عنوان مقاله:

Proposed the region-selective N-acylation of dihydropyrimidinones: Employing the density functional theory (DFT) method

محل انتشار:

دومین کنفرانس ملی توسعه دانش بنیان صنایع نفت، گاز و پتروشیمی و ششمین کنفرانس روز مهندسی پتروشیمی بندر امام (سال: 1394)

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خلاصه مقاله:

The aim of present studies is to focus on the structural optimization and calculated the thermodynamic parameters of some N-acyl dihydropyrimidinones by using density functional theory (DFT). The collected data showed that the substitution on the aryl ring can be effective on the thermodynamic properties. Furthermore, in this work we investigated the regionselective of N-acylation of some 3,4- dihydropyrimidininones by DFT methods

کلمات کلیدی:

N-acylation, DFT, region-seletive, 3,4-dihydropyrimidinone