

HIGH-RESOLUTION INFRARED SPECTROSCOPY OF JET COOLED HCB_r SINGLET BROMOCARBENE DIRADICAL

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First high-resolution mid infrared rovibrational spectral data on jet cooled bromocarbene (HCB_r) diradical are obtained using quantum shot noise limited laser absorption methods. The HCB_r diradical is generated by coflowing bromoform (HCB_r₃) in a mixture of Ne, He, and H₂ through a pulsed slit discharge beam source and is subsequently cooled down to approximately 40 K in a slit-jet supersonic expansion. Interestingly, optimization of the HCB_r radical requires the presence of H₂, presumably due to decomposition of HCB_r₃ by H atom chemistry in the discharge. Rotationally resolved absorption spectra of the CH stretch $\nu_1 = 1 \leftarrow 0$ fundamental are analyzed, resulting in precise determination of ground and excited state rovibrational constants for both ⁷⁹Br and ⁸¹Br isotopologues. The results for the ground state are in good agreement with previous high resolution near IR electronic studies in the Sears group^a. The ν_1 band origin is now unambiguously assigned at 2799 cm⁻¹, which agrees well with previous LIF/dispersed fluorescence studies of Reid and coworker^b.

^aJournal of Molecular Spectroscopy 202, 131–143 (2000)

^bJ. Chem. Phys. 124, 134302 (2006)