SUBMILLIMETER-WAVE SPECTRA of NCS

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The observation of the pure rotational spectra of NCS has been carried out for the $v_2 = 1$ and 2 states as well as for the $X^2\Pi$ ground state up to $J = 53.5$ in the submillimeter wave region. For the ground state, the analysis was straightforward. The measured transition frequencies were fit to a standard effective Hamiltonian for $^2\Pi$ vibronic states, and the improved molecular constants were obtained.

Rotational spectra in the excited bending vibrational states had not been analyzed in detail because of difficulties due to large Renner-Teller effect and anharmonic interactions. The $v_2 = 1$ vibronic state splits into four vibronic sub-states, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $\mu^2\Sigma$ and $\kappa^2\Sigma$. After various attempts, we obtained a reasonable fit for the $^2\Delta_{5/2}$ and $\mu^2\Sigma$ states, two of the lower components among the four vibronic states in $v_2 = 1$, to the experimental accuracy. On the other hand, inclusion of the higher vibronic components degrades the quality of the fit significantly, suggesting that the interaction with the (020) and/or (001) states should be taken into consideration. However, due to limited intensity of the spectra, the transitions in these vibronic states have not been fully identified. It makes full analysis and coherent interpretation difficult. In this talk, we will discuss where we are now and how we can proceed from here in near future.