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Structure and properties of molecular and ionic clusters in vapour over caesium fluoride

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Abstract

The properties of neutral molecules Cs2F2, Cs3F3, and Cs4F4, and positive and negative cluster ions Cs2F+, CsF2−, Cs3F2+, Cs2F3−, Cs4F3+, and Cs5F4+ were studied by several of quantum chemical methods implementing density function theory and Möller–Plesset perturbation theory of second and fourth orders. For all species, the equilibrium geometrical structure and vibrational spectra were determined. Different isomers have been revealed for the trimer neutral molecule Cs3F3; pentaatomic, both positive and negative, Cs3F2+, Cs2F3−; and heptaatomic Cs4F3+ ions. The most abundant isomers in the saturated vapour were determined. Enthalpies of dissociation reactions and enthalpies of formation of the species were obtained.

Keywords: caesium fluoride, cluster ions, quantum chemical methods, geometrical structure, vibrational spectra, enthalpies of formation