Units for magnetic dipole-dipole interaction

The magnetic dipole-dipole interaction equation (see below) contains the constant factor:

$$\frac{\mu_0}{4\pi}\beta_{\mathrm{e}}{}^2\left(=\frac{\mu_0}{4\pi}\mu_{\mathrm{B}}{}^2\right)$$

The Bohr magneton (magnetic moment of an electron) uses either of the symbols β_{e} or μ_{B}, with the former seeming to be more popular in EPR and the latter in standard physics.
https://en.wikipedia.org/wiki/Bohr_magneton

(There is a similar situation with the nuclear magneton symbolized as either β_{N} (β_{n}) or μ_{N} https://en.wikipedia.org/wiki/Nuclear_magneton).

$$\beta_{\mathrm{e}}\left(=\mu_{\mathrm{B}}\right)=\frac{e\hbar}{2m_{\mathrm{e}}}=\frac{eh}{[4\pi]m_{\mathrm{e}}}$$

units: C J s kg^{-1} (charge on electron in C; *h* in J s; mass of electron in kg)

https://en.wikipedia.org/wiki/Vacuum_permeability

$$\mu_0 = 4\pi\times10^{-7}\,\mathrm{Hm^{-1}}$$

$$\frac{\mu_0}{4\pi} = 1\times10^{-7}\,\mathrm{Hm^{-1}}$$

(Note that this is for magnetic properties; for electric properties there is the vacuum permittivity https://en.wikipedia.org/wiki/Vacuum_permittivity).

vacuum permeability in henry per meter:
https://en.wikipedia.org/wiki/Henry_(unit)
H = J A^{-2} = J s^2 C^{-2} (A = C s^{-1})
units: H m^{-1} = J s^2 C^{-2} m^{-1}

So now one can determine the units for the entire constant factor:

$$\frac{\mu_0}{4\pi}\beta_{\mathrm{e}}{}^2$$

units: (J s^2 C^{-2} m^{-1}) (J s C kg^{-1})^2 = J^3 s^4 kg^{-2} m^{-1}

Alternatively, using β_{e} (μ_{B}) as commonly defined in J T^{-1}:
https://en.wikipedia.org/wiki/Tesla_(unit)
(J s^2 C^{-2} m^{-1}) (J T^{-1})^2 = J^3 s^2 C^{-2} T^{-2} m^{-1} = J^3 s^2 C^{-2} (kg C^{-1} s^{-1})$^{-2}$ m^{-1} = J^3 s^4 kg^{-2} m^{-1}

J^3 s^4 kg^{-2} m^{-1} = J (kg m^2 s^{-2})^2 s^4 kg^{-2} m^{-1} = J m^3

Numerical value for $\frac{\mu_0}{4\pi}\beta_{\mathrm{e}}{}^2$:
$(1 \times 10^{-7}) \times (9.274009994 \times 10^{-24})^2 = 8.600726 \times 10^{-54}$ J m^3

So this gives in the desired energy $\times$ volume (distance cubed) SI units, but not in convenient molecular/spectroscopic units.

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Convert to molecular/spectroscopic units – cm^{-1} per $(Å)^3$ by dividing by hc:

8.600726×10^{-54} J $m^3 \times (10^{10}$ Å/m$)^3 \times (6.626070 \times 10^{-34}$ J s$)^{-1} \times (2.99792 \times 10^{10}$ cm s$^{-1})^{-1}$
= 0.43297 cm^{-1} $Å^3$

Equations for magnetic dipole-dipole interaction:

$$D_{xx_{\mathrm{dip}}} = g_x^{\ 2} \frac{\mu_0}{4\pi} \beta_{\mathrm{e}}^{\ 2} \left(\frac{1}{r^3}\right), D_{yy_{\mathrm{dip}}} = g_y^{\ 2} \frac{\mu_0}{4\pi} \beta_{\mathrm{e}}^{\ 2} \left(\frac{1}{r^3}\right), D_{zz_{\mathrm{dip}}} = g_z^{\ 2} \frac{\mu_0}{4\pi} \beta_{\mathrm{e}}^{\ 2} \left(\frac{-2}{r^3}\right)$$

$$D_{xx,yy,zz_{\mathrm{dip}}} = 0.433\left[g_{x,y,z}^{\ 2}\right]\left(\frac{1}{r^3}\right)\left[1,1,-2\right]$$

so for e.g., r = 4.0 Å, (g = 2.0) the dipolar coupling is:

$0.433 \times 4.0 \times (1/64)$ = [+0.027, +0.027, –0.054] cm^{-1}, [+T, +T, –2T], where

$$D_{\mathrm{dip}} = \frac{1}{2}\left(2D_{zz_{\mathrm{dip}}} - \left[D_{xx_{\mathrm{dip}}} + D_{yy_{\mathrm{dip}}}\right]\right), E_{\mathrm{dip}} = \frac{1}{2}\left[D_{xx_{\mathrm{dip}}} - D_{yy_{\mathrm{dip}}}\right]$$

$D_{\mathrm{dip}} = -3T = -0.081$ cm^{-1}; $E_{\mathrm{dip}} = 0$ (r = 4.0 Å, g = 2.0).