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# Ionic species in vapour over barium diiodide: Quantum chemical study of structure and thermodynamic properties

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## Ionic species in vapour over barium diiodide: Quantum chemical study of structure and thermodynamic properties

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### Abstract

The cluster ions Ba2I3+, Ba3I5+ and Ba4I7+ were detected earlier in saturated vapour over barium diiodide using high temperature mass spectrometric technique. In this work the structure and thermodynamic properties of the species BaI3–, Ba2I3+, Ba3I5+, Ba4I7+, and Ba5I9+ have been studied theoretically by using the density functional theory (DFT/B3P86) and Møller–Plesset perturbation theory (MP2 and MP4) with triple-zeta valence basis sets. The enthalpies of ion molecular reactions have been determined both theoretically and based of available experimental data; the enthalpies of formation of the cluster ions are found as follows (in kJ mol–1):  $-709 \pm 6$ , (BaI3–),  $-96 \pm 10$  (Ba2I3+),  $-654 \pm 15$  (Ba3I5+),  $-1177 \pm 20$  (Ba4I7+) and  $-1686 \pm 20$  (Ba5I9+).

#### **Keywords**

Cluster ions; Geometrical structure; Vibrational spectra; Barium diiodide; Enthalpies of formation; Thermodynamic functions; DFT; MP2 and MP4