THE ROTATIONAL SPECTROSCOPY OF 2-FORMYLTHIOPHENE UP TO 750 GHZ IN ITS GROUND AND TWO VIBRATIONALLY EXCITED STATES

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The rotational spectrum of 2-formylthiophene ($C_5$, $\mu_a = 3.9$ D, $\mu_b = 2.4$ D) has been observed from 2 to 750 GHz and over 8500 transitions have been observed, measured, and least-squares fit for the ground vibrational state. The extensive frequency coverage allowed measurement of transitions up to $J = 180$ and $K_a = 72$. Spectroscopic constants have been obtained for a complete sextic distorted-rotor A- and S-reduced Hamiltonians, in the $I'$ representation. The first two vibrationally excited states of 2-formylthiophene are the torsional mode ($\nu_{27}$, $A''$, 122 cm$^{-1}$) and the in-plane C-C-O bend ($\nu_{19}$, $A'$, 173 cm$^{-1}$) of the formyl group. These two vibrationally excited states exhibit rotational transitions with frequencies perturbed by $a$- and $b$-axis Coriolis coupling despite an energy gap of nearly 50 cm$^{-1}$. Rotational transitions for the first two vibrationally excited states have been assigned, measured, and least-squares fit to a two-state Hamiltonian, which will provide an accurate and precise energy gap and Coriolis-coupling constants for these two modes.