

Title: Microwave spectroscopy of molecule of olfactory interest: conformational analysis and computational methods

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In this project, the conformational study of the cis-3-hexen-1-ol and cis-3-hexenylacetate compounds is carried out in order to find some kind of relationship between their more stable conformers and their smell.

Initially, a conformational search was carried out using the Maestro 10.2 program for each of the compounds. Later on, the help of the GAUSSIAN16 suite of program, subsequent optimizations of the conformers obtained in each case were performed and the respective allocation of the vibrational frequencies.

A rearrangement of the conformers obtained based on their energies was made with the aim of being able to identify them by groups according to their stability. This also helped us to identify the most stable conformers of each compound in a more visual way.

As all the conformers obtained during the conformational search had dipole moment, they could be studied by rotational spectroscopy. Rotational transitions were measured using microwave spectroscopy. Finally, the lines obtained from the already predicted ones were assigned as corresponding to the most stable conformers within each group.

The instrument used for spectroscopic measurements is the Pulsed-Jet Fourier Transform Microwave Spectrometer. It is an instrument designed following the guidelines of Andresen et al. and Grabow et al. and with some details of the spectrometer of Professor Alonso from University of Valladolid.