THE PRECISE EQUILIBRIUM STRUCTURE DETERMINATION OF CHLOROBENZENE (C_6H_5Cl) BY MICROWAVE AND MILLIMETER-WAVE ROTATIONAL SPECTROSCOPY

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The rotational spectra of many isotopologues of chlorobenzene (C_6H_5Cl) have been collected over portions of the 2 to 360 GHz frequency region. Several deuterium-enriched samples were generated via Grignard reaction of bromochlorobenzenes with a D_2O quench. The measured transitions of 22 isotopologues were least-squares fit to A- and S-reduced, sextic distorted-rotor Hamiltonians. The resultant rotational constants of all available isotopologues, with CCSD(T)/cc-pCVTZ corrections for vibration-rotation interaction and electron-mass distribution, were used to determine a highly precise semi-experimental equilibrium (${r_e}^{SE}$) structure of chlorobenzene. The preliminary ${r_e}^{SE}$ structure proved critical for finding ^{13}C-atom isotopologues of the deuterium-substituted species in the available rotational spectra by enabling more accurate predictions of the rotational constants for these very low-abundance species. Transitions for several more isotopologues are expected to be available in the collected data. The highly accurate and precise ${r_e}^{SE}$ structure will be compared to a CCSD(T)/cc-pCV5Z equilibrium (r_e) and ${r_e}^{SE}$ structures of other molecules determined with the same methodology.