

hyperfine coupling

The interaction between the spin magnetic moment of an unpaired electron and the nuclear spin magnetic moments resulting in the splitting of the α (spin up) and β (spin down) energy levels in an external magnetic field and, thus, in the multiplet pattern of the ESR spectra of radical-like species and transition metal compounds. Two main contributions to the hyperfine coupling are usually considered, Fermi contact and dipolar interactions. The contact interaction is isotropic and related to the unpaired spin density at the nucleus, $|\psi_{\sigma}|^2$. The dipolar interaction is anisotropic, and related to r^{-3} , where r is the distance between the atom holding the unpaired electron and the nucleus with non-zero spin.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1945