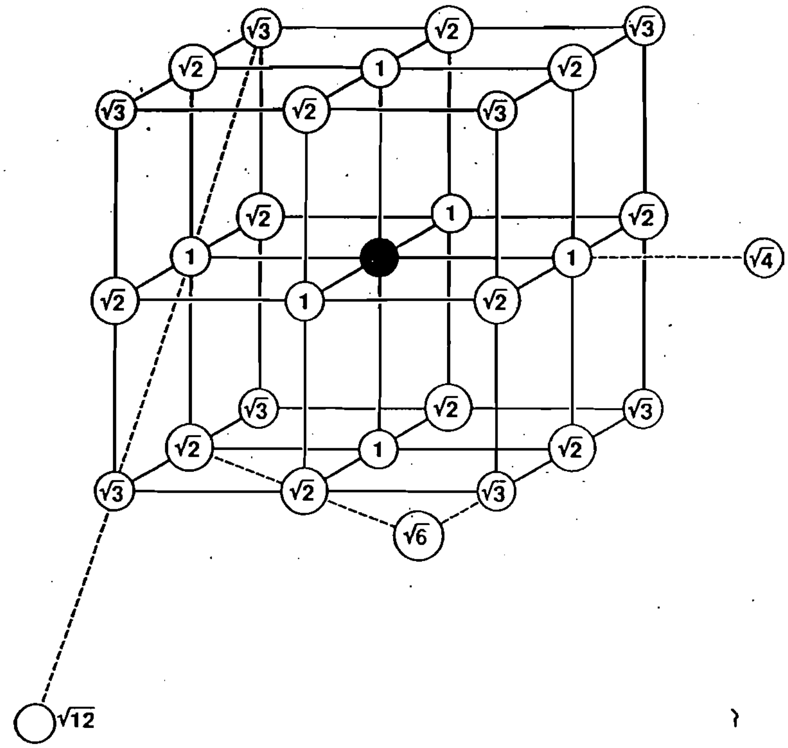



**Figure 5.2.**

The first coordination shell plus examples from other shells for the NaCl structure.

**Table 5.2.** Values of the Madelung constant for various structures.

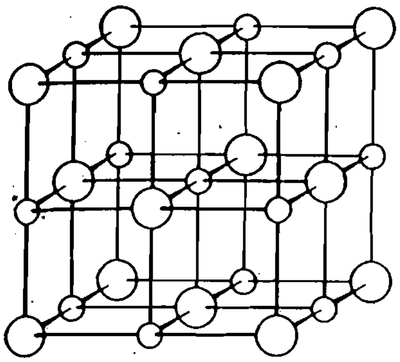
| | |
|---|---|
| Zinc blende (ZnS) | 1.63806 |
| Wurtzite (ZnS) | 1.64132 |
| Sodium chloride | 1.747558 |
| Cesium chloride | 1.762670 |
| Cuprite ($Cu_2O$) | 4.3224 |
| $\beta$-Quartz ($SiO_2$) | 4.4394 |
| High quartz ($SiO_2$) | 4.4633 |
| Cadmium iodide | 4.71 |
| Anatase ($TiO_2$) | 4.800 |
| Rutile ($TiO_2$) | 4.816 |
| Fluorite ($CaF_2$) | 5.03878 |
| Antifluorite | 5.03878 |
| Corundum ($Al_2O_3$) | 25.0312 |

**Table 5.3.** Lattice energies of the alkali halides.[a]

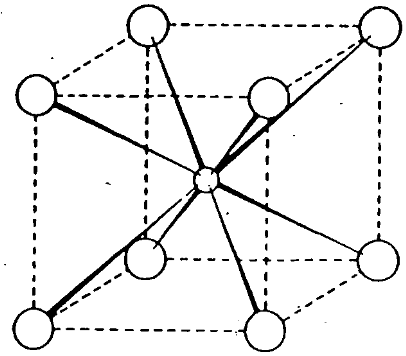
| alide | $r_e \times 10^8$ (cm) | $\chi \times 10^{12}$ (dynes/cm$^2$)$^{-1}$ | $n$ | $-E_0$ (kcal/mole)[b] Equation (5.35) | Experimental |
|---|---|---|---|---|---|
| F | 2.014 | 1.53 | 5.86 | 238 | 238 |
| Cl | 2.570 | 3.48 | 6.66 | 191 | 192 |
| Br | 2.746 | 4.28 | 7.00 | 180 | 182 |
| I | 3.010 | 7.2 | 6.15 | 161 | 170 |
| aF | 2.330 | (1.90) | (8.00) | 217 | 214 |
| aCl | 2.849 | 4.16 | 8.16 | 178 | 179 |
| aBr | 2.982 | 5.09 | 8.02 | 169 | 171 |
| aI | 3.236 | 7.1 | 7.98 | 156 | 160 |
| F | 2.679 | 3.3 | 8.05 | 189 | 189 |
| Cl | 3.149 | 5.64 | 8.87 | 163 | 163 |
| Br | 3.304 | 6.66 | 9.08 | 155 | 156 |
| I | 3.538 | 8.54 | 9.29 | 146 | 148 |
| bF | 2.815 | (3.64) | (8.80) | 178 | 181 |
| bCl | 3.286 | 7.4 | 8.12 | 154 | 158 |
| bBr | 3.434 | 7.95 | 8.72 | 152 | 151 |
| bI | 3.663 | 9.58 | 9.49 | 141 | 143 |
| sF | 3.005 | (3.07) | (13.0) | 177 | 172 |
| [illegible] | 3.559 | 5.9 | 13.1 | 148 | 142 |
| [illegible] | 3.716 | 7.0 | 13.2 | 142 | 142 |
| [illegible] | 3.952 | 9.3 | 12.7 | 133 | 135 |

[a] Taken from E. A. Moelwyn-Hughes, *Physical Chemistry*, p. 557, Pergamon Press, 1961. ased upon calculations by M. Born and J. Mayer, *Z. Phys.*, 75, 1 (1932) and J. Sherman, *hem. Rev.*, 11, 93 (1932).

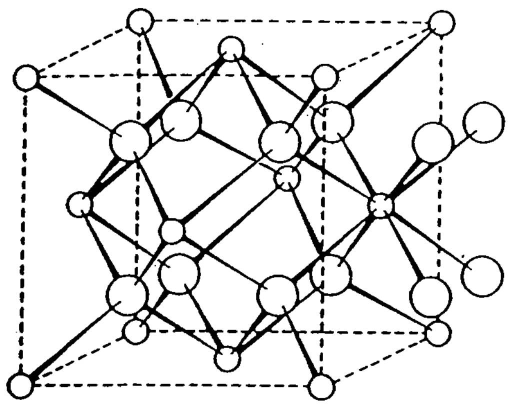
[b] Equation (5.35) has been multiplied by Avogadro's number to convert to moles.



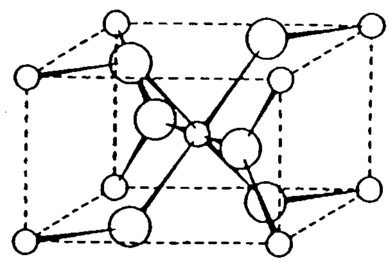
Rock-salt (NaCl)



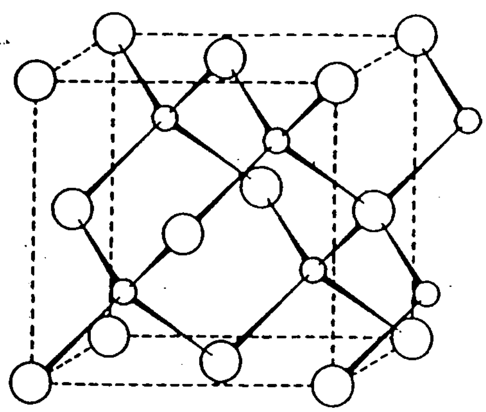
Cesium chloride (CsCl)



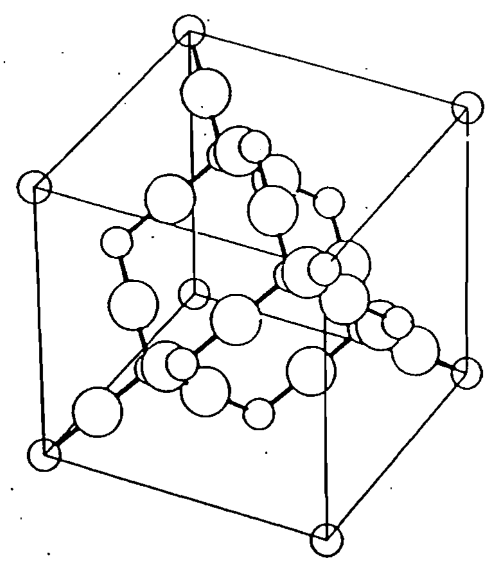
Fluorite ($CaF_2$)



Rutile ($TiO_2$)



Zinc blende (cubic ZnS)



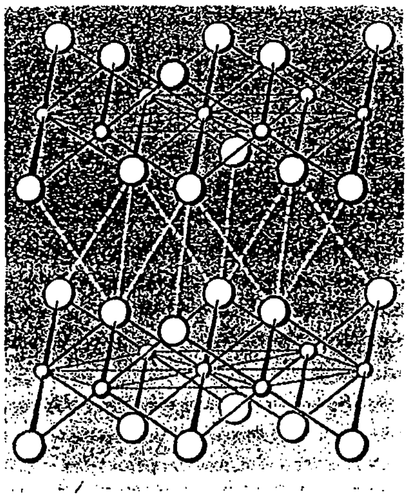
β-cristabolite

**Table 5.13.** Values of $r_+/r_-$ for the alkali halides.

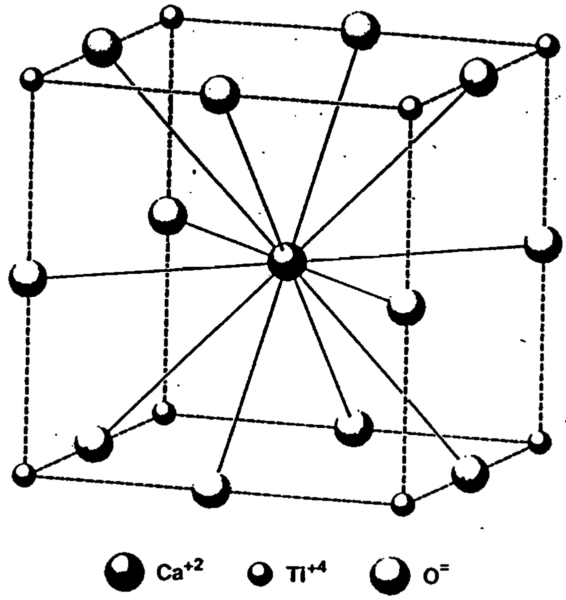
| | $Li^+$ | $Na^+$ | $K^+$ | $Rb^+$ | $Cs^+$ |
|---|---|---|---|---|---|
| $F^-$ | 0.51 | 0.73 | 1.00 | 1.12 | 1.28 |
| $Cl^-$ | 0.38 | 0.54 | 0.74 | 0.82 | 0.94 |
| $Br^-$ | 0.35 | 0.50 | 0.68 | 0.76 | 0.87 |
| $I^-$ | 0.31 | 0.44 | 0.60 | 0.68 | 0.77 |

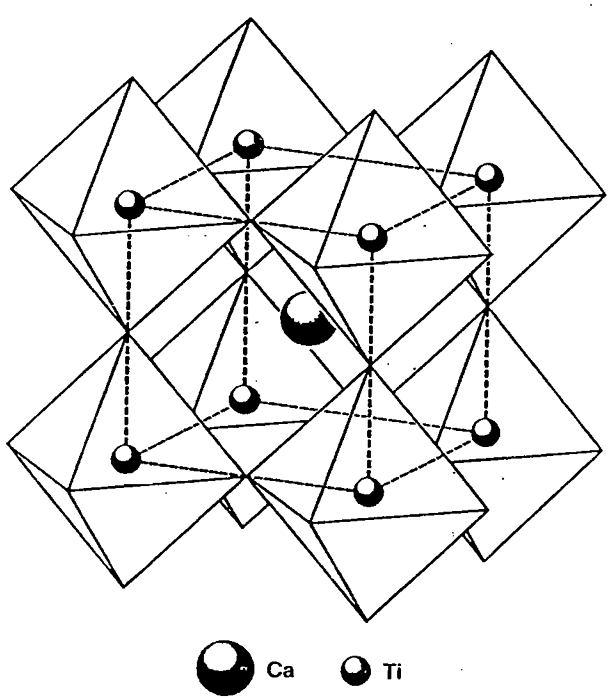
**Table 2.13 – Radius ratios for some $MX_2$ halides**

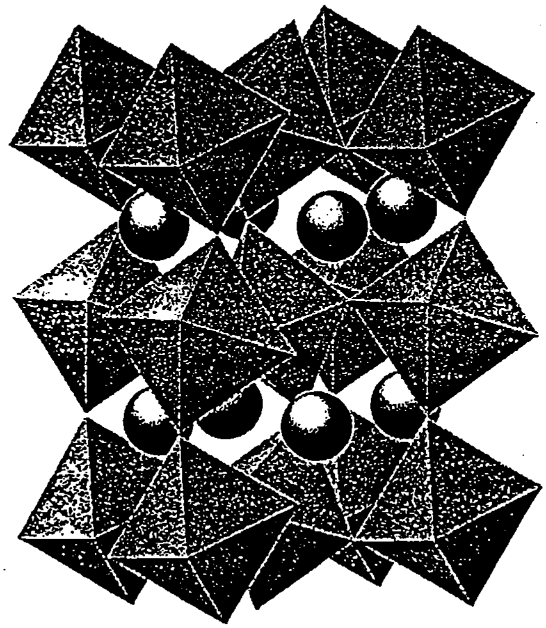
| Fluorite | | Rutile | | β-Cristobalite | |
|---|---|---|---|---|---|
| $BaF_2$ | 1.25 | $CaCl_2$ | 0.69 | $BeF_2$ | 0.23 |
| $SrF_2$ | 1.11 | $CaBr_2$ | 0.63 | | |
| $BaCl_2$ | 0.88 | $MgF_2$ | 0.73 | | |
| $CaF_2$ | 0.99 | | | | |
| $SrCl_2$ | 0.78 | | | | |
| $>0.73$ | | 0.73–0.41 | | $<0.41$ | |

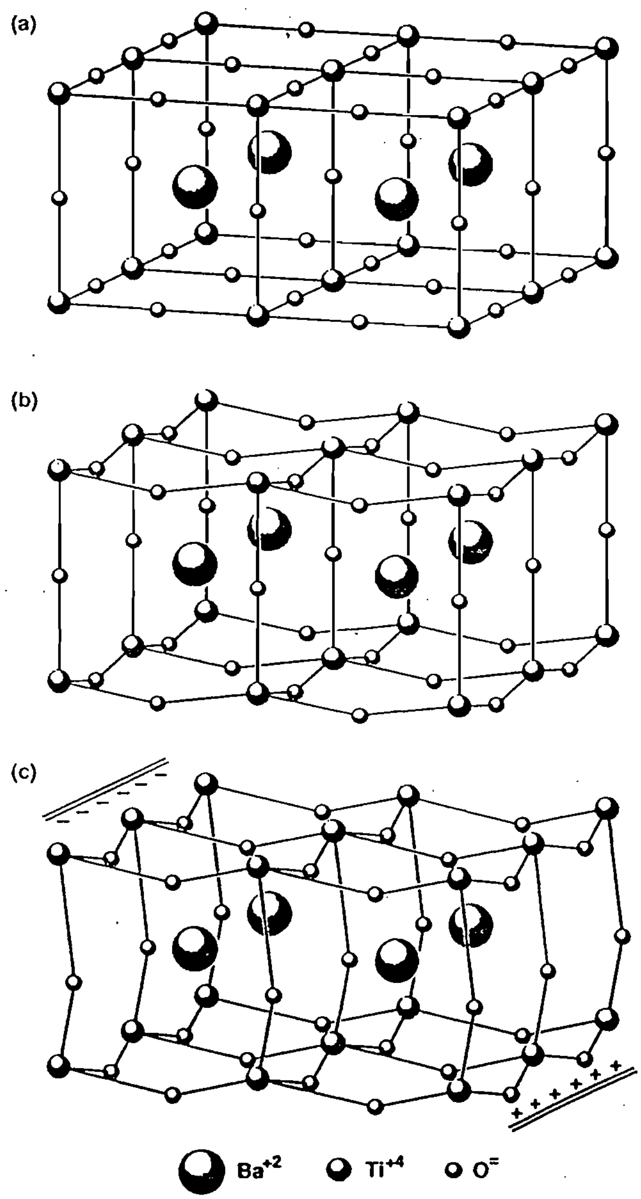


$CdI_2$

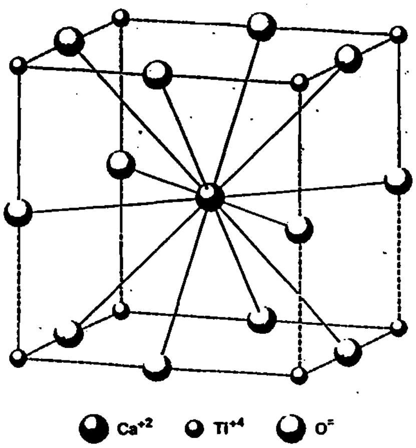

Ca+2
Ti+4
O=

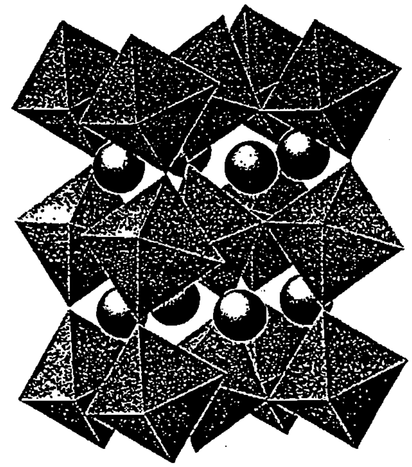

Ca
Ti

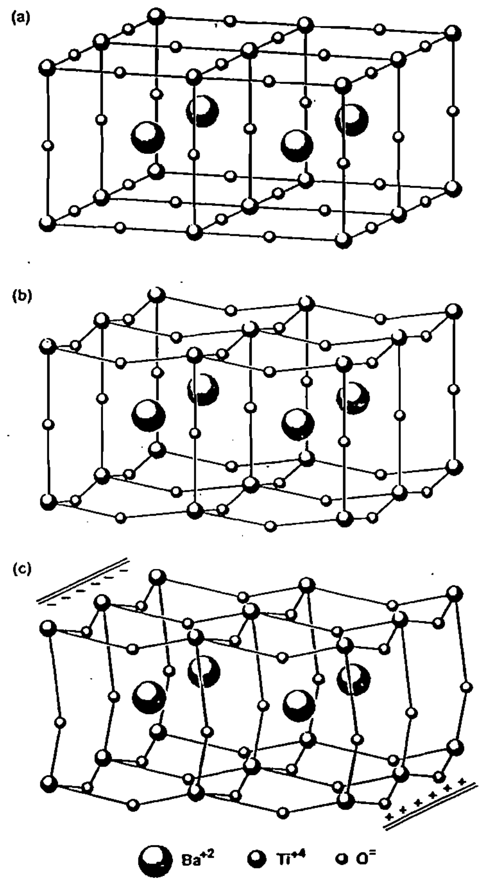


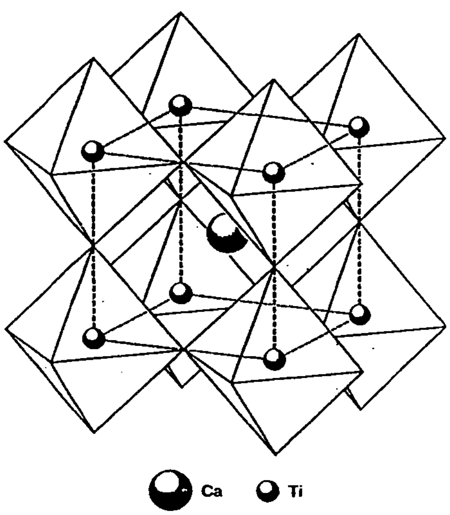


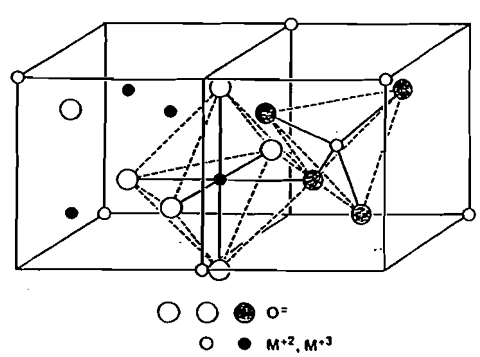
(a)
(b)
(c)
Ba+2
Ti+4
O=

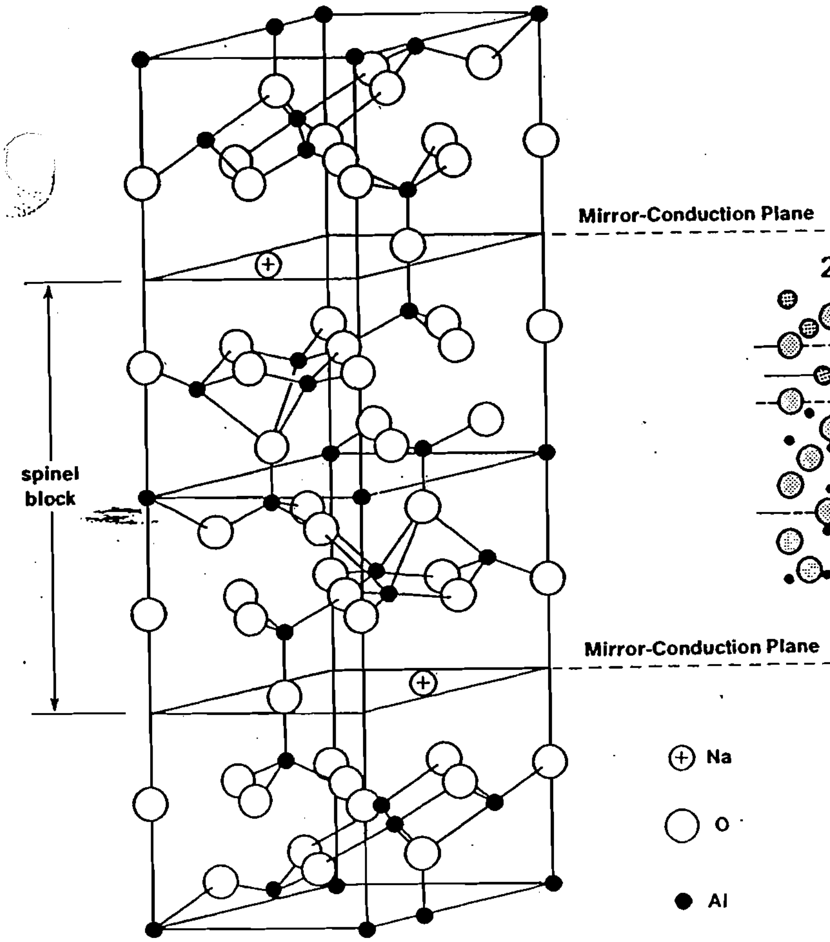

$Ca^{+2}$
$Ti^{+4}$
$O^{=}$

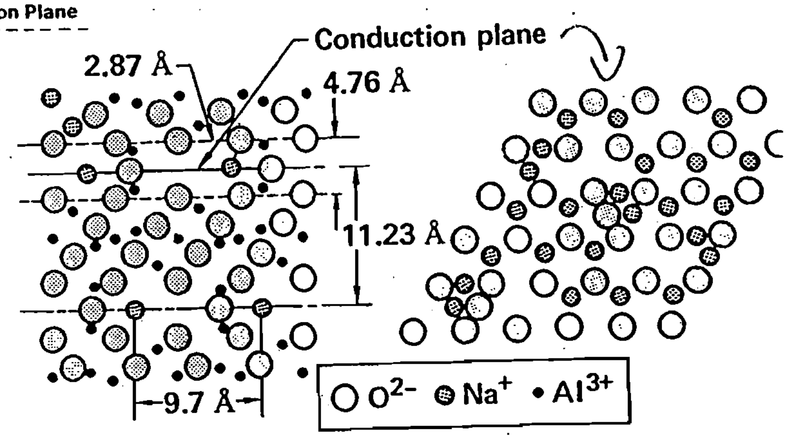



(a)
(b)
(c)
$Ba^{+2}$
$Ti^{+4}$
$O^{=}$


Ca
Ti


$O^{=}$
$M^{+2}$, $M^{+3}$



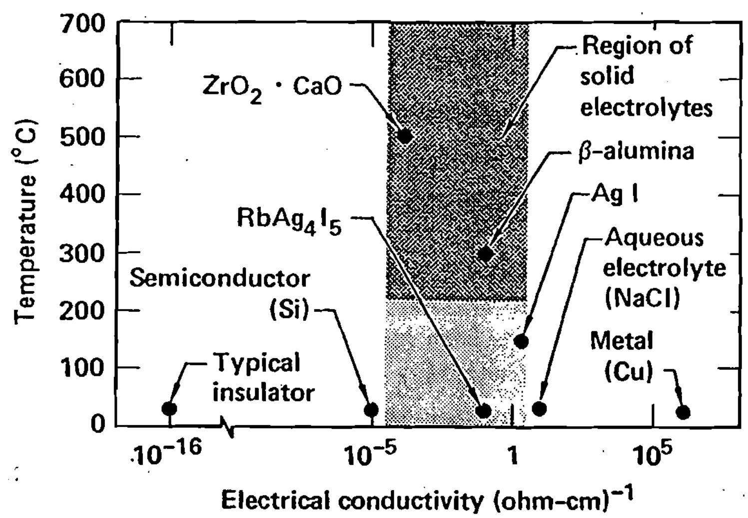




Figure 5.27.

Electrical conductivities of several common substances and representative solid electrolytes are shown at temperatures where the materials might be used. β-Alumina is the sodium form, in which $Na^+$ is the mobile species. In silver iodide, $Ag^+$ is responsible for the electrical conductivity, as it is in $RbAg_4I_5$. [After Shriver and Farrington, *C&E News*, 63, 42 (1985).]

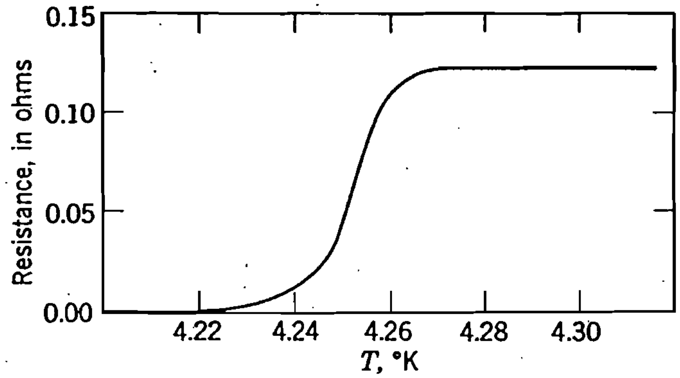
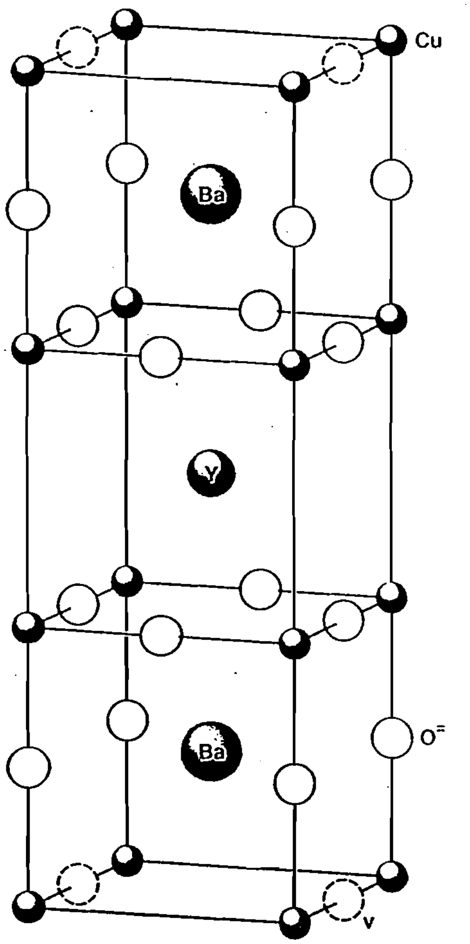
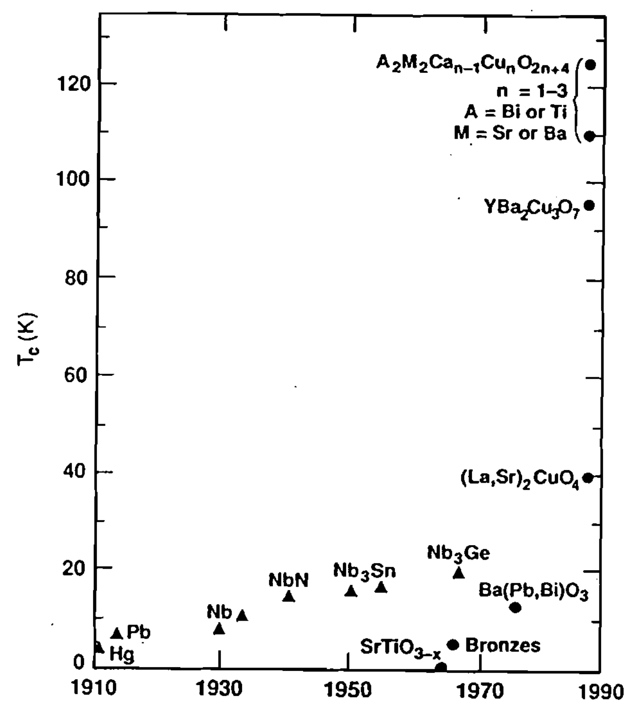


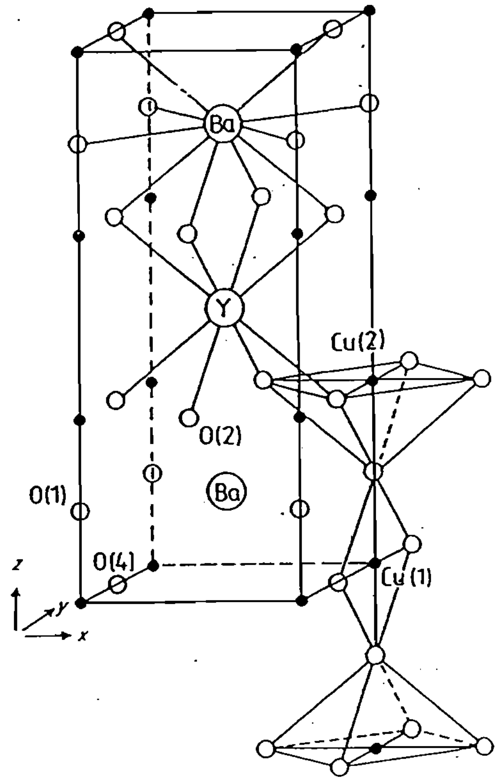

Figure 11.1 Electrical resistivity of mercury as a function of temperature. (H. Kamerlingh Onnes, Leiden Comm. Vol. 122b, 1911.)




'gure 5.19.

The 1-2-3 structure has three cubic units. $O^{2-}$ ions are absent from the vertical edges of the Y cell. They are also missing from the terminal horizontal planes $YBa_2Cu_3O_6$, but there are two $O^{2-}$, shown in dashed circles, in $YBa_2Cu_3O_7$.



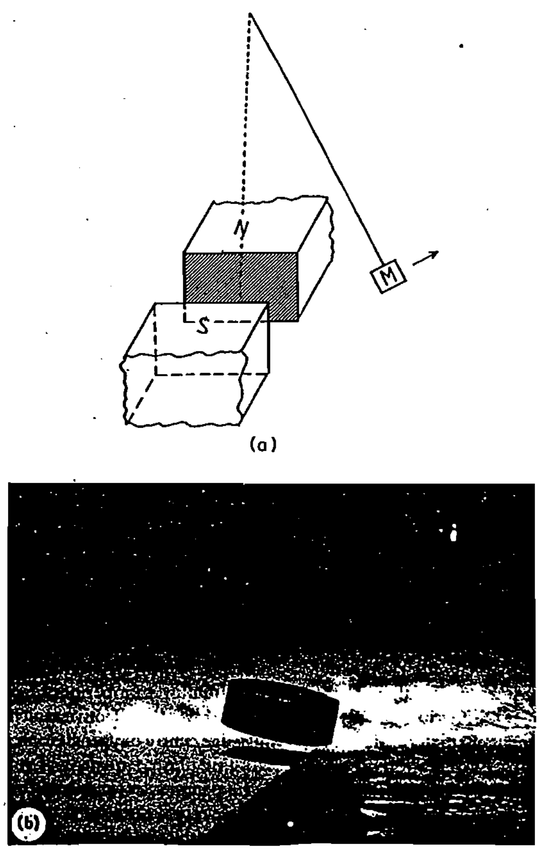




**Fig. 7.5** (a) The Meissner effect showing a superconducting material, M, being repelled from a magnetic field, (b) levitation of a sample of $YBa_2Cu_3O_7$ above a magnet. Photograph provided by R. Treviño and C. Piña, UNAM, Mexico.