The $A^2\Pi_u$ - $X^2\Pi_g$ electronic transition of Br_2^+

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Abstract

The $A^2\Pi_u$ - $X^2\Pi_g$ electronic transition of Br_2^+ has been studied in the 500 – 720 nm wavelength range using the cryogenic cylindrical ion trap velocity map imaging spectrometer. Vibrationally resolved photofragment excitation spectra are recorded by [1+1] photodissociation via $A^2\Pi_u$ intermediate state. Photofragment excitation spectra for all three isotopologues of Br_2^+ ($^{79}Br_2^+$,$^{79}Br^{81}Br^+$,$^{81}Br_2^+$) are recorded, which yields the vibrational assignments of the observed bands. The present results has allowed to make a full vibrational assignment of the $A^2\Pi_u$ - $X^2\Pi_g$ electronic transition of Br_2^+.

Introduction

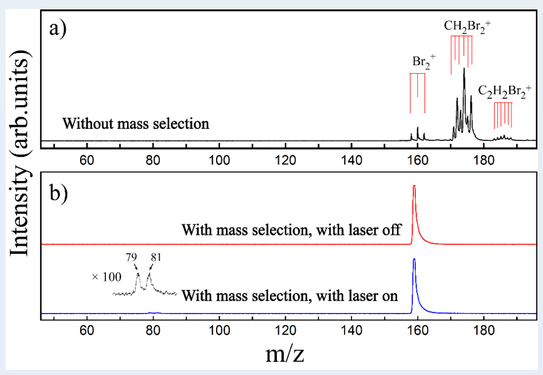
Br_2^+ ions have been received wide attention due to the role in chemical environments and industrial utilization in the past decades. Spectroscopic studies have been performed using different experimental approach aiming to investigate spectroscopic properties for the lowest several states. However, the knowledge regarding the electronic states of Br_2^+ at low energies have not been completely interpreted.

Materials and Methods

- Br_2^+: EI of $CHBr_3$/He gas mixture (5 bar) is prepared to generate isotopologues.
- The photodissociation spectra are recorded using TOF-Mass spectrometer.

$$Br_2^+ \xrightarrow{(1+1)h\nu} Br^+ + Br$$

- Br_2^+ isotopologues are selected by quadrupole mass filter (QMF).



TOF spectra after fragmentation of Br_2^+.

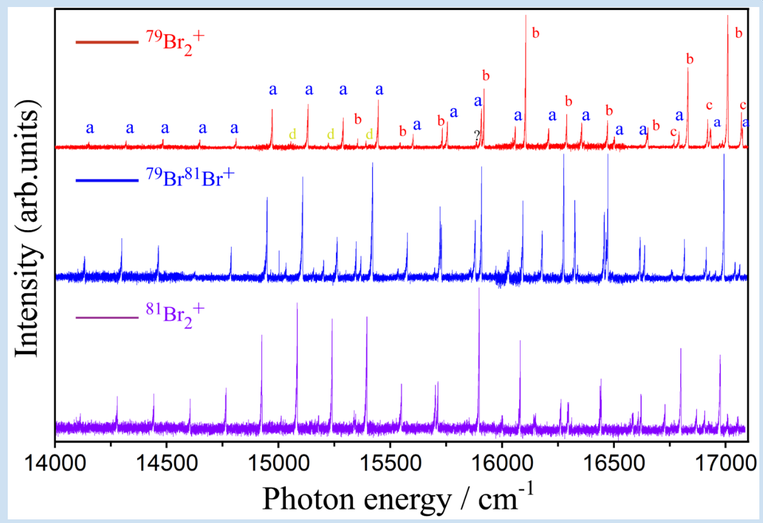
RESULTS AND DISCUSSION

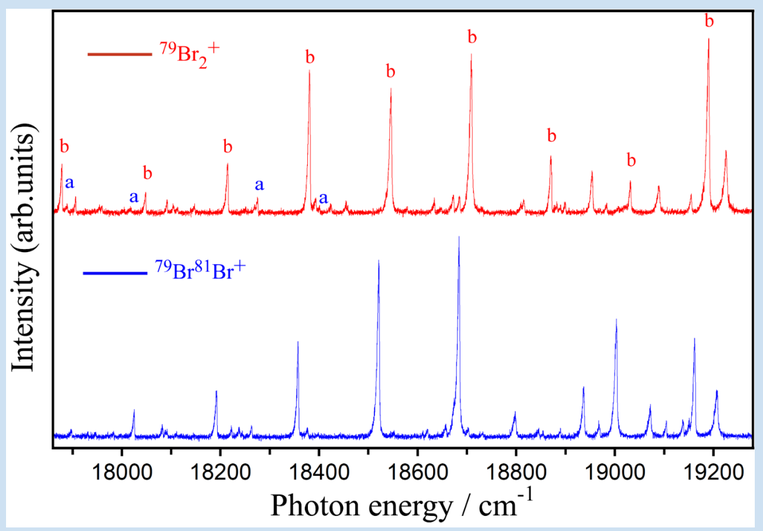
$A^2\Pi_{3/2,u}$ - $X^2\Pi_{3/2,g}$

or

$A^2\Pi_{1/2,u}$ - $X^2\Pi_{1/2,g}$

Some unknown vibrational bands ?

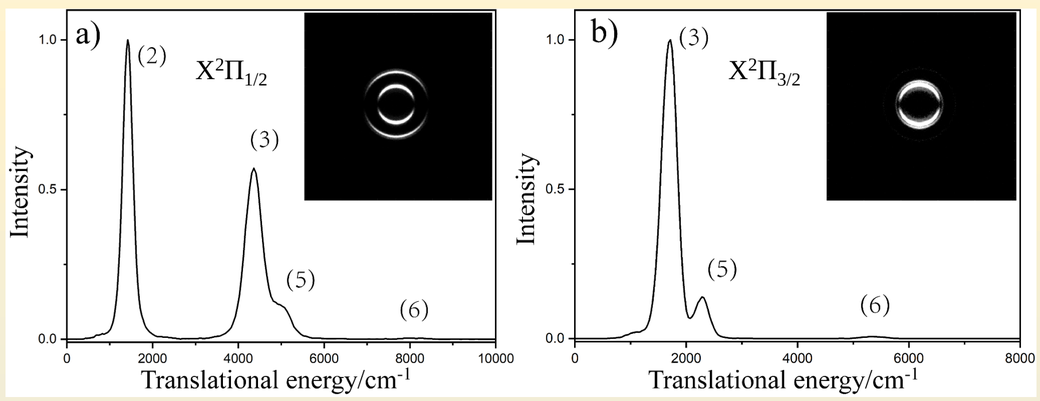




The photofragment excitation spectra for all three isotopologues of Br_2^+cation ($^{79}Br_2^+$,$^{79}Br^{81}Br^+$,$^{81}Br_2^+$) are recorded in the 500 – 720 nm wavelength range.

- Two main series of vibrational bands are distinguished from regular vibrational intervals with photofragment excitation spectra.

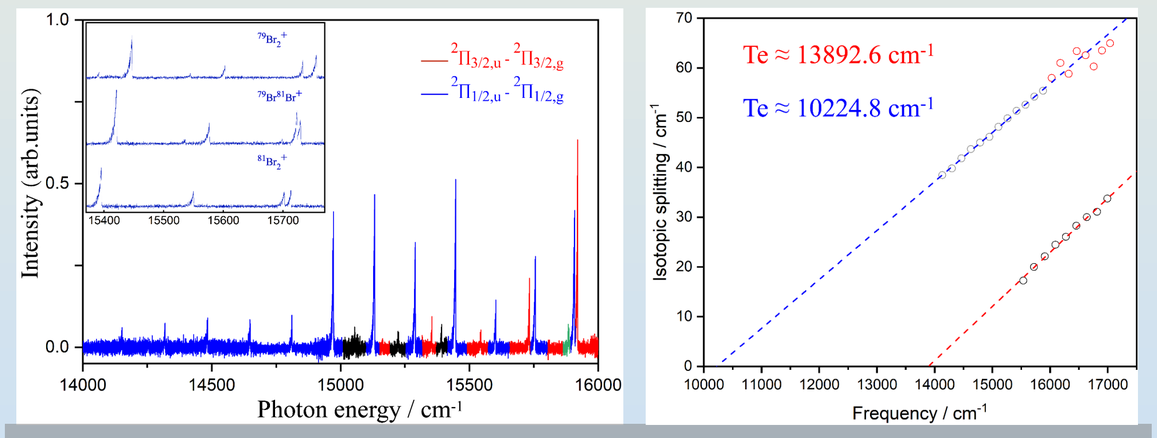
Identification of $X^2\Pi_{3/2}$ and $X^2\Pi_{1/2}$ states using VMI



TKER spectra of photofragment products of Br^+. a) E_{hv} = 15908 cm^{-1}; b) =15919 cm^{-1} ,TKER $= 2h\nu + 1/2\,\omega e - D_i - E_{so}(Br^+)_{\mathrm{int}} - E_{so}(Br)_{int}$.

- The total energy release spectra show the difference images due to the transition from $X^2\Pi_{3/2}$ or $X^2\Pi_{1/2}$ ground states.

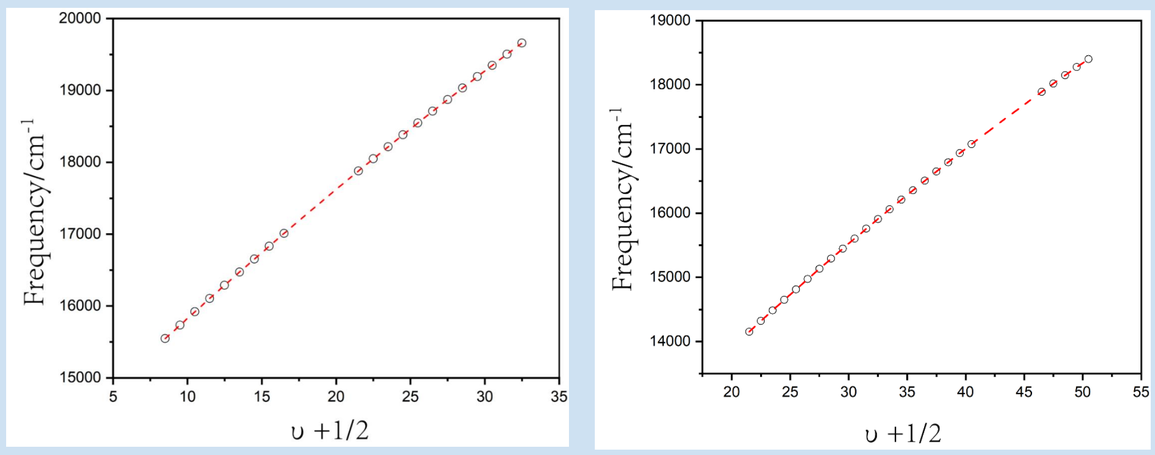
Isotopic Shifts



Isotopic splittings between 79-79 and 81-81 peaks against frequencies of the corresponding 79-81 peaks of Br_2^+.

- Estimated T_e value are deduced from isotopic shifts.

Vibrational Assignments



Curve fitting for each vibrational numbering.

- Vibrational assignments are confirmed by the well curve fitting.

CONCLUSION

1. The $A^2\Pi_u$ - $X^2\Pi_g$ electronic transition of Br_2^+ has been identified.

2. The molecular parameters are confirmed.

Acknowledgements

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