# STRUCTURE AND SPECTROSCOPIC CONSTANTS OF $\tilde{X}^2\Pi$ NCS: AN *AB INITIO* MOLECULAR ORBITAL STUDY

TSUNEO HIRANO and UMPEI NAGASHIMA, *Grid Technology Research Center, Institute of Advanced Industrial Science and Technology, 6-9-3 Ueno, Taito-ku, Tokyo 110-0015, Japan*; TINA ERICA ODAKA and PER JENSEN, *FB 9 – Theoretische Chemie, Bergische Universität – Gesamthochschule Wuppertal, D-42097 Wuppertal, Germany*.

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,[a] but there has been a discrepancy between theoretically predicted and experimentally determined rotational constants.[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*.[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[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 $NC^{34}S$ could be 5959 MHz.

[a]T. Amano and T. Amano, *J. Chem. Phys.*, **95**, 2275-2279 (1991); and references therein .

[b]M. Ouazbir, G. Chambaud, P. Rosmus and P.J. Knowles, *Phys. Chem. Chem. Phys.*, **1**, 2649-2655 (1999).