

TORSION - ROTATION - VIBRATION EFFECTS IN THE GROUND AND FIRST EXCITED STATES OF METHACROLEIN AND METHYL VINYL KETONE

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Methacrolein and methyl vinyl ketone are the two major oxidation products of isoprene emitted in the troposphere. New spectroscopic information is provided with the aim to allow unambiguous identification of these molecules, characterized by a large amplitude motion associated with the methyl top. State-of-the-art millimeter-wave spectroscopy experiments coupled to quantum chemical calculations have been performed. Comprehensive sets of molecular parameters have been obtained. The torsion-rotation-vibration effects will be discussed in detail.

From the atmospheric application point of view the results provide precise ground state molecular constants essential as a foundation (by using the Ground State Combination Differences method) for the analysis of high resolution spectrum, recorded from 600 to 1600 cm^{-1} . The infrared range can be then refitted using appropriate Hamiltonian parameters.

The present work is funded by the French ANR through the PIA under contract ANR-11-LABX-0005-01 (Labex CaPPA), by the Regional Council Nord-Pas de Calais and by the European Funds for Regional Economic Development (FEDER).