



Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: 3659

Type: Oral (Non-Student) / Orale (non-étudiant(e))

Spinning the Top at the Light Source – Torsional FTIR Synchrotron Spectra of the CD₃SH Species of Methyl Mercaptan

Monday 19 June 2023 16:00 (15 minutes)

The far-infrared spectrum of CD₃SH has been recorded from 60 to 450 cm⁻¹ at the FIR beamline of the Canadian Light Source in Saskatoon in order to explore the evolution of the torsional structure in climbing up the ladder of torsional states. So far, the torsion-rotation levels have been extensively mapped up to the third excited torsional state, and we hope to push the assignments further up to the $v_t = 4$ state and beyond to where the ground torsional ladder is passing through the lower vibrational levels with the possibility of interesting torsion-vibration interactions. Here the torsional levels are high above the potential barrier to internal rotation and are essentially free rotor states following the parabolic curves of our “Universal Spectral Predictor”. We wish to explore how well the free rotor pattern can be modeled in order to gain predictive power for extrapolation up to higher states and potentially address the long-standing torsional problem of simultaneous global fitting of ground and vibrational states.

Keyword-1

FTIR molecular spectroscopy

Keyword-2

Torsion in CD₃SH

Keyword-3

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Session Classification: (DAMOPEC) M3-2 Atomic- and molecular physics - laser spectroscopy | Physique atomique et moléculaire - spectroscopie laser (DPAMPC)

Track Classification: Technical Sessions / Sessions techniques: Atomic, Molecular and Optical Physics, Canada / Physique atomique, moléculaire et photonique, Canada (DAMOPEC-DPAMPC)