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Important Calculators of Vibrational Spectroscopy Formulas

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List of 21 Important Calculators of Vibrational Spectroscopy Formulas

Important Calculators of Vibrational Spectroscopy

1) Anharmonic Potential Constant

Open Calculator

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

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

2) Anharmonicity Constant given First Overtone Frequency

Open Calculator

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

ex $$0.237179 = \frac{1}{3} \cdot \left(1 - \left(\frac{0.75Hz}{2 \cdot 1.3Hz}\right)\right)$$

3) Anharmonicity Constant given Fundamental Frequency

Open Calculator

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

ex $$0.497308 = \frac{130Hz - 0.7Hz}{2 \cdot 130Hz}$$

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4) Anharmonicity Constant given Second Overtone Frequency

Open Calculator

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

$$0.217949 = \frac{1}{4} \cdot \left(1 - \left(\frac{0.50\text{Hz}}{3 \cdot 1.3\text{Hz}}\right)\right)$$

5) First Overtone Frequency

Open Calculator

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

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

6) Fundamental Frequency of Vibrational Transitions

Open Calculator

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

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

7) Maximum Vibrational Number using Anharmonicity Constant

Open Calculator

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

$$0.15625 = \frac{(15/\text{m})^2}{4 \cdot 15/\text{m} \cdot 100\text{J} \cdot 0.24}$$

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8) Maximum Vibrational Quantum Number

Open Calculator

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

ex $$1.583333 = \left(\frac{15/m}{2 \cdot 0.24 \cdot 15/m}\right) - \frac{1}{2}$$

9) Rotational Constant for Vibrational State

Open Calculator

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

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

10) Rotational Constant Related to Equilibrium

Open Calculator

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

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

11) Second Overtone Frequency

Open Calculator

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

ex $$0.156Hz = (3 \cdot 1.3Hz) \cdot (1 - 4 \cdot 0.24)$$

12) Total Degree of Freedom for Linear Molecules

Open Calculator

fx $\mathrm{Fl} = 3 \cdot \mathrm{z}$

ex $105 = 3 \cdot 35$

13) Total Degree of Freedom for Nonlinear Molecules

Open Calculator

fx $\mathrm{Fn} = 3 \cdot \mathrm{z}$

ex $105 = 3 \cdot 35$

14) Vibrational Degree of Freedom for Linear Molecules

Open Calculator

fx $\mathrm{vibd_l} = (3 \cdot \mathrm{z}) - 5$

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

15) Vibrational Degree of Freedom for Nonlinear Molecules

Open Calculator

fx $\mathrm{vibd_{nl}} = (3 \cdot \mathrm{z}) - 6$

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

16) Vibrational Frequency given First Overtone Frequency

Open Calculator

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

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

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17) Vibrational Frequency given Fundamental Frequency

Open Calculator

fx $$\nu_{vib} = \frac{\nu_{0->1}}{1 - 2 \cdot x_e}$$

ex $$1.346154\text{Hz} = \frac{0.7\text{Hz}}{1 - 2 \cdot 0.24}$$

18) Vibrational Frequency given Second Overtone Frequency

Open Calculator

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

ex $$0.006667\text{Hz} = \frac{0.50\text{Hz}}{3} \cdot (1 - (4 \cdot 0.24))$$

19) Vibrational Quantum Number using Rotational Constant

Open Calculator

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

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

20) Vibrational Quantum Number using Vibrational Frequency

Open Calculator

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

ex $$1.2\text{E}\hat{}35 = \left(\frac{100\text{J}}{[hP] \cdot 1.3\text{Hz}}\right) - \frac{1}{2}$$

21) Vibrational Quantum Number using Vibrational Wavenumber

Open Calculator

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

ex $$2.3E\hat{}36 = \left(\frac{100J}{[hP]} \cdot 15/m\right) - \frac{1}{2}$$

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Variables Used

- B_e Rotational Constant Equilibrium *(Per Meter)*
- B_v Rotational Constant vib *(1 per Meter)*
- E_{vf} Vibrational Energy *(Joule)*
- **Fl** Degree of Freedom Linear
- **Fn** Degree of Freedom Non Linear
- **v** Vibrational Quantum Number
- v_0 Vibration Frequency *(Hertz)*
- $v_{0->1}$ Fundamental Frequency *(Hertz)*
- $v_{0->2}$ First Overtone Frequency *(Hertz)*
- $v_{0->3}$ Second Overtone Frequency *(Hertz)*
- v_{max} Max Vibrational Number
- v_{vib} Vibrational Frequency *(Hertz)*
- $vibd_l$ Vibrational Degree Linear
- $vibd_{nl}$ 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

- Constant: **[hP]**, 6.626070040E-34 Kilogram Meter² / Second
  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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- **Important Calculators of Vibrational Spectroscopy Formulas**
- **Vibrational Energy Levels Formulas**

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