

INTERNAL ROTATION ANALYSIS AND STRUCTURE DETERMINATION OF R-CARVONE

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When the spectrum of R-carvone was collected at Missouri S&T in preparation for a three-wave mixing experiment, splittings within the rotational transitions were observed that were unassigned in both the original study of S-carvone by Moreno et al.^a and the monoterpenoid study by Loru et al.^b As reported at the 75th annual ISMS, it was discovered that these splittings were due to internal rotations caused by two non-equivalent methyl rotors. This prompted a reinvestigation into the pure rotational spectrum of R-carvone using chirped-pulse, Fourier transform microwave (CP-FTMW) spectroscopy within the 5-18 GHz region of the electromagnetic spectrum. Since initially reporting this finding, all parent species and singly substituted isotopologues for the six conformers of carvone have been analyzed using XIAM^c. Within this presentation, the results of the reinvestigation will be reported, including the experimentally derived molecular structures for the six conformers as well as the experimentally determined barrier heights to internal rotation.

^aMoreno, J. R. A.; Huet, T. R.; González, J. J. L. *Struct Chem.* 2013, 24, 1163.

^bLoru, D.; Vigorito, A.; Santos, A. F. M.; Tang, J.; Sanz, M. E. *Phys. Chem. Chem. Phys.* 2019, 21, 26111-26116.

^cHartwig, H.; Dreizler, H. Z. *Naturforsch.* 1996, 51a, 923-932.