Pure Rotational Spectroscopy of Sodium Chloride, NaCl, up to 930 GHz

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The pure rotational spectra of both isotopomers of NaCl, i. e. $^{23}Na^{35}Cl$ and $^{23}Na^{37}Cl$, have been recorded in high resolution with the Cologne terahertz spectrometer. A total of 189 new rotational lines have been measured in the frequency region between 200 and 930 GHz. Twenty nine of these transitions are assigned for $Na^{35}Cl$ to the vibrational ground state with $J \leq 72$, and 102 lines arise from vibrationally excited states up to the 5th vibrational state: $v = 5$. For $Na^{37}Cl$ a total of 58 rotational lines with $J \leq 76$ and $v \leq 4$ could be detected. The newly measured lines were fitted together with the published microwave and millimeter-wave transitions to obtain a refined and extended set of molecular parameters: $Na^{35}Cl$: B_0 = 6513.04908(41) MHz, D_0 = 9.338978(141) kHz, H_0 = –1.0433(144) mHz and $Na^{37}Cl$: B_0 = 6373.74158(66) MHz, D_0 = 8.943327(185) kHz, H_0 = –0.9623(162) mHz.

From the experimental data the equilibrium constants B_e, α, γ, D_e, β, δ, H_e and ε are calculated as well. The refined parameters for both isotopomers allow precise frequency predictions to be made far into the terahertz region. Thus this new and highly precise data set for NaCl is intended to support future astrophysical observations.

Key words: Rotational Spectroscopy; Sodium Chloride; NaCl; BWO; THz-Spectroscopy.