Quantum-chemical study of the effects of noncovalent interactions on the nuclear magnetic screening constants of pyrimidine base associates

Nafikova A., Aminova R., Aganov A., Reznik V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The effects of weak noncovalent interactions on the nuclear magnetic screening (NMS) constants (σ 1H), (σ 13C) and charge distribution (q_t) on atoms in van der Waals model associates of unsubstituted and substituted pyrimidines and substituted uracil are considered. The NMS constants were calculated by the UB3LYP/6-31G(d,p) with GIAO functions. The correlation dependences of the 1H and 13C σ constants on the charge q on atoms whre constructed. It were shown that they can be represented as polynomials that include the terms that are linear and quadratic relative to the charge. The relations obtained in this way are similar in form and close in magnitude to the coefficients of the known Buckingham and Augspurger functions that describe the electric field effects on the nuclear magnetic screening constants. It was found that the coefficients in these polynomials have a definite physical sense in that they characterize nuclear magnetic screening and the "screening polarizability" tensor in the unperturbed molecule and associate, respectively. The NMS constants and charge distribution in pyrimidine base associates and accordingly the coefficients that reflect their values in polynomials depend on the form, size, and composition of the associate and can vary significantly depending on the position of the pyrimidine base in the associate. © 2007 Springer Science+Business Media, Inc.

Keywords

Charge distribution, Electric fields, Nuclear magnetic screening, Pyrimidine bases, Quantum-chemical calculations, Screening polarizability, Stacking interactions, Van der Waals associates