

Important Calculators of Vibrational Spectroscopy Formulas PDF



Formulas
Examples
with Units

List of 21 Important Calculators of Vibrational Spectroscopy Formulas

1) Anharmonic Potential Constant Formula

Formula

$$\alpha_e = \frac{B_v - B_e}{v + \frac{1}{2}}$$

Example with Units

$$6 = \frac{35 \text{ 1/m} - 20 \text{ m}^{-1}}{2 + \frac{1}{2}}$$

Evaluate Formula

2) Anharmonicity Constant given First Overtone Frequency Formula

Formula

$$x_e = \frac{1}{3} \cdot \left(1 - \left(\frac{v_{0->2}}{2 \cdot v_{\text{vib}}} \right) \right)$$

Example with Units

$$0.2372 = \frac{1}{3} \cdot \left(1 - \left(\frac{0.75 \text{ Hz}}{2 \cdot 1.3 \text{ Hz}} \right) \right)$$

Evaluate Formula

3) Anharmonicity Constant given Fundamental Frequency Formula

Formula

$$x_e = \frac{v_0 - v_{0->1}}{2 \cdot v_0}$$

Example with Units

$$0.4973 = \frac{130 \text{ Hz} - 0.7 \text{ Hz}}{2 \cdot 130 \text{ Hz}}$$

Evaluate Formula

4) Anharmonicity Constant given Second Overtone Frequency Formula

Formula

$$x_e = \frac{1}{4} \cdot \left(1 - \left(\frac{v_{0->3}}{3 \cdot v_{\text{vib}}} \right) \right)$$

Example with Units

$$0.2179 = \frac{1}{4} \cdot \left(1 - \left(\frac{0.50 \text{ Hz}}{3 \cdot 1.3 \text{ Hz}} \right) \right)$$

Evaluate Formula

5) First Overtone Frequency Formula

Formula

$$v_{0->2} = (2 \cdot v_{\text{vib}}) \cdot (1 - 3 \cdot x_e)$$

Example with Units

$$0.728 \text{ Hz} = (2 \cdot 1.3 \text{ Hz}) \cdot (1 - 3 \cdot 0.24)$$

Evaluate Formula

6) Fundamental Frequency of Vibrational Transitions Formula

Formula

$$v_{0->1} = v_{\text{vib}} \cdot (1 - 2 \cdot x_e)$$

Example with Units

$$0.676 \text{ Hz} = 1.3 \text{ Hz} \cdot (1 - 2 \cdot 0.24)$$

Evaluate Formula



7) Maximum Vibrational Number using Anharmonicity Constant Formula ↻

Formula

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

Example with Units

$$0.1562 = \frac{(15 \text{ 1/m})^2}{4 \cdot 15 \text{ 1/m} \cdot 100 \text{ J} \cdot 0.24}$$

Evaluate Formula ↻

8) Maximum Vibrational Quantum Number Formula ↻

Formula

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

Example with Units

$$1.5833 = \left(\frac{15 \text{ 1/m}}{2 \cdot 0.24 \cdot 15 \text{ 1/m}} \right) - \frac{1}{2}$$

Evaluate Formula ↻

9) Rotational Constant for Vibrational State Formula ↻

Formula

$$B_v = B_e + \left(\alpha_e \cdot \left(v + \frac{1}{2} \right) \right)$$

Example with Units

$$35 \text{ 1/m} = 20 \text{ m}^{-1} + \left(6 \cdot \left(2 + \frac{1}{2} \right) \right)$$

Evaluate Formula ↻

10) Rotational Constant Related to Equilibrium Formula ↻

Formula

$$B_e = B_v - \left(\alpha_e \cdot \left(v + \frac{1}{2} \right) \right)$$

Example with Units

$$20 \text{ m}^{-1} = 35 \text{ 1/m} - \left(6 \cdot \left(2 + \frac{1}{2} \right) \right)$$

Evaluate Formula ↻

11) Second Overtone Frequency Formula ↻

Formula

$$v_{0 \rightarrow 3} = (3 \cdot v_{\text{vib}}) \cdot (1 - 4 \cdot x_e)$$

Example with Units

$$0.156 \text{ Hz} = (3 \cdot 1.3 \text{ Hz}) \cdot (1 - 4 \cdot 0.24)$$

Evaluate Formula ↻

12) Total Degree of Freedom for Linear Molecules Formula ↻

Formula

$$F_l = 3 \cdot z$$

Example

$$105 = 3 \cdot 35$$

Evaluate Formula ↻

13) Total Degree of Freedom for Nonlinear Molecules Formula ↻

Formula

$$F_n = 3 \cdot z$$

Example

$$105 = 3 \cdot 35$$

Evaluate Formula ↻

14) Vibrational Degree of Freedom for Linear Molecules Formula ↻

Formula

$$vib_d_l = (3 \cdot z) - 5$$

Example

$$100 = (3 \cdot 35) - 5$$

Evaluate Formula ↻



15) Vibrational Degree of Freedom for Nonlinear Molecules Formula

Formula

$$\text{vibd}_{\text{nl}} = (3 \cdot z) - 6$$

Example

$$99 = (3 \cdot 35) - 6$$

Evaluate Formula 

16) Vibrational Frequency given First Overtone Frequency Formula

Formula

$$\nu_{\text{vib}} = \frac{\nu_{0 \rightarrow 2}}{2} \cdot (1 - 3 \cdot x_e)$$

Example with Units

$$0.105 \text{ Hz} = \frac{0.75 \text{ Hz}}{2} \cdot (1 - 3 \cdot 0.24)$$

Evaluate Formula 

17) Vibrational Frequency given Fundamental Frequency Formula

Formula

$$\nu_{\text{vib}} = \frac{\nu_{0 \rightarrow 1}}{1 - 2 \cdot x_e}$$

Example with Units

$$1.3462 \text{ Hz} = \frac{0.7 \text{ Hz}}{1 - 2 \cdot 0.24}$$

Evaluate Formula 

18) Vibrational Frequency given Second Overtone Frequency Formula

Formula

$$\nu_{\text{vib}} = \frac{\nu_{0 \rightarrow 3}}{3} \cdot (1 - (4 \cdot x_e))$$

Example with Units

$$0.0067 \text{ Hz} = \frac{0.50 \text{ Hz}}{3} \cdot (1 - (4 \cdot 0.24))$$

Evaluate Formula 

19) Vibrational Quantum Number using Rotational Constant Formula

Formula

$$v = \left(\frac{B_v - B_e}{\alpha_e} \right) - \frac{1}{2}$$

Example with Units

$$2 = \left(\frac{35 \text{ J/m} - 20 \text{ m}^{-1}}{6} \right) - \frac{1}{2}$$

Evaluate Formula 

20) Vibrational Quantum Number using Vibrational Frequency Formula

Formula

$$v = \left(\frac{E_{\text{vf}}}{[hP] \cdot \nu_{\text{vib}}} \right) - \frac{1}{2}$$

Example with Units

$$1.2\text{E}+35 = \left(\frac{100 \text{ J}}{6.6\text{E}-34 \cdot 1.3 \text{ Hz}} \right) - \frac{1}{2}$$

Evaluate Formula 

21) Vibrational Quantum Number using Vibrational Wavenumber Formula

Formula

$$v = \left(\frac{E_{\text{vf}}}{[hP] \cdot \omega'} \right) - \frac{1}{2}$$

Example with Units

$$2.3\text{E}+36 = \left(\frac{100 \text{ J}}{6.6\text{E}-34 \cdot 15 \text{ J/m}} \right) - \frac{1}{2}$$

Evaluate Formula 



Variables used in list of Important Calculators of Vibrational Spectroscopy Formulas above

- B_e Rotational Constant Equilibrium (Per Meter)
- B_v Rotational Constant vib (1 per Meter)
- E_{vf} Vibrational Energy (Joule)
- F_l Degree of Freedom Linear
- F_n Degree of Freedom Non Linear
- v Vibrational Quantum Number
- ν_0 Vibration Frequency (Hertz)
- $\nu_{0 \rightarrow 1}$ Fundamental Frequency (Hertz)
- $\nu_{0 \rightarrow 2}$ First Overtone Frequency (Hertz)
- $\nu_{0 \rightarrow 3}$ Second Overtone Frequency (Hertz)
- ν_{max} Max Vibrational Number
- ν_{vib} Vibrational Frequency (Hertz)
- ν_{bd_l} Vibrational Degree Linear
- $\nu_{bd_{nl}}$ Vibrational Degree Nonlinear
- x_e Anharmonicity Constant
- z Number of Atoms
- α_e Anharmonic Potential Constant
- ω' Vibrational Wavenumber (1 per Meter)

Constants, Functions, Measurements used in list of Important Calculators of Vibrational Spectroscopy 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 
- **Measurement: Linear Atomic Density** in Per Meter (m^{-1})
Linear Atomic Density Unit Conversion 



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