THE MICROWAVE SPECTRUM OF 2-CHLOROETHYL RADICAL, CH_2ClCH_2

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The pure rotational spectrum of 2-chloroethyl radical, CH_2ClCH_2, has been observed for the first time using a cavity-based Fourier-transform microwave spectrometer in the frequency region of 10 GHz – 34 GHz. The radical was generated through electric discharge by applying a 1 kV voltage to the precursor molecule of either 1, 2-dichloroethane, CH_2ClCH_2Cl, or 1-chloro,2-iodoethane, CH_2ClCH_2I, where the latter gave 2-3 times stronger signal. Nine rotational transitions, both a-type and b-type, have been measured with resolved fine and hyperfine components for both ^{35}Cl and ^{37}Cl isotopic species in the ground vibrational state. The spectrum is highly congested due to the interactions of the electron spin, nuclear spin of chlorine atom, and nuclear spins of four hydrogen atoms. To aid in our analysis of the spectrum, we performed CCSD(T) calculation on the geometry optimization of the radical and a single point calculation at MP2 level to obtain the fine and hyperfine constants. We will present and discuss the corresponding assignments of features in the spectrum.