HIGH RESOLUTION INFRARED AND MICROWAVE SPECTRA OF NH_3-HCCH AND NH_3-OCS COMPLEXES: STUDIES OF WEAK C-H$\cdots$N HYDROGEN BOND AND ELECTRIC MULTIPOLE INTERACTIONS

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C-H$\cdots$N weak hydrogen bond is of much current interest. We report the first high resolution infrared spectroscopic study of a prototypical C-H$\cdots$N bonded system, i.e. NH_3-HCCH, at the vicinity of the $\nu 4$ band of NH_3. 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 NH_3-OCS complex, microwave spectrum of J up to 6 and infrared spectrum at the vicinity of the $\nu 4$ band of NH_3 have been recorded and analyzed for the first time. Comparison has been made with the previously studied isoelectronic complexes such as NH_3-N_2O[c] and NH_3-CO_2.[d] The source of the difference will be discussed with the aid of *ab initio* calculations.

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