Contribution ID: **1049** Type: **Oral (Non-Student) / orale (non-étudiant)**

FTIR Synchrotron Spectroscopy of the Lower Vibrational Modes of Methyl Mercaptan at the Canadian Light Source

Monday 13 June 2016 16:45 (15 minutes)

The Fourier transform infrared spectra of the lower infrared vibrational bands of CH_3SH have been investigated from 650 to 1200 cm^{-1} at 0.001 cm^{-1} resolution employing synchrotron radiation at the Canadian Light Source in Saskatoon. The relative band strengths and structures are remarkably different from those for the analogous CH_3OH relative, with the CSH bend being very weak and both the in-plane and out-of-plane CH_3 rocks being strong with comparable intensities. The CSH bend has parallel a-type character with no detectable b-type component. The out-of-plane CH_3 rock is a purely c-type perpendicular band, whereas the in-plane rock around is of a/b character. The K-reduced $v_t = 0$ sub-state origins for the CSH bend follow the normal oscillatory torsional pattern as a function of K with an amplitude of 0.362 cm^{-1}, as compared to 0.653 cm^{-1} for the ground state and 0.801 cm^{-1} for the C-S stretching mode. The torsional energy curves for the out-of-plane rock are also well-behaved but are inverted, with an amplitude of 1.33 cm^{-1}. In contrast, the sub-state origins for the in-plane rock do not display a clear oscillatory structure but are scattered over a range of about 2 cm^{-1}, with indications of some significant perturbations. Our sub-band assignments extend up to about $K = 10$ for all the modes and are well-determined from GSCD relations, particularly for the a/b in-plane rock for which $\Delta K = 0$, +1 and −1 transitions are all observed.

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Session Classification: M3-2 Atomic and Molecular Spectroscopy and Precision Measurements II (DAMOPC) / Spectroscopie atomique et moléculaire et mesures de précision II (DPAMPC)

Track Classification: Division of Atomic, Molecular and Optical Physics, Canada / Division de la physique atomique, moléculaire et photonique, Canada (DAMOPC-DPAMPC)