Theoretical study of the structure and stability of the Na2Cl+, NaCl 2−, Na3Cl 2+, and Na2Cl 3− ions

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Abstract

The geometrical parameters, normal vibration frequencies, and thermochemical characteristics of the Na2Cl+, NaCl 2−, Na3Cl 2+, and Na2Cl 3− ions in saturated vapors over sodium chloride were calculated by the ab initio methods including electron correlation. According to calculations, the Na2Cl+ and NaCl 2− triatomic ions have a linear equilibrium D ∞h configuration. The pentaatomic ions can exist in the form of the D ∞h linear isomer, C 2v planar cyclic isomer, or D 3h bipyramidal isomer. At ∼1000 K the Na3Cl 2+ and Na2Cl 3− ions exist predominantly in the form of the linear isomers. The energies and enthalpies of the ion-molecule reactions involving the above ions were calculated. The formation enthalpy of the ions Δf H 0(0 K) was determined: 230 ± 2 kJ/mol (Na2Cl+), −96 ± 4 kJ/mol (Na2Cl 3−), −616 ± 2 kJ/mol (NaCl 2−), and −935 ± 4 kJ/mol (Na2Cl 3−).

Keywords

Ions in vapors over sodium chloride; ab initio calculation; geometrical configuration isomers; geometrical parameters; vibrational spectra; ion molecular reactions; formation enthalpy of ions