

عنوان مقاله:

Effect of Substituents on Stability Interact Magnesium Ion Bonded Monomer and Dimers of Amino Acids: A DFT Study

محل انتشار:

سومین همایش ملی تحقیقات نوین در شیمی و مهندسی شیمی (سال: 1390)

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خلاصه مقاله:

Like many other inorganic elements the importance of magnesium in biological systems, increasingly become evident in last decade. magnesium plays a role in the stability of all polyphosphate compounds in the cells, including those associated with DNA and RNA synthesis. Study on the magnesium rule in biological systems is subject which get much attention from both the scientists and the general public. For finding the mechanisms in which Magnesium ion play its rules it is necessary to understanding its interaction with protein molecules as building block of biological systems. But calculation of its interaction to proteins gets high cost and consume huge time via the complexity of proteins structure so our activities is limited. In initial step to study Magnesium ion interaction to biological systems, it is necessary to study the nature of Magnesium ion interaction with several amino acid as building blocks of proteins. In the research the structure of the amino acids, Magnesium ion bonded to amino acids and Magnesium ion bonded dimers of amino acids were calculated. Bond length, Energy and bond length analysis were done and shows that each substitution which have the effect on the Magnesium charge, have high effect on bond strength and increases the heat of formation of them.

کلمات کلیدی:

Magnesium Ion Bonded Dimer, Amino Acids, bond length, interpretation, biological systems, substitution

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