Important Nuclear Magnetic Resonance Spectroscopy Formulas PDF

Formulas
Examples
with Units

List of 13
Important Nuclear Magnetic Resonance Spectroscopy Formulas

1) Chemical Shift in Nuclear Magnetic Resonance Spectroscopy Formula

Evaluate Formula

Formula

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

Example with Units

$$3E{+}8\,\text{ppm} = \left(\frac{13\,\text{Hz} - 10\,\text{Hz}}{10\,\text{Hz}} \right) \cdot 10^6$$

2) Effective Nuclear Charge given Shielding Constant Formula

Evaluate Formula

Formula

$$Z = z - \sigma$$

Example

$$17.5 = 18 - 0.5$$

3) Effective Transverse Relaxation Time Formula

Evaluate Formula

Formula

$$T2' = \frac{1}{\pi \cdot \Delta\nu_{1/2}}$$

Example with Units

$$21.2207\,\text{s} = \frac{1}{3.1416 \cdot 0.015\,\text{1/s}}$$

4) Gyromagnetic Ratio given Larmor Frequency Formula

Evaluate Formula

Formula

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

Example with Units

$$5.236\,\text{C/kg} = \frac{7.5\,\text{Hz} \cdot 2 \cdot 3.1416}{(1 - 0.5) \cdot 18\,\text{T}}$$

5) Hyperfine Splitting Constant Formula

Evaluate Formula

Formula

$$a = Q \cdot \rho$$

Example

$$6.3 = 2.1 \cdot 3$$

6) Local Distribution to Shielding Constant Formula

Evaluate Formula

Formula

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

Example

$$27.1 = 7 + 20.1$$

7) Magnetogyric Ratio of Electron Formula

Evaluate Formula

Formula

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

Example with Units

$$8.8E{+}10\,\text{C/kg} = \frac{1.60e{-}19\,\text{C}}{2 \cdot 9.1E{-}31\,\text{kg}}$$

8) Nuclear Larmor Frequency Formula

Evaluate Formula

Formula

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

Example with Units

$$30.5577\,\text{Hz} = \frac{12\,\text{C/kg} \cdot 16\,\text{T}}{2 \cdot 3.1416}$$

9) Nuclear Larmor Frequency given Shielding Constant Formula

Evaluate Formula

Formula

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

Example with Units

$$17.1887\,\text{Hz} = (1 - 0.5) \cdot \left(\frac{12\,\text{C/kg} \cdot 18\,\text{T}}{2 \cdot 3.1416}\right)$$

10) Observed Width at Half-Height of NMR Line Formula

Evaluate Formula

Formula

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

Example with Units

$$0.0152\,\text{1/s} = \frac{1}{3.1416 \cdot 21\,\text{s}}$$

11) Rate of Exchange at Coalescence Temperature Formula

Evaluate Formula

Formula

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

Example with Units

$$35.5431\,\text{1/s} = \frac{3.1416 \cdot 16\,\text{Hz}}{\sqrt{2}}$$

12) Shielding Constant given Effective Nuclear Charge Formula

Evaluate Formula

Formula

$$\sigma = z - Z$$

Example

$$3 = 18 - 15$$

13) Total Local Magnetic Field Formula

Evaluate Formula

Formula

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

Example with Units

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

Variables used in list of Nuclear Magnetic Resonance Spectroscopy Formulas above

- **a** Hyperfine Splitting Constant
- B_0 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
- T_2 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)*
- $\Delta v_{1/2}$ 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 in list of Nuclear Magnetic Resonance Spectroscopy Formulas above

- constant(s): **pi**, 3.14159265358979323846264338327950288 *Archimedes' constant*
- constant(s): **[Mass-e]**, 9.10938356E-31 *Mass of electron*
- 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: **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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