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Calculations of intermolecular interactions and their influences on structure and 13C, 1H magnetic shielding constants of solute molecules

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Abstract

On the basis of an improved method of molecular mechanics the spatial structures of molecular clusters modelling the solvate shell of methane in acetone and benzene, 2,9,10-trimethyl-1-3-dithia-5,6-benzocycloheptene in carbon disulfide have been calculated. The nuclear magnetic shielding constants for these structures are calculated by quantum chemical methods in the approach of the density functional theory of the B3LYP/6-31(d,p) level with the usage of gauge-invariant atomic orbitals. It is shown that the increase of the number of the solvent molecules results in better agreement of the calculated and experimental values of 1H and 13C chemical shifts.