SUBMILLIMETER-WAVE SPECTROSCOPY OF THE VAN DER WAALS BENDING BAND OF Ar-HBr

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The Ar-HBr cluster has a large amplitude intermolecular bending motion. The excited states of the van der Waals vibrations were observed by infrared[a] and far infrared[b] laser spectroscopy. The cluster has a nearly "linear" structure of Ar-HBr in the ground state (Σ_0 state), while the cluster is estimated to have a nearly "anti-linear" structure of Ar-BrH in the first excited state (Σ_1 state) of the intermolecular bending vibration.

In the present study, we have observed submillimeter-wave transitions of the Σ_1 - Σ_0 band of Ar-HBr generated in a pulsed supersonic jet expansion. The observed band origins of the Σ_1 - Σ_0 bands of Ar-H^{79}Br and Ar-H^{81}Br are 6 and 27 MHz lower than those reported by combination differences of infrared data[a]. The eQq constants in the Σ_1 states were determined for the first time to be 260.90(12) and 217.854(98) MHz for Ar-H^{79}Br and Ar-H^{81}Br, respectively, which agree well with the estimated values (238 and 199 MHz for Ar-H^{79}Br and Ar-H^{81}Br) from a potential calculation[c]. The $cos^{-1}\sqrt{\langle cos^2\theta\rangle}$ value is 144.3° in the Σ_1 state, which is different from the value, 42.1°, in the ground state, where the θ is an angle between a cluster axis and a HBr monomer axis.

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