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Structure and thermodynamic properties of cluster ions in saturated vapor over barium dibromide

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ABSTRACT

The structure and thermodynamic properties of cluster ions detected earlier in saturated vapour over barium dibromide were studied theoretically. The equilibrium geometrical parameters and vibrational spectra were computed for the ions BaBr_3^- , Ba_2Br_3^+ , Ba_3Br_5^+ , Ba_4Br_7^+ and Ba_5Br_9^+ ; the DFT and MP2 methods with triple-zeta valence basis sets were used. The enthalpies of ion molecular reactions were obtained both theoretically through the total energies of participants and based on experimental data. The theoretical results were scrutinized with respect to methods of computation (DFT, MP2, and MP4). The enthalpies of formation $\Delta_f H^0(0)$ of the ions have been determined (in kJ mol^{-1}): -858 ± 6 (BaBr_3^-); -293 ± 10 (Ba_2Br_3^+); -982 ± 20 (Ba_3Br_5^+); -1644 ± 30 (Ba_4Br_7^+); -2282 ± 17 (Ba_5Br_9^+).

Key words: barium dibromide, cluster ions, DFT, MP2, MP4, geometrical structure, vibrational spectra, enthalpies of ion molecular reactions, enthalpies of formation, thermodynamic functions.

1.0 Introduction

Cluster ions are formed by the combination via noncovalent forces of two or more atoms or molecules of one or more chemical species with an ion [1]. They attract the interests of many researchers due to their unique electronic, optical and magnetic properties [2–4]. Cluster ions have been identified as good or potential materials for application in ion thrusters [5], ion implantation technologies [6], in magnetohydrodynamic generators [7] and aerospace investigations [8,9]. Owing to their unique properties, these ions may be used as building blocks of new materials [2,4,10], candidates in assembling crystals [3] and also are useful in chemical vapor transport and deposition [11–13].

Different cluster ions had been proved to exist in saturated vapour over alkaline earth halides by means of high temperature mass spectrometric technique [14,15]. Positive and negative ionic species were produced through thermal emission from crystalline SrCl_2 and BaF_2 at elevated temperatures under the conditions of free-surface and Knudsen cell evaporation [16,17]; the ions

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