عنوان مقاله:

Theoretical Study of Molecular Mechanics Methods on MgSO4 Drug and CNC

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 3

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خلاصه مقاله:

One of the exciting classes of nano materials is Carbon Nano Cones (CNCs), which possesscharacteristics suitable for many applications as delivery vehicles of biologically importantmolecules in view of possible biomedical applications, such as drug delivery [1-7]. The goalof this study was to examine the binding of MgSO4 drug was put covalently to CNC with (5,1) structure and length of 100A to use Chem Office software and Hyper Chem [8-11] andinvestigation of Energy parameters of Drug-CNC. Geometrical optimizations of Drug-CNCwere carried out in gas phase and water solvent with HF/ 6-31g* for all atoms. Simulationwas done in MM+, AMBER and OPLS force fields by Monte Carlo method. Three importantenergy parameters– Epotential, Ekinetic, Etotal- in different temperatures (308, 310, 312, 314 and316 K) were used for computation.

کلمات کلیدی: