HIGH RESOLUTION FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE $\tilde{A}^2 \Sigma^+ - \tilde{X}^2 \Pi$ TRANSITION OF THE BrCN⁺ ION

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The BrCN⁺ ion was produced by Penning ionization of BrCN with metastable He^{*}, and the near-infrared emission in the 690 - 870 nm region was measured by Fourier transform spectrometer. Thirteen vibronic bands of the $\tilde{A}^2 \Sigma^+ - \tilde{X}^2 \Pi$ transition of ⁷⁹BrCN⁺ and ⁸¹BrCN⁺ were observed. The rotational analysis was performed for the $\tilde{A}^2 \Sigma^+(000) - \tilde{X}^2 \Pi_{\Omega}(000)$ and $\tilde{A}^2 \Sigma^+(000) - \tilde{X}^2 \Pi_{\Omega}(010)$ transitions, both for the $\Omega = 3/2$ and 1/2 spin components.

Molecular constants, including the effective rotational constant, centrifugal distortion constant, Λ -type doubling constant in the $\tilde{X}^2 \Pi_{1/2}$ state, and spin-rotation interaction constant in the $\tilde{A}^2 \Sigma^+$ state, were determined from the observed spectrum. Spin-orbit interaction constants for the $\tilde{X}^2 \Pi$ ground state were determined to be -1476.4669(48) and -1476.4841(60) cm⁻¹, respectively, for ⁷⁹BrCN⁺ and ⁸¹BrCN⁺. The r_0 -structures for the $\tilde{X}^2 \Pi$ and $\tilde{A}^2 \Sigma^+$ states of BrCN⁺ were derived to be compared with that for the $\tilde{X}^1 \Sigma^+$ state of BrCN. The geometrical change of the BrCN⁺ ion from the BrCN molecule was turned out to be small.

Due to the Renner-Teller effect, the $\tilde{X}^2 \Pi(010)$ state was split into four components, $\mu^2 \Sigma$, $\kappa^2 \Sigma$, and ${}^2 \Delta_P (P = 5/2 \text{ and } 3/2)$, and the rotational analysis was performed both for the $\tilde{A}^2 \Sigma^+ - \mu^2 \Sigma$ and $\tilde{A}^2 \Sigma^+ - \kappa^2 \Sigma$ transitions. For the $\mu^2 \Sigma$ and $\kappa^2 \Sigma$ vibronic states, Ω -type doubling constants were determined as well as the rotational constants and centrifugal distortion constants. Renner parameter ϵ for the $\tilde{X}^2 \Pi$ state was determined to be -0.185 from the Ω -type doubling constants for both the isotopic species.