

Vibrational spectroscopy of a cetane improver for biodiesel

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Biofuels represent one of the serious ways to succeed in the ecological transition. Diesel and biodiesel contains additives to facilitate the combustion reaction: these additives improve the engine performance and reduce the emissions of unburned hydrocarbons, particulates, carbon monoxide and nitrogen oxides. These constituents are called cetane improvers and the most common is 2-ethyl hexylnitrate (2-EHN) [1]. Since this additive is produced in very large quantities [2], it is important to be able to qualitatively and quantitatively identify its accidental release. The IR spectrum is needed for atmospheric detection.

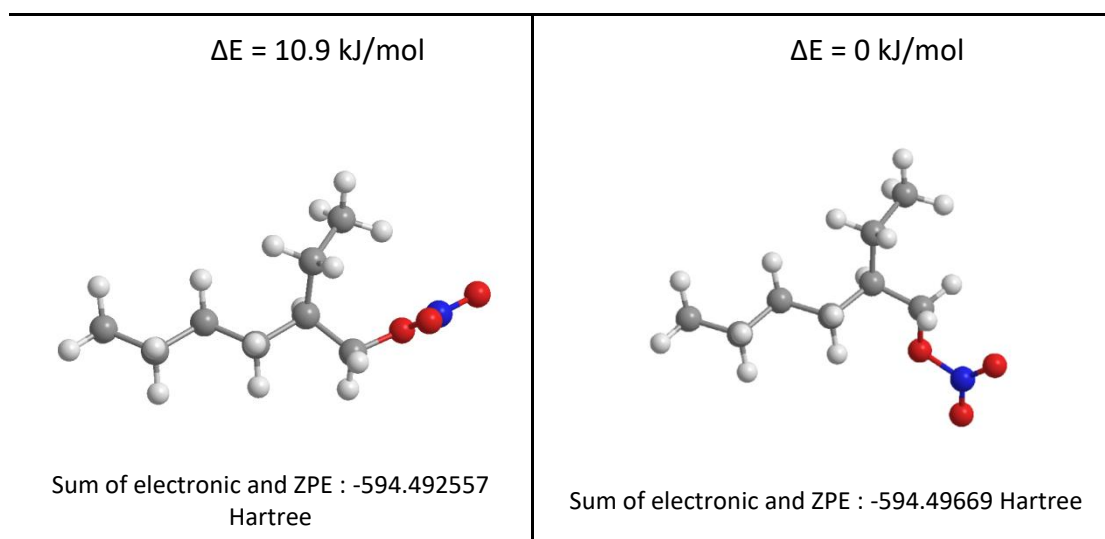


Figure 1: Some stable structures obtained for the 2-EHN with their energetics.

We have accurately measured the room temperature absorption cross section of 2-EHN, between 850 and 3000 cm^{-1} , using a FT-IR spectrometer. The main vibrational bands have been attributed, thanks to DFT calculations. Geometry optimizations also show the complexity of this flexible molecule, leading to almost iso-energetic conformers with slightly different vibrational spectra. The co-existence of all these isomers experimentally leads to particularly broad and complex absorption bands with shoulders. As an application, we also used these cross sections to probe the adsorption/desorption processes that can occur on the cell walls. All those aspects will be presented in this talk.

[1] Ickes, A. M., Bohac, S. V., & Assanis, D. N. (2009). *Energy & Fuels*, 23,10, (2009) 4943.

[2] PhD-Thesis, Elodie Nicolau. http://hal.archives-ouvertes.fr/docs/00/33/49/74/PDF/these271008-en_ligne.pdf