HIGH RESOLUTION INFRARED SPECTRA AND VIB-ROTATIONAL ANALYSIS OF THE ν_3 AND ν_4 REGIONS OF CHLORINE NITRATE IN THE TEMPERATURE RANGE 190 TO 297 K

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Chlorine nitrate plays an important role in upper atmospheric chemistry. It was first detected in the stratosphere by *Rinsland et al.*[a] by observation of the ν_4 band a-type Q-branch. There have been a number of laboratory infrared spectroscopic studies on the ν_4 band since that ime.[b] Among them is the work of *Bell, Duxbury and Stuart*[c] who used a tunable diode laser to study and model the a-type Q-branches of the two chlorine isotopic species ^{35}Cl and ^{37}Cl as well as that of the $\nu_4 + \nu_9 - \nu_9$ hot band. At room temperature, even at the high resolution of a diode laser, the bands are only partially resolved due to the overlapping of lines of the two main isotopic species and of lines from several strong hot bands. A beautifully resolved spectrum of the ν_4 region over a limited range of J and K_a was obtained later by *Xu, Blake and Sharpe*[d] from diode laser spectra of a molecular jet at about 7 K.

In this work, 29 spectra of the region 750 to 900 cm^{-1} at temperatures ranging from 190 to 297 K and air pressures ranging from zero to 156 hPa were recorded at DLR with resolutions of 0.00094 to 0.0083 cm^{-1}. Using the ground-state constants of *Müller et al.*[e] a vib-rotational analysis of the ν_4 and ν_3 fundamental bands as well the hot band, $\nu_4 + \nu_9 - \nu_9$, of the most abundant ^{35}Cl isotopomer was carried out using the spectrum recorded at 191 K with the highest resolution and a zero air pressure. The corresponding cold bands for the lesser abundant isotope were partially assigned. Upper state rotational Hamiltonian constants were determined allowing precise modeling of the contours of the ν_4 fundamental Q-branches over the temperature and pressure ranges studied as shown by comparisons with the other spectra.

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[e] H. S. P. Müller, P. Helminger, and S. H. Young, J. Mol. Spectrosc. 181, 363 (1997).