
Fluorite	$CaF_{2}$ , UO <sub>2</sub> , HgF <sub>2</sub> , LaH <sub>2</sub> , PbO <sub>2</sub>
Nickel arsenide	NiAs, NiS, FeS, PtSn, CoS
Perovskite	<b>CaTiO</b> , (distorted), SrTiO, PbZrO, LaFeO <sub>3</sub> , LiSrH <sub>3</sub> , KMnF <sub>3</sub>
Rock salt	NaCl, KBr, Rbl, AgCl, AgBr, MgO, CaO, TiO, FeO,
	NiO SnAs LIC ScN
Rutile	TiO <sub>2</sub> , MnO <sub>2</sub> , SnO <sub>2</sub> , WO <sub>2</sub> , MgF <sub>2</sub> , NiF <sub>2</sub>
Sphalerite (zinc blende)	ZnS, CuCl, CdS, HgS, GaP, InAs
Spinel	MgAl <sub>2</sub> O <sub>4</sub> , ZnFe <sub>2</sub> O <sub>4</sub> , ZnCr <sub>2</sub> S <sub>4</sub>
Wurtzite	ZnS, ZnO, BeO, MnS, AgI, AlN, SiC, NH <sub>4</sub> F







Inorganic Chemistry Chapter 1: Figure 3.48	W. H. Freeman
K⁺(g) + e⁻(g) + Cl(g)	
122 Kt/m) + of/m)	
(g) + e'(g) -355 $+\frac{1}{2}Cl_2(g)$	
425 K⁺(g) + Cl⁻(g)	<u> </u>
$K(g) + \frac{1}{2} Cl_2(g)$	
$\frac{89}{K(s) + \frac{1}{2}Cl_{2}(g)} \times \frac{438}{K(s) + \frac{1}{2}Cl_{2}(g)}$	
KCI(s)	© 2009 W.H. Freeman

-		in the A			
Compound	Structure type	$\Delta H_{\rm L}^{\rm exp}/({\rm kJ}  {\rm mol}^{-1})$	Compound type	Structure	$\Delta H_{\rm L}^{\rm exp}/({\rm kJ}{\rm mol}^{-1})$
LiF	Rock salt	1030	SrCl <sub>2</sub>	Fluorite	2125
Lil	Rock salt	757	LiH	Rock salt	858
NaF	Rock salt	923	NaH	Rock salt	782
NaCl	Rock salt	786	KH	Rock salt	699
NaBr	Rock salt	747	RbH	Rock salt	674
Nal	Rock salt	704	CsH	Rock salt	648
KCI	Rock salt	719	BeO	Wurtzite	4293
KI	Rock salt	659	MgO	Rock salt	3795
CsF	Rock salt	744	CaO	Rock salt	3414
CsCl	Caesium chloride	657	SrO	Rock salt	3217
CsBr	Caesium chloride	632	BaO	Rocksalt	3029
Csl	Caesium chloride	600	Li <sub>2</sub> O	Antifluorite	2799
MgF <sub>2</sub>	Rutile	2922	TiO <sub>2</sub>	Rutile	12150
CaF <sub>2</sub>	Fluorite	2597	CeO <sub>2</sub>	Fluorite	9627



E	Effects energie	of charg s reflect	e and s ed in m	ize on la elting po	ttice bints
	n	nelting po	oints (°c)		
NaF	993	CaF <sub>2</sub>	1423	MgO	2800
NaCl	801	SrCl <sub>2</sub>	872	CaO	2580
NaBr	747	Li <sub>2</sub> O	>1700	SrO	2430
KC1	770	Na <sub>2</sub> O	1275	BaO	1923
			(subl)		















Inorganio	c Chemistry Chapter 1: Tablo 3.	8	W. H. Freeman
	Table 3.8 Madelung	g constants	
	Structural type	А	
			•••••
	Caesium chloride	1.763	
	Fluorite	2.519	
	Rock salt	1.748	
	Rutile	2.408	
	Sphalerite	1.638	
	Wurtzite	1.641	
			© 2009 W.H. Freeman



















CHAPTER 3: TA	BLE 3.13	BLE 3.13				
Typical	Band Gaps					
	Material	$E_{\rm g}/{ m eV}$				
	Carbon (diamond)	5.47				
	Silicon carbide	3.00				
	Silicon	1.11				
	Germaniun	0.66				
	Gallium arsenide	1.35				
	Indium arsenide	0.36				
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- Pure elemental semiconductors (Si, Ge, etc.) are used for devices where light or heat can be supplied to promote electrons.
- More useful devices are made using "doped" semiconductors appropriate impurities are intentionally added to supply electrons (e.g., P) or holes (e.g., Al) which modify the band gaps and the conductivity can be controlled.



























		andee 1	mergie	s (U in k	J/mol)	or Son	ie Salts
Solid	U	Solid	U	Solid	U	Solid	U
LiF	1036 I	iC1	853	LiBr	807	LiI	757
NaF	923 1	laC1	786	NaBr	747	NaI	704
KF	821 F	C1	715	KBr	682	KI	649
$MgF_2$	2957 N	lgCl <sub>2</sub>	2526	MgBr <sub>2</sub>	2440	MgI <sub>2</sub>	2327
		1.4			A 77	0	1491
Mg(s) =	$\rightarrow Mg$	(g)			$\Delta H$		140 K.
Mg(s) - <sup>2</sup> 3(g) —	$\rightarrow Mg$ $\rightarrow 2F(g$	(g) )			$\Delta H$	• =	148 K. 159 k.
Mg(s) - <sup>2</sup> 3(g) — Mg(g) -	$\rightarrow Mg$ $\rightarrow 2F(g)$ $\rightarrow Mg$	(g) ) (*(g) +	- e <sup>-</sup>		$\Delta H$ $\Delta H$	° = ° =	148 k. 159 k. 738 k.
Mg(s) - <sup>2</sup> 2(g) — Mg(g) - Mg <sup>+</sup> (g)	$\rightarrow Mg$ $\rightarrow 2F(g)$ $\rightarrow Mg$ $\rightarrow Mg$	(g) ) ( <sup>+</sup> (g) + [g <sup>2+</sup> (g)	- e <sup>-</sup> ) + e <sup>-</sup>	-11	$\Delta H$ $\Delta H$ $\Delta H$	° = ° = ° =	148 k 159 k 738 k 1450 k
Mg(s) - F3(g) Mg(g) - Mg <sup>+</sup> (g) F(g) + 4	$\rightarrow$ Mg $\rightarrow$ 2F(g $\rightarrow$ Mg $\rightarrow$ Mg $\rightarrow$ Mg	(g) $(f^{+}(g) + f^{-}(g)$ $(g^{2+}(g) + f^{-}(g))$	- e <sup>-</sup> ) + e <sup>-</sup>		ΔH ΔH ΔH ΔH	° = ° = ° = ° =	148 k 159 k 738 k 1450 k - 328 k

