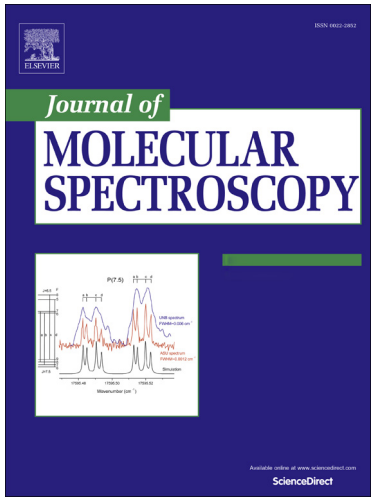


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# Rovibrational States of $HBF^+$ Isotopologues: Theory and Experiment

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**Abstract**

Near-equilibrium potential energy surfaces for $HBF^+$ isotopologues, obtained from high-level calculations beyond fc-CCSD(T), are employed in variational calculations for many rovibrational states. Calculated effective spectroscopic parameters are in excellent agreement with available experimental data and many predictions are being made, also for line intensities. The band origin of the bending vibration of $H^{11}BF^+$ is predicted at 730.7 $cm^{-1}$. Combining a difference-frequency system with glow discharge and a discharge modulation scheme, six and seven lines of the $\nu_1$ bands for $H^{11}BF^+$ and $H^{10}BF^+$, respectively, were observed. Together with data obtained from microwave spectroscopy the spectroscopic constants of $\nu_1$ could be derived through least-squares fitting.

*Keywords:* $HBF^+$, coupled-cluster theory, potential energy function, rovibrational transitions, line intensities, difference-frequency laser spectroscopy

## 1. Introduction

The number of high-resolution infrared (IR) spectra observed for molecular cations is still rather small. $HBF^+$ was among the first cations which could be studied in the middle of the 1980s. Using magnetic-field-modulated IR laser

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