# Important EPR Spectroscopy Formulas PDF

Formulas
Examples
with Units

**List of 9**
**Important EPR Spectroscopy Formulas**

## 1) Applied Magnetic Field using External Field Formula

Evaluate Formula

Formula

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

Example with Units

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

## 2) Electron Paramagnetic Resonance Frequency Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0002\,Hz = \frac{1.5 \cdot 0.0001\,A*m^2 \cdot 7E\text{-}34\,A/m}{6.6E\text{-}34}$$

## 3) Energy Difference between Two Spin States Formula

Evaluate Formula

Formula

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

Example with Units

$$1.1E\text{-}37\,1/m = (1.5 \cdot 0.0001\,A*m^2 \cdot 7E\text{-}34\,A/m)$$

## 4) Energy of Negative Spin State Formula

Evaluate Formula

Formula

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

Example with Units

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

## 5) External Magnetic Field Strength Formula

Evaluate Formula

Formula

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

Example with Units

$$6.8E\text{-}34\,A/m = \left(\sqrt{6 \cdot (6 + 1)}\right) \cdot \left(\frac{6.6E\text{-}34}{2 \cdot 3.14}\right)$$

## 6) Lande g Factor in Electron Paramagnetic Resonance Formula

Evaluate Formula

Formula

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

Example

$$1.6071 = 1.5 - \frac{\left(5 \cdot \left(5 + 1\right)\right) - \left(6 \cdot \left(6 + 1\right)\right)}{2 \cdot 7 \cdot \left(7 + 1\right)}$$

## 7) Lines Generated for Spin Half Formula

Evaluate Formula

Formula

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

Example

$$15 = 1 + 14$$

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

Evaluate Formula

Formula

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

Example with Units

$$2 = 2 \cdot e^{\frac{1.5 \cdot 0.0001\ A*m^2 \cdot 7E\text{-}34\ A/m}{8.3145\ J/K*mol}}$$

## 9) Number of Lines Generated Formula

Evaluate Formula

Formula

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

Example

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

## Variables used in list of EPR Spectroscopy Formulas above

- $B$ 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
- $l_{no.}$ 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)*
- $\mu$ Bohr Magneton *(Ampere Square Meter)*
- $v_{epr}$ Electron Paramagnetic Resonance Frequency *(Hertz)*
- $\sigma$ Local Fields

## Constants, Functions, Measurements used in list of EPR Spectroscopy Formulas above

- constant(s): **[Molar-g]**, 8.3145
  *Molar gas constant*
- constant(s): **e**, 2.71828182845904523536028747135266249
  *Napier's constant*
- constant(s): **[hP]**, 6.626070040E-34
  *Planck constant*
- Functions: **sqrt**, sqrt(Number)
  *A square root function is a function that takes a non-negative number as an input and returns the square root of the given input number.*
- 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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