RELATIVISTIC SPIN-ORBIT COUPLING EFFECTS ON SECONDARY ISOTOPE SHIFTS OF ^{13}C NUCLEAR SHIELDING IN CX_2 (X = O, S, Se, Te)

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Rovibrational corrections, temperature dependence, and isotope shifts of the ^{13}C nuclear shielding in CX_2 -molecules (X = O, S, Se, Te) are calculated [1]. The relativistic heavy-atom spin-orbit (SO) effect on these properties is considered for the first time for the secondary isotope effects. The nuclear shielding hypersurface (in terms of nuclear displacements) is calculated using a density-functional theory method [2] including both second- and third-order SO-contributions [3]. *Ab initio* multiconfiguration self-consistent field calculations [4, 5] are done at the equilibrium geometry for all systems for comparison. The results are compared with both present and earlier experimental data on CS_2 [1] and CSe_2 [6].

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