عنوان مقاله:

DFT Calculations on host–guest system based on glycoluril clip and phenol and its hydroxyphenol analogues

محل انتشار:

همایش منطقه ای شیمی (سال: 1389)

تعداد صفحات اصل مقاله: 1

نویسندگان:

E. Vessally - *Islamic Azad University, Miyaneh Branch, Miyaneh, Iran*

A. Mohammadiyan - *Payame Noor University (PNU), Zanjan, Iran*

خلاصه مقاله:

Molecular recognition continues to be of major interest in the fields of host–guest chemistry and biomimetic chemistry [1]. Depending upon the need for selectivity in the recognition process, several types of interactions can play a role. In aqueous solution, the hydrophobic effect is often the main driving force for host–guest complex formation [2]. The selectivity of binding can be improved if additional interactions are involved, such as hydrogen bonding, electrostatic interactions, van der Waals forces, aryl stacking interactions and metal-to-ligand interactions. The approach of using a combination of interactions is particularly important for receptors in organic solvents, because here the hydrophobic effect is lacking. Rebek and Nolte, amongst others, have used this approach to develop host systems that can bind guests based on hydrogen bonding and aryl stacking. In this work, we introduced a host–guest system based on glycoluril clip and phenol and its hdroxyphenol analogues. DFT calculations were carried out on these host–guest system by using B3LYP/6-31G(d) level of theory. The DFT calculations clarified a more interaction between glycoluril clip and ortho- and meta-hydroxyphenol than para- hydroxyphenol. The results will be presented and discussed.

کلمات کلیدی: