INTERNAL ROTATION ANALYSIS AND STRUCTURAL 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 unreported in the original study of S-carvone by Moreno et al.[a] It was discovered that these splittings were due to internal rotations caused by two non-equivalent methyl rotors. This promoted a re-investigation 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. Spectral analyses were performed using a combination of the SPFIT[b] and XIAM[c] software packages. Current work on the parent and singly substituted isotopologue species for the EQ1 and EQ2 conformers will be reported. In addition, the potential energy barrier heights to internal rotation for both rotors have been analyzed and will be discussed.

[a]Moreno, J. R. A.; Huet, T. R.; González, J. J. L. Struct Chem. 2013, 24, 1163.
[b]Pickett, H. M. J. Mol. Spectrosc. 1991, 148, 371-377.
[c]H. Hartwig and H. Dreizler, Z. Naturforsch 51a, 923-932 (1996).