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

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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).