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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 ± 6, (BaI3−), −96 ± 10 (Ba2I3+), −654 ± 15 (Ba3I5+), −1177 ± 20 (Ba4I7+) and −1686 ± 20 (Ba5I9+).

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