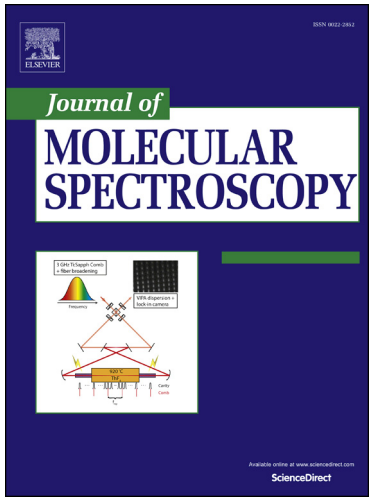

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Newly Assigned Microwave Transitions and a Global Analysis of the Combined Microwave/Millimeter Wave Rotational Spectra of 9-Fluorenone and Benzophenone

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Abstract:
Microwave spectra of 9-fluorenone and benzophenone have been observed using a broadband chirped-pulse Fourier Transform Microwave (cp-FTMW) Spectrometer. An analysis of the microwave spectra allowed for the assignment of 178 *b*-type rotational transitions for 9-fluorenone in the 8.0 – 13.0 GHz region, the assignment of 166 *b*-type transitions for benzophenone in the 8.0 – 14.0 GHz region, and effectively quadrupled the total number of pure rotational transitions observed for these molecules. This new microwave data and the previously published millimeter wave data of Maris et al have been analyzed together in a global fit, where the resulting rotational constants accurately reproduce the spectra over the entire 8 to 80 GHz region for both molecules. In addition, the resulting constants have been found to be consistent with the expected planar C_{2v} structure for 9-fluorenone and the paddle-wheel like C_2 structure of benzophenone. The rotational constants of the combined global fit have allowed for a more precise determination of the inertial defects (Δ) and second moments of inertia (P_{cc}) for 9-fluoreneone and benzophenone. Specific focus has been paid to the second moment of benzophenone, which when used in conjunction with theory strongly suggests an $\sim$32.9° torsional angle out of the *ab*-plane for the paddle-wheel structure of the gas phase molecule.