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**Cluster ions in saturated vapor over barium difluoride:  
structure and thermodynamic properties**

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**ABSTRACT**

Different cluster ions detected earlier in saturated vapor over barium fluoride have been studied here theoretically. The equilibrium geometrical parameters and vibrational spectra were obtained for the ions  $\text{BaF}_3^-$ ,  $\text{Ba}_2\text{F}_3^+$ ,  $\text{Ba}_3\text{F}_5^+$ ,  $\text{Ba}_4\text{F}_7^+$ , and  $\text{Ba}_5\text{F}_9^+$ . The DFT/B3P86 and MP2 methods were implemented with the TZVP basis sets including the diffuse and polarized basis functions. Along with cluster ions, the dimer molecule  $\text{Ba}_2\text{F}_4$  properties were examined; the existence of isomeric forms was confirmed and the relative concentration of the isomers was evaluated. The enthalpies of ion molecular reactions were obtained both theoretically and based on experimental data. The enthalpies of formation  $\Delta_f H^\circ(0)$  of the species were determined (in  $\text{kJ mol}^{-1}$ ):  $-1356 \pm 4$  ( $\text{BaF}_3^-$ );  $-1039 \pm 12$  ( $\text{Ba}_2\text{F}_3^+$ );  $-2179 \pm 16$  ( $\text{Ba}_3\text{F}_5^+$ );  $-3277 \pm 35$  ( $\text{Ba}_4\text{F}_7^+$ );  $-4316 \pm 22$  ( $\text{Ba}_5\text{F}_9^+$ );  $-1859 \pm 7$  ( $\text{Ba}_2\text{F}_4$ ).

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

**1. Introduction**

An interest in the structure and properties of gaseous alkaline earth halide cluster ions has not declined due to a variety of applications. Heavy ions are applicable in ion thrusters [1], where accelerated ion beams generate a propellant force. Also ion beams may be used in magneto-hydrodynamic (MHD) generators [2], ion implantation technologies [3] and aerospace investigations [4,5]. The molecular and ionic clusters may serve as building blocks of novel materials [6–8], useful in assembling crystals [9]; and also useful in chemical vapor transport and deposition [10–12]. The understanding of behavior of alkaline earth metals in the presence of halogens, their effect as impurities or additives in combustion systems also require information on the cluster ions in vapor phase [13].

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