

A computational study on etherification mechanism of 4,5 - dihydroxy - 1,3 -bis (hydroxymethyl) imidazolidin - 2 - one with primary alcohols in acidic and parched condition

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Abstract

Etherification mechanism of 4,5-dihydroxy-1,3-bis (hydroxymethyl) imidazolidin-2-one (DMDHEU) with primary alcohols in acidic and parched condition were investigated by using density functional theory combined with comparison and reference to results of experiment and spectral analysis. Geometry and energy of reactants, products, actived complexes and carbocation intermediate were optimized at B3LYP/6-311g(d,p) level. Energy level diagram is compatible with type of cation – molecule reaction. Reactants and products form actived complexes with H⁺ and water, in this state H⁺ is occupied by both alcohol and water or ether and water. This state has lower energy level compared to both of the following cases: H⁺ is only occupied by water; and H⁺ is only occupied by the product or reactant. Computational results indicate that the etherification reaction follows unimolecular nucleophilic substitution (SN1) mechanism; substituent group –R in primary alcohol R-CH₂OH (-R = -H, -CH₃, -CH₂CH₃, -Vinyl, -CH₂NHCH₃, -CH₂OCH₃, -CH₂Cl) only affect to energy barrier of step releasing H₃O⁺ Ec but no effect to energy barrier of activation step Ea = 12.8 kcal/mol; value of Ec is much higher than value of Ea which were verified and confirmed through experiment results.

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