Calculation of CD spectra and magnetic shielding ternsors of proteins with the generalized hybrid orbital (GHO) QM/MM method

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The use of generalized hybrid orbitals (GHO) of Gao and coworkers [1] grants useful QM/MM approaches to molecular biology. Electronic properties of proteins can be calculated on-the-fly in a molecular dynamics simulation with analytic energy gradient of GHO-MP2 [2]. We present the CD (circular dichroism) spectrum of insulin [3] as an example. Rotatory strengths of insulin are calculated at GHO-CC2 [4] for selected frames and thermally averaged. The simulated spectrum is compared with experimental data. The GHO method is also applied for magnetic shielding tensors using GIAO (gauge-including atomic orbital) [5]. The gauge-origin independency problem is treated utilizing the one-centered character of auxiliary orbitals in GHO-SCF and GHO-MP2. Carbon chemical shifts are calculated for the retinal chromophore in visual rhodopsin.

All of the above-mentioned QM/MM methods are available in our GELLAN quantum chemistry program package.

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