# THE MADELUNG CONSTANT AND CRYSTAL LATTICE ENERGY

If $U$ is the crystal lattice energy and $M$ is the Madelung constant, then[a]

$$U = \frac{NMz_i z_j e^2}{r}(1 - 1/n)$$

| Substance | Ion type | Crystal form[b] | $M$ |
|---|---|---|---|
| Sodium chloride, NaCl | $M^+$, $X^-$ | FCC | 1.74756 |
| Cesium chloride, CsCl | $M^+$, $X^-$ | BCC | 1.76267 |
| Calcium chloride, $CaCl_2$ | $M^{++}$, $2X^-$ | Cubic | 2.365 |
| Calcium fluoride (fluorite), $CaF_2$ | $M^{++}$, $2X^-$ | Cubic | 2.51939 |
| Cadmium chloride, $CdCl_2$ | $M^{++}$, $2X^-$ | Hexagonal | 2.244[c] |
| Cadmium iodide (α), $CdI_2$ | $M^{++}$, $2X^-$ | Hexagonal | 2.355[c] |
| Magnesium fluoride, $MgF_2$ | $M^{++}$, $2X^-$ | Tetragonal | 2.381[c] |
| Cuprous oxide (cuprite), $Cu_2O$ | $2M^+$, $X^{--}$ | Cubic | 2.22124 |
| Zinc oxide, ZnO | $M^{++}$, $X^{--}$ | Hexagonal | 1.4985[c] |
| Sphalerite (zinc blende), ZnS | $M^{++}$, $X^{--}$ | FCC | 1.63806 |
| Wurtzite, ZnS | $M^{++}$, $X^{--}$ | Hexagonal | 1.64132[c] |
| Titanium dioxide (anatase), $TiO_2$ | $M^{4+}$, $2X^{--}$ | Tetragonal | 2.400[c] |
| Titanium dioxide (rutile), $TiO_2$ | $M^{4+}$, $2X^{--}$ | Tetragonal | 2.408[c] |
| β-Quartz, $SiO_2$ | $M^{4+}$, $2X^{--}$ | Hexagonal | 2.2197[c] |
| Corundum, $Al_2O_3$ | $2M^{3+}$, $3X^{--}$ | Rhombohedral | 4.1719 |

[a] $N$ is Avogadro's number, $z_i$ and $z_j$ are the integral charges on the ions (in units of $e$), and $e$ is the charge on the electron in electrostatic units ($e = 4.803 \times 10^{-10}$ esu). $r$ is the shortest distance between cation-anion pairs in centimeters. Then $U$ is in ergs (1 erg = $10^{-7}$ J).

[b] FCC = face centered cubic; BCC = body centered cubic.

[c] For tetragonal and hexagonal crystals the value of $M$ depends on the details of the lattice parameters.

The Born Exponent, $n$ is:

| Ion type | $n$ |
|---|---|
| He, $Li^+$ | 5 |
| Ne, $Na^+$, $F^-$ | 7 |
| Ar, $K^+$, $Cu^+$, $Cl^-$ | 9 |
| Kr, $Rb^+$, $Ag^+$, $Br^-$ | 10 |
| Xe, $Cs^+$, $Au^+$, $I^-$ | 12 |

For a crystal with a mixed-ion type, an average of the values of $n$ in this table is to be used (6 for LiF, for example).