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FTIR Synchrotron Spectroscopy of the S-H Stretching Band of Methyl Mercaptan –An Interstellar and Biogenic Molecule

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The infrared Fourier transform spectrum of the S-H stretching fundamental band of CH_3SH at 2604 cm^{-1} has been recorded using synchrotron radiation at the FIR beamline of the Canadian Light Source in Saskatoon. This band is an order of magnitude weaker than the corresponding O-H stretch of methanol, with a very different structure. It is a hybrid band predominantly of perpendicular b-type, with a smaller parallel a-component. With both ΔK = +1 and ΔK = -1 sub-bands present, the assignments are well-determined from ground-state combination relations, but are complicated by the presence of many J-localized perturbations. Upper-state term values have been determined for K = 0-14, and the substate origins have been fitted to a Fourier model. The oscillation amplitude of the torsional curves is 0.545 cm^{-1} compared to 0.652 cm^{-1} for the ground state, indicating a reduction of the order of 16% in the torsional barrier height V_3.

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