عنوان مقاله:

A Theoretical Charge Density Investigation on Histidine-Histidine Dipeptide in Gas Phase

محل انتشار:

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نویسنده:

خلاصه مقاله:

In the present work, an extensive theoretical calculation study on Histidine-Histidine dipeptide in gas phase is done by using DFT method with Gaussian ۹۸ program. Through investigations on the molecular geometries of this molecule it is found that there is six rings in the molecules not two rings. The presence of four intramolecular hydrogen bonds is responsible for the formation of additional four rings besides two imidazole rings which gives more stability to the molecule. The quantum theory of atoms in molecules (QTAIM) proves these strong intramolecular hydrogen bonds in the title dipeptide.

کلمات کلیدی:

Dipeptides, Histidine, Hydrogen Bonding, DFT, QTAIM

لینک ثابت مقاله در پایگاه سیویلیکا: