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Nuclear Magnetic Resonance Spectroscopy Formulas

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List of 13 Nuclear Magnetic Resonance Spectroscopy Formulas

Nuclear Magnetic Resonance Spectroscopy

1) Chemical Shift in Nuclear Magnetic Resonance Spectroscopy

$$\text{fx } \delta = \left(\frac{\nu - \nu^\circ}{\nu^\circ} \right) \cdot 10^6$$

[Open Calculator !\[\]\(a870788d6ed9b8fd294b7654a8c8526b_img.jpg\)](#)

$$\text{ex } 8\text{ppm} = \left(\frac{13\text{Hz} - 10\text{Hz}}{10\text{Hz}} \right) \cdot 10^6$$

2) Effective Nuclear Charge given Shielding Constant

$$\text{fx } Z = z - \sigma$$

[Open Calculator !\[\]\(c50c8b7b2cc2cf9ff925edec0ee94c0d_img.jpg\)](#)

$$\text{ex } 17.5 = 18 - 0.5$$

3) Effective Transverse Relaxation Time

$$\text{fx } T_2' = \frac{1}{\pi \cdot \Delta\nu_{1/2}}$$

[Open Calculator !\[\]\(f60b7a900783ac3fd531bfd9c111be6d_img.jpg\)](#)

$$\text{ex } 21.22066\text{s} = \frac{1}{\pi \cdot 0.015/\text{s}}$$



4) Gyromagnetic Ratio given Larmor Frequency

$$\text{fx } \gamma = \frac{\nu_L \cdot 2 \cdot \pi}{(1 - \sigma) \cdot B_0}$$

[Open Calculator !\[\]\(cbe80b694ebd74fcfe136a095b608235_img.jpg\)](#)

$$\text{ex } 5.235988\text{C/kg} = \frac{7.5\text{Hz} \cdot 2 \cdot \pi}{(1 - 0.5) \cdot 18\text{T}}$$

5) Hyperfine Splitting Constant

$$\text{fx } a = Q \cdot \rho$$

[Open Calculator !\[\]\(3e2231b1ad3ca8da8658228c00dd08e0_img.jpg\)](#)

$$\text{ex } 6.3 = 2.1 \cdot 3$$

6) Local Distribution to Shielding Constant

$$\text{fx } \sigma_{\text{local}} = \sigma_d + \sigma_p$$

[Open Calculator !\[\]\(0d5ec72f61334709c3fc9450209b754f_img.jpg\)](#)

$$\text{ex } 27.1 = 7 + 20.1$$

7) Magnetogyric Ratio of Electron

$$\text{fx } \gamma_e = \frac{e}{2 \cdot [\text{Mass-e}]}$$

[Open Calculator !\[\]\(b64b40baaee5acddc1eab8538ba84754_img.jpg\)](#)

$$\text{ex } 8.8\text{E}^{-10}\text{C/kg} = \frac{1.60\text{e-}19\text{C}}{2 \cdot [\text{Mass-e}]}$$



8) Nuclear Larmor Frequency

$$\text{fx } \nu_L = \frac{\gamma \cdot B_{\text{loc}}}{2 \cdot \pi}$$

[Open Calculator !\[\]\(e78f798d4ea5c530c9db49e7d26e6b95_img.jpg\)](#)

$$\text{ex } 30.55775\text{Hz} = \frac{12\text{C/kg} \cdot 16\text{T}}{2 \cdot \pi}$$

9) Nuclear Larmor Frequency given Shielding Constant

$$\text{fx } \nu_L = (1 - \sigma) \cdot \left(\frac{\gamma \cdot B_0}{2 \cdot \pi} \right)$$

[Open Calculator !\[\]\(05be7c7a8995decd503647c99211f7c2_img.jpg\)](#)

$$\text{ex } 17.18873\text{Hz} = (1 - 0.5) \cdot \left(\frac{12\text{C/kg} \cdot 18\text{T}}{2 \cdot \pi} \right)$$

10) Observed Width at Half-Height of NMR Line

$$\text{fx } \Delta\nu_{1/2} = \frac{1}{\pi \cdot T_2}$$

[Open Calculator !\[\]\(fe3aebe81acea8d45108cd2768939da7_img.jpg\)](#)

$$\text{ex } 0.015158/\text{s} = \frac{1}{\pi \cdot 21\text{s}}$$

11) Rate of Exchange at Coalescence Temperature

$$\text{fx } k_c = \frac{\pi \cdot \Delta\nu}{\sqrt{2}}$$

[Open Calculator !\[\]\(899d8b7697d64725bf017d3296cfcf1b_img.jpg\)](#)

$$\text{ex } 35.54306/\text{s} = \frac{\pi \cdot 16\text{Hz}}{\sqrt{2}}$$



12) Shielding Constant given Effective Nuclear Charge

fx $\sigma = Z - Z$

Open Calculator 

ex $3 = 18 - 15$

13) Total Local Magnetic Field

fx $B_{\text{loc}} = (1 - \sigma) \cdot B_0$

Open Calculator 

ex $9\text{T} = (1 - 0.5) \cdot 18\text{T}$



Variables Used

- **a** Hyperfine Splitting Constant
- **B₀** Magnitude of Magnetic Field in Z-Direction (Tesla)
- **B_{loc}** Local Magnetic Field (Tesla)
- **e** Charge of Electron (Coulomb)
- **k_c** Rate of Exchange (1 Per Second)
- **Q** Empirical Constant in NMR
- **T₂** Transverse Relaxation Time (Second)
- **T₂'** Effective Transverse Relaxation Time (Second)
- **Z** Atomic Number
- **Z** Effective Nuclear Charge
- **γ** Gyromagnetic Ratio (Coulomb per Kilogram)
- **γ_e** Magnetogyric Ratio (Coulomb per Kilogram)
- **δ** Chemical Shift (Parts per Million)
- **Δv** Peak Separation (Hertz)
- **Δv_{1/2}** Observed Width at Half-Height (1 per Second)
- **v** Resonance Frequency (Hertz)
- **v_L** Nuclear Larmor Frequency (Hertz)
- **v[°]** Resonance Frequency of Standard Reference (Hertz)
- **ρ** Spin Density
- **σ** Shielding Constant in NMR
- **σ_d** Diamagnetic Contribution
- **σ_{local}** Local Contribution



- σ_p Paramagnetic Contribution



Constants, Functions, Measurements used

- **Constant:** **pi**, 3.14159265358979323846264338327950288
Archimedes' constant
- **Constant:** **[Mass-e]**, 9.10938356E-31
Mass of electron
- **Function:** **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:** **Time** in Second (s)
Time Unit Conversion 
- **Measurement:** **Electric Charge** in Coulomb (C)
Electric Charge Unit Conversion 
- **Measurement:** **Frequency** in Hertz (Hz)
Frequency Unit Conversion 
- **Measurement:** **Magnetic Field** in Tesla (T)
Magnetic Field Unit Conversion 
- **Measurement:** **Radiation Exposure** in Coulomb per Kilogram (C/kg)
Radiation Exposure Unit Conversion 
- **Measurement:** **Salinity** in Parts per Million (ppm)
Salinity Unit Conversion 
- **Measurement:** **Vorticity** in 1 per Second (1/s)
Vorticity Unit Conversion 
- **Measurement:** **Time Inverse** in 1 Per Second (1/s)
Time Inverse Unit Conversion 



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