

HIGH RESOLUTION INFRARED AND MICROWAVE SPECTRA OF NH₃-HCCH AND NH₃-OCS COMPLEXES:
STUDIES OF WEAK C-H ···N HYDROGEN BOND AND ELECTRIC MULTIPOLE INTERACTIONS

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C-H ···N weak hydrogen bond is of much current interest. We report the first high resolution infrared spectroscopic study of a prototypical C-H ···N bonded system, i.e. NH₃-HCCH, at the vicinity of the ν_4 band of NH₃. The spectrum has been recorded using an infrared spectrometer equipped with an astigmatic multipass cell aligned for 366 passes and a room temperature external cavity quantum cascade laser at the 6 μm region. The perpendicular band spectrum of symmetric top rotor observed is consistent with the previous microwave^a and infrared^b studies at 3 μm . We also extended the previous microwave measurement to higher J and K .

For the related NH₃-OCS complex, microwave spectrum of J up to 6 and infrared spectrum at the vicinity of the ν_4 band of NH₃ have been recorded and analyzed for the first time. Comparison has been made with the previously studied isoelectronic complexes such as NH₃-N₂O^c and NH₃-CO₂.^d The source of the difference will be discussed with the aid of *ab initio* calculations.

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