

Important Vibrational Energy Levels Formulas PDF



Formulas Examples with Units

List of 15 Important Vibrational Energy Levels Formulas

1) Anharmonicity Constant given Dissociation Energy Formula ↶

Formula

$$x_e = \frac{(\omega')^2}{4 \cdot D_e \cdot \omega'}$$

Example with Units

$$0.375 = \frac{(151/\text{m})^2}{4 \cdot 10\text{ J} \cdot 151/\text{m}}$$

Evaluate Formula ↶

2) Dissociation Energy given Vibrational Wavenumber Formula ↶

Formula

$$D_e = \frac{\omega'^2}{4 \cdot x_e \cdot \omega'}$$

Example with Units

$$15.625\text{ J} = \frac{151/\text{m}^2}{4 \cdot 0.24 \cdot 151/\text{m}}$$

Evaluate Formula ↶

3) Dissociation Energy of Potential Formula ↶

Formula

$$D_{ae} = E_{vf} \cdot v_{\max}$$

Example with Units

$$550\text{ J} = 100\text{ J} \cdot 5.5$$

Evaluate Formula ↶

4) Dissociation Energy of Potential using Zero Point Energy Formula ↶

Formula

$$D_e = D_0 + E_0$$

Example with Units

$$9\text{ J} = 5\text{ J} + 4\text{ J}$$

Evaluate Formula ↶

5) Energy of Vibrational Transitions Formula ↶

Formula

$$E_t = \left(\left(v + \frac{1}{2} \right) - x_e \cdot \left(\left(v + \frac{1}{2} \right)^2 \right) \right) \cdot ([\text{hP}] \cdot v_{\text{vib}})$$

Evaluate Formula ↶

Example with Units

$$8.6\text{E-34 J} = \left(\left(2 + \frac{1}{2} \right) - 0.24 \cdot \left(\left(2 + \frac{1}{2} \right)^2 \right) \right) \cdot (6.6\text{E-34} \cdot 1.3\text{ Hz})$$



6) Maximum Vibrational Quantum Number given Dissociation Energy Formula

Formula

$$v_m = \frac{D_e}{E_{vf}}$$

Example with Units

$$0.1 = \frac{10J}{100J}$$

Evaluate Formula 

7) Vibrational Energy Formula

Formula

$$E_t = \left(v + \frac{1}{2} \right) \cdot ([hP] \cdot v_{vib})$$

Example with Units

$$2.2E-33J = \left(2 + \frac{1}{2} \right) \cdot (6.6E-34 \cdot 1.3Hz)$$

Evaluate Formula 

8) Vibrational energy using Anharmonicity constant Formula

Formula

$$E_{xe} = \frac{(\omega')^2}{4 \cdot x_e \cdot \omega' \cdot v_{max}}$$

Example with Units

$$2.8409J = \frac{(151/m)^2}{4 \cdot 0.24 \cdot 151/m \cdot 5.5}$$

Evaluate Formula 

9) Vibrational Energy using Dissociation Energy Formula

Formula

$$E_{DE} = \frac{D_e}{v_{max}}$$

Example with Units

$$1.8182J = \frac{10J}{5.5}$$

Evaluate Formula 

10) Vibrational Energy using Vibrational Wave Number Formula

Formula

$$E_{wn} = \left(v + \frac{1}{2} \right) \cdot \omega'$$

Example with Units

$$37.5J = \left(2 + \frac{1}{2} \right) \cdot 151/m$$

Evaluate Formula 

11) Vibrational Frequency given Vibrational Energy Formula

Formula

$$v_{ve} = \frac{E_{vf}}{v + \frac{1}{2}} \cdot [hP]$$

Example with Units

$$2.7E-32Hz = \frac{100J}{2 + \frac{1}{2}} \cdot 6.6E-34$$

Evaluate Formula 

12) Vibrational Wavenumber given Vibrational Energy Formula

Formula

$$\omega'_{ve} = \frac{E_{vf}}{v + \frac{1}{2}}$$

Example with Units

$$40 = \frac{100J}{2 + \frac{1}{2}}$$

Evaluate Formula 



13) Zero Point Dissociation Energy Formula

Formula

$$D_0 = D_e - E_0$$

Example with Units

$$6\text{J} = 10\text{J} - 4\text{J}$$

Evaluate Formula 

14) Zero Point Energy Formula

Formula

$$E_0 = \left(\frac{1}{2} \cdot \omega' \right) - \left(\frac{1}{4} \cdot x_e \cdot \omega' \right)$$

Example with Units

$$6.6\text{J} = \left(\frac{1}{2} \cdot 15\text{ 1/m} \right) - \left(\frac{1}{4} \cdot 0.24 \cdot 15\text{ 1/m} \right)$$

Evaluate Formula 

15) Zero Point Energy given Dissociation Energy Formula

Formula

$$E_0 = D_e - D_0$$

Example with Units

$$5\text{J} = 10\text{J} - 5\text{J}$$

Evaluate Formula 



Variables used in list of Vibrational Energy Levels Formulas above

- D_0 Zero Point Dissociation Energy (Joule)
- D_{ae} Actual Dissociation Energy of Potential (Joule)
- D_e Dissociation Energy of Potential (Joule)
- E_0 Zero Point Energy (Joule)
- E_{DE} Vibrational Energy given DE (Joule)
- E_t Vibrational Energy in Transition (Joule)
- E_{vf} Vibrational Energy (Joule)
- E_{wn} Vibrational Energy given wavenumber (Joule)
- E_{xe} Vibrational Energy given xe constant (Joule)
- v Vibrational Quantum Number
- v_m Maximum Vibrational Number
- v_{max} Max Vibrational Number
- v_{ve} Vibrational Frequency given VE (Hertz)
- v_{vib} Vibrational Frequency (Hertz)
- x_e Anharmonicity Constant
- ω' Vibrational Wavenumber (1 per Meter)
- ω'_{ve} Vibrational Wavenumber given VE

Constants, Functions, Measurements used in list of Vibrational Energy Levels Formulas above

- **constant(s):** [hP], 6.626070040E-34
Planck constant
- **Measurement: Energy** in Joule (J)
Energy Unit Conversion 
- **Measurement: Frequency** in Hertz (Hz)
Frequency Unit Conversion 
- **Measurement: Wave Number** in 1 per Meter (1/m)
Wave Number Unit Conversion 



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Formulas 

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