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Madelung Constant Formulas

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List of 10 Madelung Constant Formulas

Madelung Constant

1) Madelung Constant given Repulsive Interaction Constant

Open Calculator

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

ex $$1.702967 = \frac{4.1E\hat{}\text{-}29 \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot 0.9926}{\left((0.3C)^2\right) \cdot \left([Charge\text{-}e]^2\right) \cdot \left((60A)^{0.9926-1}\right)}$$

2) Madelung Constant using Born Lande Equation

Open Calculator

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

ex $$1.688737 = \frac{-3500J/mol \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot 60A}{\left(1 - \left(\frac{1}{0.9926}\right)\right) \cdot \left([Charge\text{-}e]^2\right) \cdot [Avaga\text{-}no] \cdot 4C \cdot 3C}$$

3) Madelung Constant using Born-Mayer equation

Open Calculator

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

ex $1.716794 = \frac{-3500\text{J/mol} \cdot 4 \cdot \pi \cdot [\text{Permitivity-vacuum}] \cdot 60\text{A}}{[\text{Avaga-no}] \cdot 4\text{C} \cdot 3\text{C} \cdot \left([\text{Charge-e}]^2\right) \cdot \left(1 - \left(\frac{60.44\text{A}}{60\text{A}}\right)\right)}$

4) Madelung Constant using Kapustinskii Approximation

Open Calculator

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

ex $1.76 = 0.88 \cdot 2$

5) Madelung Constant using Madelung Energy

Open Calculator

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

ex $1.704092 = \frac{-(\text{-5.9E^-21J}) \cdot 4 \cdot \pi \cdot [\text{Permitivity-vacuum}] \cdot 60\text{A}}{\left((0.3\text{C})^2\right) \cdot \left([\text{Charge-e}]^2\right)}$

6) Madelung Constant using Total Energy of Ion

Open Calculator

$$M = \frac{\left(E_{tot} - \left(\frac{B_M}{r_{0-\{born\}}^n}\right)\right) \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot r_0}{-(q^2) \cdot \left([Charge\text{-}e]^2\right)}$$

ex

$$1.695387 = \frac{\left(7.02E\text{^}\text{-}23J - \left(\frac{4.1E\text{^}\text{-}29}{(60A)^{0.9926}}\right)\right) \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot 60A}{-\left((0.3C)^2\right) \cdot \left([Charge\text{-}e]^2\right)}$$

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

Open Calculator

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

ex

$$1.692481 = \frac{(7.02E\text{^}\text{-}23J - 5.93E\text{^}\text{-}21J) \cdot 4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot 60A}{-\left((0.3C)^2\right) \cdot \left([Charge\text{-}e]^2\right)}$$

8) Madelung Energy

Open Calculator

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

ex

$$-5.9E\text{^}\text{-}21J = -\frac{1.7 \cdot \left((0.3C)^2\right) \cdot \left([Charge\text{-}e]^2\right)}{4 \cdot \pi \cdot [Permitivity\text{-}vacuum] \cdot 60A}$$

9) Madelung Energy using Total Energy of Ion

Open Calculator

fx $E_M = E_{tot} - E$

ex -5.9E^-21J = 7.02E^-23J − 5.93E^-21J

10) Madelung Energy using Total Energy of Ion given Distance

Open Calculator

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

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

Variables Used

- 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

- Constant: **pi**, 3.14159265358979323846264338327950288
  Archimedes' constant
- Constant: **[Avaga-no]**, 6.02214076E23
  Avogadro's number
- Constant: **[Charge-e]**, 1.60217662E-19 Coulomb
  Charge of electron
- Constant: **[Permitivity-vacuum]**, 8.85E-12 Farad / Meter
  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

Check other formula lists

- **Madelung Constant Formulas**

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