THE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM AND POTENTIAL ENERGY CALCULATIONS FOR AN AROMATIC CLAISEN REARRANGEMENT MOLECULE, ALLYL PHENYL ETHER

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Claisen rearrangement ethers are a fundamental organic, pericyclic rearrangement reaction reagent. In the mechanism of a Claisen rearrangement, a vinyl allyl ether is needed to provide the necessary Lewis acid/base sites on the molecule for the rearrangement and are simply heated. This rearrangement was first discovered by heating up the title molecule, allyl phenyl ether.[a] However, much like the Diels-Alder, Cope, and other pericyclic reactions, conformation and coordination of chemical groups is key to the Claisen mechanism. In this study, the authors present some structural characteristics of allyl phenyl ether from an analysis of the microwave spectra in the 8-14 GHz region using a CP-FTMW spectrometer. This is, to the authors knowledge, the first known microwave region study of the title molecule. Three conformers have been observed and assigned to date and will be discussed. Along with the rotational spectra, geometry calculations and potential energy surfaces performed at the MP2/6-311G++(3d,2p) level will be discussed and compared to the experimental results. Modeling the Claisen aromatic rearrangement mechanism using CP-FTMW spectroscopy will also be discussed.

[a] L. Claisen *Chemische Berichte* **45**, 3157, October 1912.