STEROID HORMONES IN THE GAS PHASE: THEIR PROBLEMS AND AN APPROACH

S. V. M. CALIEBE, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany, Institute of Physical Chemistry, Christian-Albrechts-Universität, Kiel, Germany; P. PINACHO, Physical Chemistry, University of the Basque Country (UPV/EHU), Bilbao, Spain; M. SCHNELL, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany, Institute of Physical Chemistry, Christian-Albrechts-Universität, Kiel, Germany

Steroid hormones are considered to be large molecules in the context of rotational spectroscopy, which leads to multiple challenges to study them, both experimental and in analysis. In order to understand the pathways and mechanisms of steroid hormones in the human body, one approach to study them and their interactions with other molecules is to investigate their fragments that represent parts of the overall molecule. Here, we will present the rotational spectroscopy study on the male steroid hormone androsterone¹ and compare it to a structural fragment of it, decahydro-2-naphthol. Further, we will show results for a second steroid hormone fragment set: the female hormone estrone² and 5,6,7,8-tetrahydro-2-naphthol. The comparison between the monomers will help with future work on complexes with the fragments. Studying complexes generates knowledge on interactions of the fragment with different solvents, functional groups, and molecules, which should lead to a better understanding of substrate-receptor interactions.

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¹doi:10.1021/acs.jpclett.2c03203, S.V.M. Caliebe, P. Pinacho, M. Schnell, Steroid hormone androsterone observed in the gas phase by rotational spectroscopy, J. Phys. Chem. Lett. 13, 11913-11917 (2022).

²doi:10.1039/D1CP04903H, P. Pinacho, S.V.M. Caliebe, M.M. Quesada-Moreno, S. Zinn, M. Schnell, Unexpected discovery of estrone in the rotational spectrum of estradiol: a systematic investigation of a CP-FTMW spectrum, Phys. Chem. Chem. Phys 24, 5539-5545 (2022).