عنوان مقاله:

ATURAL BOND ORBITAL, STRUCTURAL PROPERTIES, DENSITYFUNCTIONAL THEORY (DFT) CALCULATIONS AND CHARGEDISTRIBUTION FOR THE 2-[(1H-PYRROL-2-YL) METHYL]-1HPYRROLECOMPOUND

محل انتشار:

سومین همایش ملی فن آوری های نوین شیمی و مهندسی شیمی (سال: 1393)

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خلاصه مقاله:

Pyrroles are a significant class of heterocycles due to their uses as bioactivecompounds and there have general application in the arena of materials chemistry. In this paper,the optimized geometries and frequencies of the stationary point and the minimum-energy pathsof 2-[(1H-Pyrrol-2-yl) methyl]-1H-pyrrole are calculated by using the DFT (B3LYP) methodswith LANL2DZ basis sets. B3LYP/LANL2DZ calculation results indicated that some selectedbond length, bond angles values calculation spectrum for the C9H10N2 some similarity betweencalculated and experimental results.

کلمات کلیدی:

DFT, B3LYP/LANL2DZ, Calculation, HOMO, LUMO, Pyrrole Derivatives

لینک ثابت مقاله در پایگاه سیویلیکا: