COMPUTATIONAL SPECTROSCOPY OF NCS IN THE RENNER-DEGENERATE ELECTRONIC STATE $\tilde{X}\,^2\Pi$

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$\tilde{X}\,^2\Pi$ NCS is a Renner-degenerate linear molecule whose rovibronic spectrum is greatly complicated by the Renner effect and all-pervading resonances. As an alternative avenue to understanding this spectrum, we have calculated values of the ro-vibronic energies, intensities, and rotational constants by direct numerical solution of the rovibronic Schrödinger equation with the RENNER program.[a] All values obtained are in good agreement with the available experimental data. Rovibronic spectra are also simulated. The Renner calculations are based on three-dimensional potential energy surfaces and dipole moment surfaces computed *ab initio* for NCS in the $\tilde{X}\,^2\Pi$ electronic ground state at the core-valence, full-valence MR-SDCI+Q/[aug-cc-pCVQZ(N, C, S)] level of theory.

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[a]J. Freund, S. C. Galleguillos Kempf, P. Jensen, U. Nagashima, T. Hirano, *J. Mol. Spectrosc.* **345**, 31–38 (2018). DOI: 10.1016/j.jms.2017.11.010; T. Hirano, U. Nagashima, P. Jensen, J. Mol. Spectrosc., (2018), https://doi.org/10.1016/j.jms.2017.12.011.