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_s, μ_a = 3.9 D, μ_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^r representation. The first two vibrationally excited states of 2-formylthiophene are the torsional mode (ν_{27}, A$''$, 122 cm^{-1}) and the in-plane C-C-O bend (ν_{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.