GLOBAL ANALYSIS OF BROADBAND ROTATION AND VIBRATION-ROTATION SPECTRA OF SULFUR DICYANIDE

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The successful analysis of the quantum monodromy induced features in the rotational spectrum of the NCNCS molecule[a] prompted a quest for similar behaviour in its vibration-rotation spectrum and several high-resolution FT-IR spectra were recorded on the IFS125HR interferometer at the Canadian Light Source.[b] The sulfur dicyanide, $S(CN)_2$, molecule is a precursor to NCNCS and the analysis of its spectrum proved to be a prerequisite to a search for the elusive NCNCS transitions. The CLS spectra provided the opportunity to augment the previous extensive analysis of the FASSST rotational spectrum of $S(CN)_2$[c] with vibration-rotation data, in particular from the ν_4 fundamental at 121 cm^{-1} and its related hot-band series. A global fit of the two data sets allowed retaining the detailed analysis of the previously reported perturbations in the $3\nu_4$ triad and $4\nu_4$ tetrad of states, while allowing for determination of precise energies of all low-lying vibrational states of $S(CN)_2$. In this way we have determined wavenumbers for five lowest fundamentals of this experimentally difficult molecule and obtained an extensive set of benchmark data for calibration of anharmonic force field calculations of such quantities as the vibration-rotation changes in rotational constants, and anharmonicity coefficients. Comparisons with results of several such calculations are presented.

[a] B.P.Winnewisser, et al., *Phys. Chem. Chem. Phys.* **12**, 8158 (2010).
[b] M.Winnewisser et al., 67^{th} OSU Symposium on Molecular Spectroscopy, The Ohio State University, Ohio 2012, TF-01.
[c] Z.Kisiel et al., *J. Mol. Spectrosc.* **246**, 39 (2007).