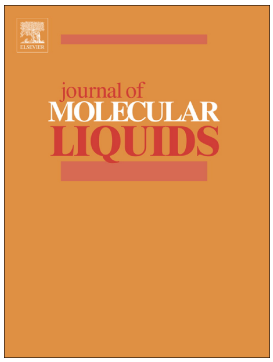

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Hydrogen bonding interaction of ascorbic acid with nicotinamide: experimental and theoretical study

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Abstract

The interactions of ascorbic acid (AA) with nicotinamide (NA) were investigated by cyclic voltammetry (CV), ^{1}H nuclear magnetic resonance (^{1}H NMR), density functional theory (DFT) and atoms in molecules (AIM) analysis. Changes in the anodic peak potential of AA and the ^{1}H NMR chemical shifts of NA indicated the formation of hydrogen bonding between AA and NA. The DFT and AIM results confirmed the mainly interaction sites are the hydrogen atoms on enediol of AA, and the nitrogen atom on the pyridine ring and the carbonyl oxygen atom on the amide group of NA.

Keywords: nicotinamide; ascorbic acid; interaction; hydrogen bonding

1. Introduction

Ascorbic acid (vitamin C, AA) is one of the most important vitamins with antioxidant properties that widely exist in various fruits and vegetables. AA plays a crucial role in healthy and biological metabolism in the body. It takes part in free radical scavenging, cancer prevention, collagen synthesis, iron absorption, wound healing, cholesterol metabolism and immunity improvement [1,2]. Deficiency of ascorbic acid in human may cause scurvy, anemia, gum problems, muscle degradation and neurotic disorders [3]. As an antioxidant, AA is widely used in food, pharmaceutical formulations and cosmetic applications [4,5].

Nicotinamide (vitamin B3, NA) is an essential micronutrient, which is most abundant in foods such as meats, legumes, nuts, grains, coffee and tea. NA is involved in a wide range of biological processes, including energy metabolism, cell respiration, cholesterol and steroids synthesis, signal transduction and genome integrity maintenance [6]. Deficiency of NA is characterised by pellagra, acne, stomatitis, glottiditis and photosensitive dermatitis, therefore, it is used for treating various skin

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