QUANTUM MECHANICAL AND CONFORMATIONAL STUDIES OF TRIACETYLENE-CONTAINING ESTERS OF TRI(PROPYN-2-YL)TRIMESATE, TRI(BUTYN-3-YL)TRIMESATE AND TRI(PENTYN-4-YL)TRIMESATE

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Abstract

By the advanced of computers, computational methods based on quantum chemical calculations are widely used to determine structural and spectroscopic properties of compounds. In quantum theory, the system is described by wave functions. Once the wave functions are found by solving the Schrödinger equation, any electronic, atomic or molecular characteristics can be calculated from these functions (approximations have to be made).

The purpose of this work has been to study a series of new triacetylenes (Figure 1) which was synthesised by reactions of trimesic acid or trimesic acid chloride with (2-propyn-1-ol), (3-butyn-1-ol), (4-pentyn-1-ol) and (5-hexyn-1-ol), respectively. Different semi-empirical and \textit{ab-initio} methods are used to calculate structural and spectroscopic properties, including FT IR, FT Raman, UV-Vis, \textsuperscript{1}H and \textsuperscript{13}C NMR spectra of the title compounds. These theoretical results were compared with the experimental data obtained. The result of this work provides an easy access to solve structure of the compounds.

![Figure 1: General structure of compounds under investigation](image_url)