CHIRPED PULSE-FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF ETHYL 3-METHYL-3-PHENYLGLYCIDATE (STRAWBERRY ALDEHYDE)

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Strawberry aldehyde (C_{12} O_3 H_{14}), a common artificial flavoring compound, has two non-interconvertible conformational families defined by the relative stereochemistry around its epoxide carbons. In one family, referred to as the *trans* because the two large substituents (a phenyl ring and an ethyl ester) are on opposite sides of the epoxide ring, these two substituents are unable to interact with each other. However, in the *cis* family, there is a long-range interaction that is difficult to accurately capture in electronic structure calculations. Three *trans* and two *cis* conformations have been assigned by broadband chirped pulse Fourier transform microwave spectroscopy, along with the C-13 isotopomers in natural abundance for one conformer from each of the families. The agreement of the rotational constants, relative dipole moments, and relative energies between theory and experiment is excellent, even at relatively crude levels of theory, for the *trans* family, but is quite poor for the *cis* conformers. In addition, due to the reactivity of strawberry aldehyde and the high temperature to which it must be heated to yield a suitable vapor pressure, several decomposition products have been assigned, and more, as of yet unassigned, are likely to be present. This project demonstrates some of the challenges in performing large-molecule rotational spectroscopy.