

Convergent ab initio Study of BH₃ Electron Attachment

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The lowest energy anion of BH₃ has previously been studied by photoelectron spectroscopy and matrix isolation infrared absorption spectroscopy.¹⁻² However, a theoretical description of the anion is deceptively challenging. Previous work has found the anion to be unstable to electron detachment in the vicinity of its *D*_{3h} minimum energy structure—becoming stable at stretched *D*_{3h} geometries. Only upon correction for zero-point vibrational energy (ZPVE), does the anion fall energetically below the neutral.³ In this work, BH₃ is studied with EOM-EA-CC methods up to CCSDTQP, predicting its adiabatic electron affinity and photoelectron spectrum. Particular attention is given to converging the critically-important ZPVE with respect to expansion of the basis set (both in diffuseness and angular momentum).

References

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