High-Resolution Fourier Transform Infrared Spectrum of 1,3-Difluoroallene: a Candidate for the Detection of Molecular Parity Violation

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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 them to be different by a very small parity violating energy difference $\Delta_{pv}E$ on the order of sub-feV to feV. This small effect has not yet been measured: such experiments constitute a major challenge of physical-chemical stereochemistry with possible 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 [3], is the analysis of 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 [1-5] (see Table 2 of [2]). Here we report the high-resolution Fourier Transform Infrared (FTIR) spectroscopy and detailed analysis in the range 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 [6−9].

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