

# $^{13}\text{C}$ -NMR chemical shift of deuterated benzene

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The isotope effect induced by the deuterium substituted species is observed in molecular properties, such as geometry, kinetics, and electronic state of molecules through nuclear-electron interaction. Theoretical considerations and experimental alignments have been studied on the basis of *ab initio* molecular orbital (MO), density functional (DF) theories, and other empirical strategies. The Born-Oppenheimer (BO) approximation with the nuclear vibrational wavefunction can treat the isotope effect because the nuclear mass effect accounts for the average distance of vibrational motion partially.

Recently, multi-component quantum chemical theory [1–3] has been available to describe nuclear wavefunction and electronic wavefunction simultaneously, even in H/D isotope effect [4–6]. Dios and Jameson have proposed combination nuclear vibrational states with Gauge Independent Atomic Orbital (GIAO) method [9] to determine isotope shifts of nuclear magnetic resonance (NMR) shielding constant [10].

In this study, we focus on NMR shielding constants of the H/D isotopomer and/or isotopologue of benzene with the average distances obtained as the expectation value of the Morse vibrational wavefunction. Primary and secondary H/D isotope NMR shifts calculated by using GIAO with CCSD/cc-pVTZ and B3LYP/cc-pVTZ methods are discussed with additivities of experimental results.

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