

عنوان مقاله:

Microsolvation of CH⁺ in helium: An ab initio study

محل انتشار:

سومین همایش ملی تکنولوژی های نوین در شیمی، پتروشیمی و نانو ایران (سال: 1395)

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خلاصه مقاله:

In the present study, microsolvation and interaction of the CH⁺ cation with He_n=1-8 clusters are investigated by means of ab initio calculations at MP2/aug-cc-pVTZ and QCISD/aug-cc-pVTZ levels. Stabilization energy of the studied complexes including BSSE and ZPE corrections are in the range of 1.8 and 11.6 kJ/mol. A good linear correlation is found between the stabilization energy and stretching frequency shift ($\Delta\nu$) in the studied complexes. According to energy decomposition analysis, it is found that polarization effects are the major source of the attraction in these complexes

کلمات کلیدی:

Microsolvation; CH⁺; He; ab-initio; EDA

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