Much is not known for NCS, while its sister molecule NCO is a quite familiar molecule for high resolution molecular spectroscopy and is known as one of the typical molecules to show the Renner effect. Molecular constants of $\tilde{X}^{2}\Pi$ NCS are known, but there has been a discrepancy between theoretically predicted and experimentally determined rotational constants.\textsuperscript{b} At the MR-SDCI+Q and MR-ACPF levels with the full-valence active space, our calculated $B_0$ values were smaller by at least 0.4 % than experimentally observed $B_0$ value, as is the case reported by Ouazbir, et al.\textsuperscript{b} When the core-valence correlation is included, this situation was improved to give an error of 0.05% in $B_e$ and $B_0$. The predicted $B_e$ and $B_0$, though preliminary at the moment, at the level of core-valence MR-SDCI+Q/aug-cc-pCVQZ are 6113.9 and 6103.5 MHz, respectively, against the experimental $B_0$ value\textsuperscript{a} of 6106.62162(25) MHz. The N-C and C-S equilibrium bond lengths are predicted to be 1.178 and 1.632 Å, respectively, and hence the $B_0$ of the isotopemer NC$^{24}$S could be 5959 MHz.

\textsuperscript{a}T. Amano and T. Amano, \textit{J. Chem. Phys.}, \textbf{95}, 2275-2279 (1991); and references therein.