ROTATIONAL AND PHOTOELECTRON SPECTROSCOPIES MEET QUANTUM CHEMISTRY: N,N-DIETHYLHYDROXYLAMINE

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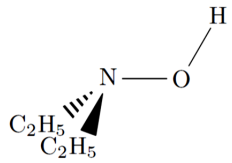
We report a combination of quantum mechanical calculations and different spectroscopic techniques used to investigate in the gas phase N,N-diethylhydroxylamine (DEHA), an important scavenger compound. The molecule has been first studied by rotational spectroscopy using Pulsed Jet Fourier Transform Microwave (PJ-FTMW) spectrometer in the 6.5-18.5 GHz frequency range and Stark modulated Free Jet Absorption Millimeter-Wave (FJ-AMMW) spectrometer in the 59.6-74.4 GHz range. Three conformers have been overall observed. They are all characterized by the hydroxyl hydrogen atom being in trans isomerism with respect to the bisector of the CNC angle. For the global minimum, also the ^{13}C and ^{15}N isotopologues have been observed in natural abundance, allowing for a partial structure determination. Ultraviolet Photoelectron Spectroscopy (UPS) and X-ray Photoelectron spectroscopy (XPS) measurements have been performed at the Gas Phase Photoemission beamline (GasPhase) of the Elettra Synchroton light laboratory (Trieste, Italy). The core (C(1s), N(1s) and O(1s)) photoemission spectra have been assigned with the support of SAC-CI/cc-pVTZ calculations. Density Functional Theory (DFT) approaches, including Time-Dependent DFT, have been exploited to reproduce the outer valence electron binding energies and peaks profiles, through the calculation of the Huang-Rhys factors. Interestingly, the structure of the first ionized cation is not that of an amine but it is similar to an N-oxoammonium compound.



trans-DEHA