عنوان مقاله:

A hybrid density functional theory (DFT) and ab initio study of α-Acyloxycarboxamides Derived from Indane-۱, ۲, ۳-trione

محل انتشار:

کنفرانس ملی سنتز آلی و شیمی دارویی (سال: 1392)

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خلاصه مقاله:

α-acyloxycarboxamides are synthesized from three component Passerinireaction between indane-۱,۲,۳-trione, isocyanides, and thiophenecarboxylic acids inquantitative yields. The structures of the final products were confirmed by IR, ۱H and۱۳C NMR spectroscopy, mass spectrometry, and elemental analysis. The B۳LYP/HFcalculations for computation of ۱H and ۱۳C NMR chemical shifts have been carriedout for the title compounds at the ۶-۳۱۱+G** and ۶-۳۱۱++G** basis set levels withinGIAO and CSGT approaches by DFT and HF methods. Predicted ۱H and ۱۳C NMRchemical shifts have been assigned and compared with experimental ۱H and ۱۳C NMRspectra and they are supported each other.

کلمات کلیدی:

DFT, HF, NMR spectra, Passerini reaction, isocyanide

لینک ثابت مقاله در پایگاه سیویلیکا: