

Theoretical study of anharmonic resonances in HBS⁺

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Streszczenie

A theoretical study of spin-rovibronic levels of HBS⁺ in the X²II 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⁻¹, and predictions of rovibronic levels up to 4000 cm⁻¹ 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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