

2017-10-01

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

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Elsevier B.V.

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<https://doi.org/10.1016/j.comptc.2017.08.022>

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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  $\text{Ba}_2\text{I}_3^+$ ,  $\text{Ba}_3\text{I}_5^+$  and  $\text{Ba}_4\text{I}_7^+$  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  $\text{BaI}_3^-$ ,  $\text{Ba}_2\text{I}_3^+$ ,  $\text{Ba}_3\text{I}_5^+$ ,  $\text{Ba}_4\text{I}_7^+$ , and  $\text{Ba}_5\text{I}_9^+$  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  $\text{kJ mol}^{-1}$ ):  $-709 \pm 6$ , ( $\text{BaI}_3^-$ ),  $-96 \pm 10$  ( $\text{Ba}_2\text{I}_3^+$ ),  $-654 \pm 15$  ( $\text{Ba}_3\text{I}_5^+$ ),  $-1177 \pm 20$  ( $\text{Ba}_4\text{I}_7^+$ ) and  $-1686 \pm 20$  ( $\text{Ba}_5\text{I}_9^+$ ).

## Keywords

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