عنوان مقاله:

The theoretical investigation of interaction energy between pyridine derivatives and bisphenyl glycolurile molecular clip

محل انتشار:

همایش ملی شیمی پاک (سال: 1393)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

The glycolurils and thioglycolurils have a great deal of attention due to their practical applications, such as fertilizers, polymer crosslinking, explosives, stabilizers of organic compounds against photo-degradation, combinatorial chemistry, radioiodination agents for biomolecules, psychotropic agents, catalysts, bleaching activators, and they have also been applied for the monomer in supramolecular chemistry[1-3]. In this research, the theoretical calculations were performed due to determine the interaction energy between a glycoluril, GL, as a host molecular clip and pyridine diol derivatives as the guest molecules (host-guest complex. The theoretical calculations on GL pyridine derivatives and pyridine diol were done, using a hybrid functional closed-shell RB3LYP and the 6-31G* basis set, employing the Gaussian 09. The energetic and geometric parameters, especially the bond lengths were investigated for GL, pyridine and pyridine diol derivatives and their parameters compared to glycoluril, GL molecule (host-guest complex hydroxy pyridine).

کلمات کلیدی: