Numbers and Conversions Useful in EPR

Free electron g value g_e = **2.0023193**

Boltzmann Constant k = **0.69504 cm^{-1} / K**

Calculating the g value from the frequency and magnetic field:

$g = (h/\mu_B)\,\nu / H$ = **714.4775** · ν [GHz] / H [G] = **0.7144775** · ν [GHz] / H [kG]

$g = (h/\mu_B)\,\nu / B$ = **0.07144775** · ν [GHz] / B [T] (1 T = 10^4 G)

Converting a hyperfine constant A from Gauss (that is the splitting seen in a spectrum) to cm^{-1} or MHz:

A [cm^{-1}] = (μ_B / hc) · g · A [G] = **4.66864478 × 10^{-5}** · g · A [G]

A [cm^{-1}] = (μ_B / hc) · g · A [mT] = **4.66864478 × 10^{-4}** · g · A [mT] (10 G = 1 mT)

A [MHz] = (μ_B / h) · g · A [G] = **1.39962** · g · A [G]

A [MHz] = (μ_B / h) · g · A [mT] = **13.9962** · g · A [mT] (10 G = 1 mT)

Note that the g value to which an EPR line belongs must be used in the conversion.

A [MHz] = A [cm^{-1}] · **2.9979 × 10^4**

Zero-Field Splitting parameters D, E and higher-rank parameters B_m^n are often expressed in Gauss instead of cm^{-1}. This is convenient because the parameters expressed in Gauss can often be directly read out of the spectra. The conversion is:

D [cm^{-1}] = (g_e · μ_B / hc) · D [G] = **9.34811756 × 10^{-5} [cm^{-1}/G]** · D [G]

D [cm^{-1}] = (g_e · μ_B / hc) · D [T] = **0.934811756 [cm^{-1}/T]** · D [T] (1 T = 10^4 G)

Coefficient appearing in calculation of the dipolar interaction between electrons with the distance given in Ångstroms:

$D_{dip} = -(\mu_0\,\mu_B^2 / 4\pi) \times (3g^2 / r^3)$

$\mu_0\,\mu_B^2 / 4\pi$ = **0.43297** cm^{-1} · Å^3

Some numbers useful in calculations involving the magnetic susceptibility:

$N\mu_B$ = **5584.939** erg / Gauss
in formulas for magnetization

$N\mu_B^2$ = **0.26074** cm^{-1}
for calculating the Temperature Independent Paramagnetism (TIP, $N\alpha$)

$N\mu_B^2/3k$ = **0.1250486** cgs emu · K
appearing in the famous formula $\chi = (N\mu_B^2/3kT) \cdot g^2 \cdot S(S + 1)$

See also
https://www.nist.gov/pml/fundamental-physical-constants
http://kirste.userpage.fu-berlin.de/chemistry/general/constants_en.html