THE 130-360 GHZ ROTATIONAL SPECTRUM OF THE CHLORINE ISOTOPOLOGUES OF CHLOROBENZENE AND ITS EXCITED VIBRATIONAL STATES

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We collected the rotational spectrum of chlorobenzene ($\mathrm{C_6H_5Cl}$, μ = 1.7117(14) D) in the frequency range of 130 – 360 GHz. For the [^{35}Cl]- and [^{37}Cl]- isotopologues, the ground states and a total of at least 15 excited vibrational states have been analyzed and fit as distorted rotors to sextic, A-reduced Hamiltonians with low-errors ($\sigma_{fit} < 50$ kHz). This analysis allowed for precise determination of the vibration-rotation interaction constants for each vibrationally excited state and demonstrated these constants are in quite close agreement with their predicted (B3LYP/6-311+G(2d,p)) values. For the lowest-energy vibrational states, transitions with high K_a and low J include hyperfine-resolved transitions of sufficient intensity to determine the quadrupole coupling constants. These data provide an exhaustive analysis of all accessible vibrational states in our frequency region and expand upon previously measured microwave transitions of chlorobenzene.