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Mwanga, Stanley F.

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Molecular and ionic clusters existing in vapor over cesium chloride: Structure and thermodynamic properties

Stanley F. Mwangi, Tatiana P. Pogrebnaya, Alexander M. Pogrebnoi

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Abstract

The properties of neutral molecular Cs_2Cl_2 , Cs_3Cl_3 and Cs_4Cl_4 and the positively charged ionic clusters Cs_4Cl_3^+ and Cs_5Cl_4^+ existing in vapor over cesium chloride have been studied. The DFT method with B3LYP5 and B3P86 functionals, and Møller–Plesset perturbation theory of the second and fourth order have been used. The effective core potential with Def2-QZVP basis set for cesium and full electron basis set cc-pVTZ for chlorine were implemented. The geometrical parameters and vibrational frequencies of species have been determined. Isomers of two kinds have been revealed for Cs_3Cl_3 and Cs_4Cl_3^+ species, and their relative concentrations in vapor were evaluated. The dissociation reactions of the clusters with elimination of CsCl molecule were examined and enthalpies of reactions and enthalpies of formation of the species have been determined.

Keywords

Cesium chloride; Molecular and ionic clusters; Geometrical structure; Vibrational spectra; Thermodynamic properties