عنوان مقاله:

Design of methyldopa structure and calculation of itsproperties by quantum mechanic

محل انتشار:

اولین کنفرانس ملی کاربرد نانوتکنولوژی در صنایع نفت و پتروشیمی (سال: 1391)

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خلاصه مقاله:

Methyldopa(MTD), α-methyl-3,4-methyl-dihydroxyphenylalanine, is anantihypertensive agent. The structure was optimized at the DFT and MP2 levels of theory. Weperformed nonempirical quantum mechanical calculations at the BLYP and B3LYP/3-21G , 6-31G, and 6-31G levels of theory in the gas phase and differentsolvents(water,ethanol,methanol) at temperature of 298.15 K. Finally, we employed the densityfunctional .theory (DFT) to calculate nuclear magnetic resonance spectra and infrared spectra

کلمات کلیدی:

Density functional theory (DFT), Methyldopa (MTD), Quantum mechanical

لینک ثابت مقاله در پایگاه سیویلیکا: