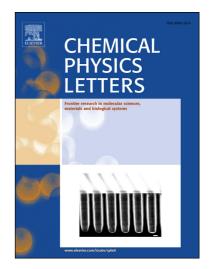
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Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol

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Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol

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Abstract

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We examine the reaction of ethanol with glyoxal to form hemiacetal by means of the high-level G4(MP2) procedure. In this reaction, an intermolecular proton transfer is coupled with the formation of a covalent C–O bond between the two molecules. We find a novel catalytic reaction mechanism in which an H₂SO₄ catalyst reduces the barrier height from $\Delta H^{\ddagger}_{298} = 140.2$ to 16.3 kJ mol⁻¹. It is well established that H₂SO₄ can effectively catalyse intramolecular proton transfers. This letter shows that H₂SO₄ can catalyse an intermolecular proton transfer that is coupled with a covalent bond formation.

Keywords: Sulfuric acid catalyst, Intermolecular proton transfer, Glyoxal, G4(MP2), CCSD(T).

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