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Vibrational Energy Levels Formulas

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List of 15 Vibrational Energy Levels Formulas

Vibrational Energy Levels

1) Anharmonicity Constant given Dissociation Energy

Open Calculator

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

ex $$0.375 = \frac{(15/\text{m})^2}{4 \cdot 10\text{J} \cdot 15/\text{m}}$$

2) Dissociation Energy given Vibrational Wavenumber

Open Calculator

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

ex $$15.625\text{J} = \frac{(15/\text{m})^2}{4 \cdot 0.24 \cdot 15/\text{m}}$$

3) Dissociation Energy of Potential

Open Calculator

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

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

4) Dissociation Energy of Potential using Zero Point Energy

Open Calculator

fx $$D_e = D_0 + E_0$$

ex $$9J = 5J + 4J$$

5) Energy of Vibrational Transitions

Open Calculator

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

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

6) Maximum Vibrational Quantum Number given Dissociation Energy

Open Calculator

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

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

7) Vibrational Energy

Open Calculator

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

ex $$2.2E\hat{}\text{-}33J = \left(2 + \frac{1}{2}\right) \cdot ([hP] \cdot 1.3Hz)$$

8) Vibrational energy using Anharmonicity constant

Open Calculator

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

ex $$2.840909\text{J} = \frac{(15/\text{m})^2}{4 \cdot 0.24 \cdot 15/\text{m} \cdot 5.5}$$

9) Vibrational Energy using Dissociation Energy

Open Calculator

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

ex $$1.818182\text{J} = \frac{10\text{J}}{5.5}$$

10) Vibrational Energy using Vibrational Wave Number

Open Calculator

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

ex $$37.5\text{J} = \left(2 + \frac{1}{2}\right) \cdot 15/\text{m}$$

11) Vibrational Frequency given Vibrational Energy

Open Calculator

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

ex $$2.7\text{E}\hat{}\text{-}32\text{Hz} = \frac{100\text{J}}{2 + \frac{1}{2}} \cdot [hP]$$

12) Vibrational Wavenumber given Vibrational Energy

Open Calculator

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

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

13) Zero Point Dissociation Energy

Open Calculator

fx $$D_0 = D_e - E_0$$

ex $$6J = 10J - 4J$$

14) Zero Point Energy

Open Calculator

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

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

15) Zero Point Energy given Dissociation Energy

Open Calculator

fx $$E_0 = D_e - D_0$$

ex $$5J = 10J - 5J$$

Variables Used

- 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

- 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

Check other formula lists

- **Vibrational Energy Levels Formulas**

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