CONTINUATION OF THE PURSUIT OF THE FAR-INFRARED SPECTRUM OF NCNCS, AT THE CANADIAN LIGHT SOURCE

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The molecule cyanogen iso-thiocyanate, NCNCS, has proved to be the most revealing model system for studying the effects of molecular quantum monodromy[a]. In two previous measuring campaigns in May 2011 and May 2012 at the Canadian Light Source (CLS) at the University of Saskatchewan we have obtained a rich collection of high-resolution infrared band systems for both $S(CN)_2$ and its isomer NCNCS which is our target molecule. We found experimentally that NCNCS is the more stable isomer. Some results for $S(CN)_2$ are reported in the adjacent talk in this session. However, the isomerization between $S(CN)_2$ and NCNCS and other reaction products make the attainment of a pure sample of NCNCS difficult and time consuming. We have not yet obtained a satisfactory high-resolution recording of the quasi-linear bending mode in the far infrared in the two allotments of beam time so far available to us. Our theoretical preparations for the project include recent refinements of predictions of intensities in the low-lying bending mode band system, which will be shown. The experimental aspects of obtaining an optimal sample of NCNCS in order to observe the rotational resolved spectrum in the CLS campaign scheduled for May 2013, and an initial report of the results, will also be discussed.

[a] B. P. Winnewisser, M. Winnewisser, I. R. Medvedev, F. C. De Lucia, S. C. Ross and J. Koput, Phys. Chem. Chem. Phys., **12**, 8158 (2010)