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EPR Spectroscopy Formulas

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List of 9 EPR Spectroscopy Formulas

EPR Spectroscopy

1) Applied Magnetic Field using External Field

Open Calculator

fx $$B_{eff} = B \cdot (1 - \sigma)$$

ex $$7E\hat{}\text{-}34A/m = 7E\hat{}\text{-}34A/m \cdot (1 - 0.002)$$

2) Electron Paramagnetic Resonance Frequency

Open Calculator

fx $$\nu_{epr} = \frac{g_j \cdot \mu \cdot B}{[hP]}$$

ex $$0.000158Hz = \frac{1.5 \cdot 0.0001A*m^2 \cdot 7E\hat{}\text{-}34A/m}{[hP]}$$

3) Energy Difference between Two Spin States

Open Calculator

fx $$\Delta E_{+1/2\text{-}1/2} = (g_j \cdot \mu \cdot B)$$

ex $$1.1E\hat{}\text{-}37/m = (1.5 \cdot 0.0001A*m^2 \cdot 7E\hat{}\text{-}34A/m)$$

4) Energy of Negative Spin State

Open Calculator

fx $$E_{-1/2} = -\left(\frac{1}{2} \cdot (g_j \cdot \mu \cdot B)\right)$$

ex $$-5.3E\hat{}-38/m = -\left(\frac{1}{2} \cdot (1.5 \cdot 0.0001A*m^2 \cdot 7E\hat{}-34A/m)\right)$$

5) External Magnetic Field Strength

Open Calculator

fx $$B = \left(\sqrt{s_{qno} \cdot (s_{qno} + 1)}\right) \cdot \left(\frac{[hP]}{2 \cdot 3.14}\right)$$

ex $$6.8E\hat{}-34A/m = \left(\sqrt{6 \cdot (6 + 1)}\right) \cdot \left(\frac{[hP]}{2 \cdot 3.14}\right)$$

6) Lande g Factor in Electron Paramagnetic Resonance

Open Calculator

fx $$g_j = 1.5 - \frac{(l_{no.} \cdot (l_{no.} + 1)) - (s_{qno} \cdot (s_{qno} + 1))}{2 \cdot J \cdot (J + 1)}$$

ex $$1.607143 = 1.5 - \frac{(5 \cdot (5 + 1)) - (6 \cdot (6 + 1))}{2 \cdot 7 \cdot (7 + 1)}$$

7) Lines Generated for Spin Half

Open Calculator

fx $$N_{I = 1/2} = 1 + N_{nuclei}$$

ex $$15 = 1 + 14$$

8) No. of Particles in Upper State using Boltzmann Distribution

Open Calculator

fx $$N_{upper} = N_{lower} \cdot e^{\frac{g_j \cdot \mu \cdot B}{[Molar\text{-}g]}}$$

ex $$2 = 2 \cdot e^{\frac{1.5 \cdot 0.0001 A*m^2 \cdot 7E\hat{}\text{-}34 A/m}{[Molar\text{-}g]}}$$

9) Number of Lines Generated

Open Calculator

fx $$N_{lines} = (2 \cdot N_{nuclei} \cdot I) + 1$$

ex $$113 = (2 \cdot 14 \cdot 4) + 1$$

Variables Used

- **B** External Magnetic Field Strength *(Ampere per Meter)*
- B_{eff} External applied Magnetic Field *(Ampere per Meter)*
- $E_{-1/2}$ Energy of Negative Spin State *(1 per Meter)*
- g_j Lande g Factor
- **I** Spin Value
- **J** Total Angular Momentum Quantum No
- $I_{no.}$ Orbital Quantum Number
- $N_{I=1/2}$ Lines Generated for Spin Half
- N_{lines} Number of Lines Generated
- N_{lower} Lower State Particles
- N_{nuclei} Number of Equivalent Nuclei
- N_{upper} Upper State Particles
- s_{qno} Spin Quantum Number
- $\Delta E_{+1/2-1/2}$ Energy Difference between Spin States *(1 per Meter)*
- **μ** Bohr Magneton *(Ampere Square Meter)*
- v_{epr} Electron Paramagnetic Resonance Frequency *(Hertz)*
- **σ** Local Fields

Constants, Functions, Measurements used

- Constant: **[Molar-g]**, 8.3145 Joule/Kelvin Mole
  Molar gas constant
- Constant: **e**, 2.71828182845904523536028747135266249
  Napier's constant
- Constant: **[hP]**, 6.626070040E-34 Kilogram Meter² / Second
  Planck constant
- Function: **sqrt**, sqrt(Number)
  Square root function
- Measurement: **Frequency** in Hertz (Hz)
  Frequency Unit Conversion
- Measurement: **Magnetic Field Strength** in Ampere per Meter (A/m)
  Magnetic Field Strength Unit Conversion
- Measurement: **Wave Number** in 1 per Meter (1/m)
  Wave Number Unit Conversion
- Measurement: **Magnetic Moment** in Ampere Square Meter (A*m²)
  Magnetic Moment Unit Conversion

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