

Quadrant II – Transcript and Related Materials

Programme: Bachelor of Science (First Year)

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Paper Title: Inorganic Chemistry and Organic Chemistry (Section A)

Unit: 2

Module Name: Statement of Born-Landé Equation for Calculation of Lattice Energy, Born-Haber Cycle and its Applications

Module No: 18

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Notes

Born-Landé equation:

The Born-Landé equation which was proposed by Max Born and Alfred Landé in 1918 is used to calculate the lattice energy of a crystalline ionic compound. As per this equation, the lattice energy could be derived from the electrostatic potential of the ionic lattice and a repulsive potential energy term.

$$U = - \frac{N_A M z^+ z^- e^2}{4\pi\epsilon_0 r_0} \left(1 - \frac{1}{n}\right)$$

Born-Landé Equation

where:

- U = Lattice energy
- N_A = Avogadro constant
- M = Madelung constant (depends on geometry of the crystal)
- z^+ = numeric charge number of cation
- z^- = numeric charge number of anion
- e = elementary charge, 1.6022×10^{-19} C
- ϵ_0 = permittivity of free space
 $4\pi\epsilon_0 = 1.112 \times 10^{-10}$ C²/(J·m)
- r_0 = distance to closest ion
- n = Born exponent (typically a number between 5 and 12, which is determined from compressibility of the solid, or derived theoretically)

Example:

- Calculate the lattice energy of NaCl using Born–Landé equation.

Solution:

Given

$$M = 1.747$$

$$Z^- = -1 \text{ (the Cl}^- \text{ ions charge)} = 1 \text{ (consider the absolute value)}$$

$$Z^+ = +1 \text{ (the charge of the Na}^+ \text{ ion)}$$

$$N_A = 6.022 \times 10^{23} \text{ ion pairs mol}^{-1}$$

$$C = 1.60210 \times 10^{-19} \text{C (the charge on the electron)}$$

$$\pi = 3.14$$

$$\epsilon_0 = 8.785 \times 10^{-12} \text{ C}^2 \text{ J}^{-1} \text{ m}^{-1}$$

$$r_0 = 281 \times 10^{-12} \text{ m, the sum of radii of Born-Landé equation.}$$

$$n = 8, \text{ the average of the values for Na}^+ \text{ and Cl}^-$$

$$U_{NaCl} = - \frac{6.022 \times 10^{23} \times 1.747 \times 1 \times 1 \times (1.6021 \times 10^{-19})^2}{4 \times 3.14 \times 8.785 \times 10^{-12} \times 281 \times 10^{-12}} \left(1 - \frac{1}{8}\right) = -755 \text{ kJ/mol}$$

Similarly, lattice energy for other ionic solids can be obtained from Born–Landé equation:

Comp	Cal. (kJ/mol)	Expt. (kJ/mol)
NaCl	-755	-786
LiF	-1007	-1046
CaCl ₂	-2170	-2255

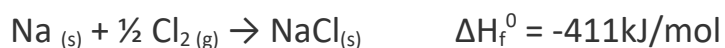
(Experimental values of lattice energy are also shown for comparison)

Born-Haber cycle and its applications

Born-Haber cycle is a thermochemical cycle which is used to determine the lattice energy of an ionic crystal indirectly.

Born Haber cycle of sodium chloride NaCl:

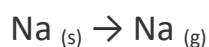
The heat of formation (ΔH_f^0) of solid crystalline sodium chloride from the sodium metal and chlorine gas can be obtained experimentally.



The formation of solid crystalline sodium chloride from solid sodium metal and gaseous chlorine goes through several processes. Heat change involved in all the processes (except that of lattice energy) can be obtained experimentally.

The processes involved in the formation of sodium chloride are given as follows:

1. Solid sodium atom in metallic sodium sublimates to gaseous atom by absorbing heat energy (ΔH_{sub}).



Sublimation energy $\Delta H_{\text{sub}} = + 107 \text{kJ/mol}$

2. Sodium atom in gaseous state absorbs the ionization energy to release one electron and forms gaseous sodium ion.



Ionization energy $\Delta H_{\text{IE}} = +502 \text{kJ/mol}$

3. Gaseous diatomic chlorine molecule breaks into two individual atoms by absorbing bond energy, such that half of the bond energy of chlorine molecule is absorbed by each chlorine atom.



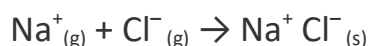
Bond dissociation energy of chlorine = $\frac{1}{2} \Delta H_{\text{diss}} = \frac{1}{2} \times 242 = +121\text{kJ/mol}$

4. Chlorine atom in gaseous state accepts an electron to form chloride ion and releases energy equivalent to electron affinity.



Electron affinity = $\Delta H_{\text{EA}} = -355\text{kJ/mol}$

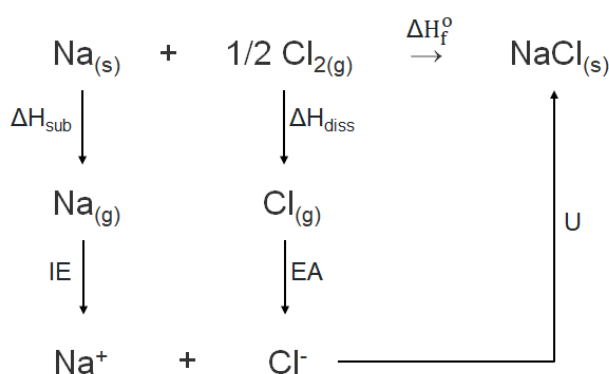
5. The sodium ion and chloride ion in gaseous state combine to form solid crystalline sodium chloride and releases energy equivalent to lattice energy.



Lattice energy = U (cannot be directly measured by experiment)

Adding the enthalpy of all the processes, give the net enthalpy of formation of solid crystalline sodium chloride from sodium and chlorine in their standard conditions of solid and gas respectively. This should be equal to the experimentally obtained enthalpy of formation of solid sodium chloride.

The enthalpies are represented as a cycle in the figure given below:



Born Haber cycle of sodium chloride NaCl

Therefore, $\Delta H_f^{\circ} = \Delta H_{\text{sub}} + \Delta H_{\text{IE}} + \frac{1}{2} \Delta H_{\text{dis}} + \Delta H_{\text{EA}} + U$ or

$$-411 = 107 + 502 + \left(\frac{1}{2} \times 242\right) - 355 + U$$

$$U = -786 \text{ kJ/mol (Lattice energy of sodium chloride solid)}$$

This is how Born-Haber cycle can be used to experimentally determine the lattice energy for a crystalline ionic solid, indirectly.