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Review of calculation of magnetic hyperfine Interactions for a molecular system HO-KI JEONG, Sengban Patent & Science Laboratory, Albany, NY 12205, JUNHO JEONG, Sengban Patent & Science Laboratory, Albany, NY 12205 and SUNY at Albany, Albany, NY 12222 — Magnetic hyperfine interactions related to the nuclear and the electron spins of a molecular system consist of dipole-dipole interaction and the Fermi contact interaction. And it installed in the Gaussian program is to use to analyze NMR, ESR, μSR, and EPR experimental data. However, the Fermi contact term, important effect in a molecule, of magnetic hyperfine interaction has physical and mathematical problems on the vector potential definition. By contrasting the definitions of vector potential derived by the electromagnetic field theory with by the dipole-dipole interaction theory, it will be proved that the Fermi contact term cannot exist mathematically and physically. Most theoretical scientists have mistake is to choose wrong initial coordinates.

Junho Jeong
Sengban Patent & Science Laboratory, Albany, NY 12205
and State University of New York at Albany, Albany NY 12222

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