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5.4. Mercury-199 NMR

Sommario/riassunto

Relativistic effects, though minor in light atoms, increase rapidly in magnitude as the atomic number increases. For heavy atom species, it becomes necessary to discard the Schrodinger equation in favor of the Dirac equation. Construction of an effective many-body Hamiltonian that accurately accounts for both relativistic and electron correlation effects in many-electron systems is a challenge. It is only in the past 20-25 years that relativistic quantum chemistry has emerged as a field of research in its own right, and it seems certain that relativistic many-electron calculations of molecular