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Structural and thermodynamic characteristics of ionic associates in vapors over sodium bromide and iodide

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Structural and thermodynamic characteristics of ionic associates in vapors over sodium bromide and iodide

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Abstract

Nonempirical methods are used to calculate the geometric parameters, the frequencies of normal vibrations, and thermochemical characteristics of ions existing in saturated vapors over sodium bromide and iodide: Na2X+, NaX 2−, Na3X 2+, and Na2X 3− (X = Br, I). According to the calculations, Na2X+ and NaX 2− triatomic ions have a linear equilibrium configuration of D ∞h symmetry. Pentaatomic ions can exist in the form of three isomers: linear with D ∞h symmetry, planar cyclic with C 2v symmetry, and bipyramidal with D 3h symmetry. At a temperature of ∼1000 K, Na3X 2+ and NaX 3− pentaatomic ions are shown to be present in vapor mainly in the form of linear isomers. The energies and enthalpies of ion molecular reactions with the participation of the above ions are calculated, and the formation enthalpies of the ions are determined, Δ f H o(0 K): 293±2 kJ/mol (Na2Br+), 354±2 kJ/mol (Na2I+), −536±2 kJ/mol (NaBr 2−, −458±2 kJ/mol (NaI 2−, 24±5 kJ/mol (Na3Br 2+, 143±5 kJ/mol (Na3I 2+, −810±5 kJ/mol (Na2Br 3−, and −675±5 kJ/mol (Na2I 3−.

Keywords
ionic associates in vapors over sodium bromide and iodide; nonempirical calculation; geometric configuration; isomers; geometric parameters; vibrational spectra; ion-molecular reactions; formation enthalpy of ions