THE HIGH-RESOLUTION FAR-INFRARED SPECTRA OF SULFUR DI-CYANIDE, $S(CN)_2$ AND THE PURSUIT OF THAT OF CYANOGEN ISO-THIOCYANATE, NCNCS

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There are only pellet low resolution infrared spectra reported in the literature for sulfur di-cyanide $S(CN)_2$, and none at all for cyanogen iso-thiocyanate, NCNCS. These two molecules are linked by a thermal isomerization reaction: NCSCN plus heat yields mainly NCNCS. Despite its difficult synthesis and its short kinetic life time, NCNCS is the best example so far of a quasi-linear molecule which clearly exhibits the distinctive monodromy-induced dislocation of the ro-vibrational energy levels. The momentum maps (monodromy plots) of various physical quantities, such as effective rotational constants, ro-vibrational energies, dipole moment components etc. for NCNCS show at the top of the punt of the two-dimensional champaign-bottle potential energy function[a] all the effects of quantum monodromy and exited state quantum phase transitions[b]. For that reason it would be highly interesting to observe for NCNCS the high-resolution FIR bands of the lowest quasi-linear bending vibration. At the Canadian Light Source in May-June 2011 we first had to obtain the far-infrared spectrum of the precursor molecule $S(CN)_2$ with the IFS125HR Bruker Fourier transform spectrometer. Six of the fundamental vibrational modes of this molecule have been observed and measured with the maximum resolution of 0.00096 cm^{-1}. The analysis of the measured and assigned band systems is presently being carried out and will be reported in this contribution. The experimental strategy for synthesizing NCNCS and observing its FIR bands in a flow system through a multi-pass infrared absorption cell will also be discussed.

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[b] D. Larese and F. Iachello, J. Mol. Struct., 1006 (2011) 611-628