SUBMILLIMETER WAVE SPECTRA OF NCS

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Rotational spectra of NCS in the excited bending vibrational states have not been analyzed in detail, because of difficulty in analysis due to large Renner - Teller effect and anharmonic interactions. We have extended the observation of the pure rotational spectra of NCS in the $v_2 = 1$ as well as in 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 including the higher order centrifugal distortion constants were obtained. The $v_2 = 1$ vibronic state splits into four vibronic sub-states, $^2\Delta_{5/2}$, $^2\Delta_{3/2}$, $\mu^2\Sigma$ and $\kappa^2\Sigma$. As a first attempt, the Δ and Σ states were fitted separately to effective Hamiltonians. The least square fittings converged by including various effective parameters concerned with the P-type doubling. However, the physical significance of these higher order parameters is not clear. It is found that the spin rotation coupling constant, γ, and the Λ-type doubling constants, p, q, are significantly different from those for the ground state. We have attempted to analyze the Δ and Σ states simultaneously by taking into account the perturbations from higher vibrational states.
An isotopic species, NC^{34}S, in the $X^2\Pi_{3/2}$ state has also been measured and r_0 structure is derived to be r_0(NC)= 1.1805(1) Åand r_0(CS)= 1.63212(7) Å.

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