

ROTATIONAL SPECTROSCOPY OF FLUORONAPHTHALENES: THE MODEL STUDY OF HALOGENATED NAPHTHALENES

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The presence of a fluorine atom in fluoronaphthalenes ($C_{10}H_7F$) induces both mesomeric and inductive effects. The mesomeric effect results in electron redistribution, making particular carbon atoms susceptible to undergo nucleophilic attack at meta-position and electrophilic attack around ortho- and para- positions, while the inductive effect creates a polar bond that affects the polarity and the stability of the molecule and makes the para-position pre-dominant for the electrophilic attack. By studying the rotational structure in both the ground and excited vibrationally states, the higher order terms of rotational constants inform on molecular distortion relatively to the equilibrium structure from a reference frame in the molecular rotation model. Furthermore, the Coriolis or rotation-vibration terms which involve both the time variation of molecular displacement and the angular velocity of the frame can be characterized to demonstrate the influence of fluorine group on the variation of molecular flexibility in vibrational states.

Our present study reports the rotational spectroscopic measurements of 1- and 2-fluoronaphthalene in the millimeter-wave spectral region using both a chirped-pulse instrument (75-110 GHz) and a frequency multiplication chain-based spectrometer (140-220 GHz). By combining newly recorded transitions of fluoronaphthalenes with existing literature data^a, a refined set of spectroscopic parameters is derived for each species both in the ground and excited vibrational states up to 300 cm^{-1} . This study could serve as a valuable database for future investigations about the role of halogen groups in aromaticity.

^aCarey, S. J., Sun, M., & Kukolich, S. G. (2014). Microwave spectra of 1-fluoronaphthalene and 2-fluoronaphthalene. *Journal of Molecular Spectroscopy*, 304, 25-27.