Important Madelung Constant Formulas PDF

Formulas
Examples
with Units

List of 10
Important Madelung Constant Formulas

1) Madelung Constant given Repulsive Interaction Constant Formula

Evaluate Formula

Formula

$$M = \frac{B_M \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot n_{born}}{\left(q^2\right) \cdot \left([Charge\text{-}e]^2\right) \cdot \left(r_0^{n_{born}-1}\right)}$$

Example with Units

$$1.703 = \frac{4.1E\text{-}29 \cdot 4 \cdot 3.1416 \cdot 8.9E\text{-}12\,F/m \cdot 0.9926}{\left(0.3\,C^2\right) \cdot \left(1.6E\text{-}19\,C^2\right) \cdot \left(60\,A^{0.9926-1}\right)}$$

2) Madelung Constant using Born Lande Equation Formula

Evaluate Formula

Formula

$$M = \frac{-U \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot r_0}{\left(1 - \left(\frac{1}{n_{born}}\right)\right) \cdot \left([Charge\text{-}e]^2\right) \cdot [Avaga\text{-}no] \cdot z^+ \cdot z^-}$$

Example with Units

$$1.6887 = \frac{-3500\,J/mol \cdot 4 \cdot 3.1416 \cdot 8.9E\text{-}12\,F/m \cdot 60\,A}{\left(1 - \left(\frac{1}{0.9926}\right)\right) \cdot \left(1.6E\text{-}19\,C^2\right) \cdot 6E{+}23 \cdot 4\,C \cdot 3\,C}$$

3) Madelung Constant using Born-Mayer equation Formula

Evaluate Formula

Formula

$$M = \frac{-U \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot r_0}{[Avaga\text{-}no] \cdot z^+ \cdot z^- \cdot \left([Charge\text{-}e]^2\right) \cdot \left(1 - \left(\frac{\rho}{r_0}\right)\right)}$$

Example with Units

$$1.7168 = \frac{-3500\,J/mol \cdot 4 \cdot 3.1416 \cdot 8.9E\text{-}12\,F/m \cdot 60\,A}{6E{+}23 \cdot 4\,C \cdot 3\,C \cdot \left(1.6E\text{-}19\,C^2\right) \cdot \left(1 - \left(\frac{60.44\,A}{60\,A}\right)\right)}$$

4) Madelung Constant using Kapustinskii Approximation Formula

Evaluate Formula

Formula

$$M = 0.88 \cdot N_{ions}$$

Example

$$1.76 = 0.88 \cdot 2$$

5) Madelung Constant using Madelung Energy Formula

Evaluate Formula

Formula

$$M = \frac{-\left(E_M\right) \cdot 4 \cdot \pi \cdot [\text{Permitivity-vacuum}] \cdot r_0}{\left(q^2\right) \cdot \left([\text{Charge-e}]^2\right)}$$

Example with Units

$$1.7041 = \frac{-\left(-5.9\text{E-}21\,\text{J}\right) \cdot 4 \cdot 3.1416 \cdot 8.9\text{E-}12\,\text{F/m} \cdot 60\,\text{A}}{\left(0.3\,\text{C}^2\right) \cdot \left(1.6\text{E-}19\,\text{C}^2\right)}$$

6) Madelung Constant using Total Energy of Ion Formula

Evaluate Formula

Formula

$$M = \frac{\left(E_{tot} - \left(\frac{B_M}{r_0^{n_{born}}}\right)\right) \cdot 4 \cdot \pi \cdot [\text{Permitivity-vacuum}] \cdot r_0}{-\left(q^2\right) \cdot \left([\text{Charge-e}]^2\right)}$$

Example with Units

$$1.6954 = \frac{\left(7.02\text{E-}23\,\text{J} - \left(\frac{4.1\text{E-}29}{60\,\text{A}^{0.9926}}\right)\right) \cdot 4 \cdot 3.1416 \cdot 8.9\text{E-}12\,\text{F/m} \cdot 60\,\text{A}}{-\left(0.3\,\text{C}^2\right) \cdot \left(1.6\text{E-}19\,\text{C}^2\right)}$$

7) Madelung Constant using Total Energy of Ion given Repulsive Interaction Formula

Evaluate Formula

Formula

$$M = \frac{\left(E_{tot} - E\right) \cdot 4 \cdot \pi \cdot [\text{Permitivity-vacuum}] \cdot r_0}{-\left(q^2\right) \cdot \left([\text{Charge-e}]^2\right)}$$

Example with Units

$$1.6925 = \frac{\left(7.02\text{E-}23\,\text{J} - 5.93\text{E-}21\,\text{J}\right) \cdot 4 \cdot 3.1416 \cdot 8.9\text{E-}12\,\text{F/m} \cdot 60\,\text{A}}{-\left(0.3\,\text{C}^2\right) \cdot \left(1.6\text{E-}19\,\text{C}^2\right)}$$

8) Madelung Energy Formula

Evaluate Formula

Formula

$$E_M = -\frac{M \cdot \left(q^2\right) \cdot \left([Charge\text{-}e]^2\right)}{4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot r_0}$$

Example with Units

$$-5.9E\text{-}21\,J = -\frac{1.7 \cdot \left(0.3\,C^2\right) \cdot \left(1.6E\text{-}19\,C^2\right)}{4 \cdot 3.1416 \cdot 8.9E\text{-}12\,F/m \cdot 60\,A}$$

9) Madelung Energy using Total Energy of Ion Formula

Evaluate Formula

Formula

$$E_M = E_{tot} - E$$

Example with Units

$$-5.9E\text{-}21\,J = 7.02E\text{-}23\,J - 5.93E\text{-}21\,J$$

10) Madelung Energy using Total Energy of Ion given Distance Formula

Evaluate Formula

Formula

$$E_M = E_{tot} - \left(\frac{B_M}{r_0^{n_{born}}}\right)$$

Example with Units

$$-5.9E\text{-}21\,J = 7.02E\text{-}23\,J - \left(\frac{4.1E\text{-}29}{60\,A^{0.9926}}\right)$$

Variables used in list of Madelung Constant Formulas above

- B_M Repulsive Interaction Constant given M
- **E** Repulsive Interaction between Ions *(Joule)*
- E_M Madelung Energy *(Joule)*
- E_{tot} Total energy of Ion in an Ionic Crystal *(Joule)*
- **M** Madelung Constant
- n_{born} Born Exponent
- N_{ions} Number of Ions
- **q** Charge *(Coulomb)*
- r_0 Distance of Closest Approach *(Angstrom)*
- **U** Lattice Energy *(Joule per Mole)*
- z^- Charge of Anion *(Coulomb)*
- z^+ Charge of Cation *(Coulomb)*
- **ρ** Constant Depending on Compressibility *(Angstrom)*

Constants, Functions, Measurements used in list of Madelung Constant Formulas above

- constant(s): **pi**, 3.14159265358979323846264338327950288 *Archimedes' constant*
- constant(s): **[Avaga-no]**, 6.02214076E+23 *Avogadro's number*
- constant(s): **[Charge-e]**, 1.60217662E-19 *Charge of electron*
- constant(s): **[Permitivity-vacuum]**, 8.85E-12 *Permittivity of vacuum*
- Measurement: **Length** in Angstrom (A) *Length Unit Conversion*
- Measurement: **Energy** in Joule (J) *Energy Unit Conversion*
- Measurement: **Electric Charge** in Coulomb (C) *Electric Charge Unit Conversion*
- Measurement: **Molar Enthalpy** in Joule per Mole (J/mol) *Molar Enthalpy Unit Conversion*

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