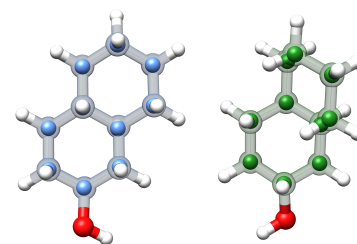


THE HORMONE ANDROSTERONE VS. ITS ANALOG DECAHYDRO-2-NAPHTHOL: DIFFERENCES AND SIMILARITIES

SWANTJE V. M. CALIEBE, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*;
PABLO PINACHO, *Physical Chemistry, University of the Basque Country (UPV/EHU), Bilbao, Spain*;
MELANIE SCHNELL, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*.

Here we report the study on the *cis* and *trans* isomers of decahydro-2-naphthol and various complexes with it. Decahydro-2-naphthol is structurally analogous to a section of the steroid hormone androsterone, which has been recently studied by rotational spectroscopy.^a For the large (from a rotational spectroscopy point of view) molecule androsterone, no experimental gas-phase structure was observed. In addition, intermolecular interactions in complexes with androsterone and smaller molecules cannot be experimentally studied due to the size of the steroid hormone. Because of that, decahydro-2-naphthol is an excellent system to indicate intermolecular interactions with other molecules and gain knowledge of the experimental gas-phase structure and thus, the conformational flexibility and arrangement in order to start to understand reaction mechanisms and functions of steroid hormones. Further, the orientations of the OH-groups in the decahydro-2-naphthol molecules were determined and also compared with the results from androsterone. The molecules were studied in the gas phase in a cold and isolated environment generated by a supersonic expansion. The spectra were recorded using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy in the 2-8 GHz frequency region. The assignment was supported by quantum-chemical calculations.



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