

## Ro-vibrational Analysis of Several Infrared Bands of [3]-Radialene

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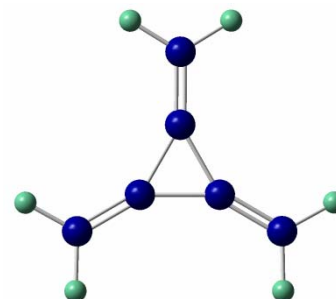
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We are engaged in the study of the high resolution infrared spectrum of trimethylene-cyclopropane, commonly known as [3]-radialene. This molecule is isomeric with benzene and is the first member of a class of alicyclic organic compounds containing exocyclic double bonds. Since this compound is not commercially available it was synthesized in-house at Oregon State University. In our initial work on this molecule, the structure was determined by electron diffraction, augmented by a ground state  $B_0$  value deduced by combination-differences from high-resolution infrared spectra. Details about the structure and the chemical bonding in [3]-radialene are reported in reference [1].



The  $3N-6$  fundamental-vibration degrees of freedom are classified according to the irreducible representation

$$\Gamma_{\text{vib}} = 4a_1'(\text{R}) + a_1'' + 3a_2' + 2a_2''(\text{IR}) + 7e'(\text{IR, R}) + 3e''(\text{R})$$

in which the infrared and Raman activities are shown in the parentheses. The  $a_1''$  and  $a_2'$  species are forbidden in both infrared absorption and Raman scattering processes.

The present work focuses on the ro-vibrational analysis of the  $\nu_9$  and  $\nu_{10}$  ( $a_2''$ ) parallel bands at 874 and 199  $\text{cm}^{-1}$  respectively, as well as of the  $\nu_{16}$  ( $e'$ ) perpendicular band at 780  $\text{cm}^{-1}$ . For each band, the possible perturbation by Coriolis interactions with nearby levels has been examined, aided by initial estimates of the state ro-vibrational parameters and the interaction constants obtained from Gaussian density functional calculations (B3LYP/cc-pVTZ). We report here the resultant upper state parameters of these three infrared active fundamentals.

[1] C. Wright, J. Holmes, J.W. Nibler, K. Hedberg, J.D. White, L. Hedberg, A. Weber, T.A. Blake, *Journal of Physical Chemistry A* **2013**, <http://dx.doi.org/10.1021/jp401813t>.