عنوان مقاله:

Monte Carlo Simulation and Quantum Calculation in Prediction the Properties of Single Carbon Nanotubes (SWNTs) with Mitotane

محل انتشار:

بیست و یکمین کنفرانس شیمی فیزیک انجمن شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Mitotane [1-(2-chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane, (o,p'-DDD)] is theonly drug approved for the treatment for adrenocortical carcinoma (ACC) and has also been usedfor various forms of glucocorticoid excess. Through still largely unknown mechanisms, mitotaneinhibits adrenal steroid synthesis and adrenocortical cell proliferation. Mitotane increases hepaticmetabolism of cortisol, and an increased replacement dose of glucocorticoids is standard of careduring mitotane treatment. In this investigation, the interaction of mitotane, with single carbonnanotubes (SWNTs), are examined, with AMBER, OPLS, CHARMM and MM+ force field inmolecular mechanic (MM) method. The calculations achieved by methods of Monte Carlosimulation in different temperatures. the calculations were carried out using HyperChemprofessional release 7.01 package of program. We investigate effects of gas phase on interactionof mitotane with single carbon nanotubes (SWNTS), utilizing these force fields. The total energy(E tot), Potential (E pot) and Kinetic (E kin) energy (kcal/mol), calculated. The calculated data asshown in tables and figures are corresponding with some behavior of nanotubes. This study canbe useful for understanding of the electrical behavior of nanotubes in the quantitative structurestudies.

کلمات کلیدی:

Quantum Monte Carlo (QMC), Molecular Mechanic (MM), Single Carbon Nanotubes (SWNTs), Force Field

لینک ثابت مقاله در پایگاه سیویلیکا:

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