AN IMPROVED HIGH-RESOLUTION ROTATIONAL ANALYSIS OF [^{35}CL]- AND [^{37}CL]-2-CHLOROETHANOL

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Chlorinated species have been detected in various extraterrestrial environments, such as the interstellar medium (ISM), Mars, and carbonaceous chondrites. In the ISM, more than 90% of known chlorine is found in HCl, which is predicted to react with other known ISM constituents, ethylene oxide (*c*-CH_2CH_2O) and 1,2-ethanediol ($HOCH_2CH_2OH$), to form the simplest stable organic chlorohydrin, 2-chloroethanol ($ClCH_2CH_2OH$).[1] The detection of 2-chloroethanol is therefore critical for modeling chlorine chemistry in the ISM and guiding future astronomical observations. To assist the detection of 2-chloroethanol in the ISM, the rotational spectrum of 2-chloroethanol was measured from 140 to 700 GHz, coinciding with the frequency ranges for radio telescopes like ALMA and NOEMA. Additional microwave spectra from 8 to 26 GHz were collected to provide new measurements of rotational transitions with resolved quadrupole coupling. Both chlorine isotopologues (^{35}Cl and ^{37}Cl) were observed for the lowest-energy gauche-gauche conformer, providing an improved set of rotational and centrifugal distortion constants up to the octic level, for the ground and several vibrationally excited states less than 500 cm^{-1}. Recent analysis of the ^{37}Cl isotopologue has resolved and refined the nuclear quadrupole coupling constants. Here, we will present an update of our spectral analysis for this potentially important interstellar species.

[1] Soliday, R. M.; Bunn, H.; Sumner, I.; Raston, P. L. Far-Infrared Synchrotron Spectroscopy and Quantum Chemical Calculations of the Potentially Important Interstellar Molecule, 2-Chloroethanol. *JPCA* **2019**, *123* (6), 1208–1216. https://doi.org/10.1021/acs.jpca.8b11333.