عنوان مقاله:

The study of substitute and intra-molecular interaction effects on NMR shielding tensors of anticancer Vorozole

محل انتشار:

همایش ملی نانو فناوری و شیمی سبز (سال: 1391)

تعداد صفحات اصل مقاله: 6

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خلاصه مقاله:

The density functional theory (DFT) has been used to analyze the effects of substitute and intra-molecular interactions on the NMR and NBO parameters of the anticancer vorozole structure. Results showed that the NMR shielding tensors are dependent on the molecular structure and chemical environment. However, their values are obviously different in the considered compounds. The obtained data demonstrated that by increasing lone pair electrons contribution of nitrogen atoms in resonance interactions and ring currents, the values of NMR chemical shielding around them increase. However, tetravalent nitrogens (N(17) and N(2)) have higher chemical shielding than trivalent (N(3), N(5), N(20) and N(21)) formers.

کلمات کلیدی:

Vorozole; Substitute effect; NMR tensors; NBO analysis