ANALYSIS OF THE HIGH-RESOLUTION FOURIER TRANSFORM INFRARED SPECTRUM OF THE CHIRAL MOLECULE 1,3-DIFLUOROALLENE: A CANDIDATE FOR THE DETECTION OF MOLECULAR PARITY VIOLATION

S. ALBERT, M. GOTTSELIG, K. KEPPLER, E. MILOGLYADOV, G. SEYFANG, G. WICHMANN, M. QUACK, *Department of Chemistry und Applied Biosciences, ETH Zurich, 8093 Zurich Switzerland*; **J. STOHNER**, *ICBC, ZHAW, 8820 Wädenswil Switzerland*

According to traditional quantum chemical theory, the ground state energies of enantiomers of chiral molecules would be identical by symmetry, whereas "electroweak quantum chemistry," including the parity violating weak nuclear force, predicts a small parity violating energy difference between them, $\Delta_{pv}E$ on the order of sub-feV to feV. Experiments to measure this yet to be measured small effect are of importance both for fundamental physics in the standard model of elementary particles and for the evolution of biomolecular homochirality in the origin of life.[1,2] An important step towards such experiments, according to the approach following a previous publication[3], is the analysis of the high-resolution spectra of suitable candidate molecules. We have identified chiral allenes in general and 1,3-difluoroallene in particular as possible candidates for such experiments[1,2,3,4,5] (see Table 2 of Ref. 2) and report here the analysis of the FTIR spectrum in the region of the antisymmetric CF-stretching fundamental ν_{12} = 1087.138308(32) cm^{-1} and the symmetric stretching fundamental ν_4 = 984.9027(3) cm^{-1} of FHC=C=CHF.
The experimental results will be discussed in the context of possible further efforts towards measuring the parity violating energy difference in chiral molecules.[6,7,8,9]

[1]M. Quack, G. Seyfang, G. Wichmann, Proc. Nobel Symposium 167 on Chiral Matter Stockholm 2021, 207 (World Scientific, Singapore 2023).
[2]M. Quack, G. Seyfang, G. Wichmann, *Chem. Sci.* 2022, **13**, 10598.
[3]M. Quack, *Chem. Phys. Lett.* 1986, **132**, 147.
[4]M. Gottselig and M. Quack, *J. Chem. Phys.* 2005, **123**, 84305-1.
[5]L. Horny and M. Quack, *Mol. Phys.* 2015, **113**, 1768.
[6]Handbook of High-resolution Spectroscopy (3 Volumes), M. Quack and F. Merkt, Eds., 2011, Wiley, Chichester, New York.
[7]M. Quack, *Bunsen-Magazin* 2022, **24**, 238.
[8]G. Wichmann, G. Seyfang, M. Quack, *Mol. Phys.* 2021, **119**, e1959073.
[9]J. A. Agner, S. Albert, P. Allmendinger, U. Hollenstein, A. Hugi, P. Jouy, K. Keppler, M. Mangold, F. Merkt, M. Quack, *Mol. Phys.* 2022, **120**, e2094297.

p-number: p223 **Submitted on Wed, 02 Aug 2023 11:22:37 +0200**