

## Theoretical study of anharmonic resonances in HBS<sup>+</sup>

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### Czasopismo

Molecular Physics

### Numer woluminu

100

### Strony

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### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

A theoretical study of spin-rovibronic levels of HBS<sup>+</sup> in the X<sup>2</sup>II ground state is reported. Vibronic energy levels are calculated variationally using highly accurate full dimensional *ab initio* potential energy surfaces. All experimental levels are reproduced within 15 cm<sup>-1</sup>, and predictions of rovibronic levels up to 4000 cm<sup>-1</sup> for four isotopomers are provided. Anharmonic resonances induced by the Renner-Teller effect and strong spin-orbit coupling are analysed in detail.

### Adres publiczny

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