

Kinetic and thermodynamic reasons for fractionation of chlorine isotopes in the process of halite sedimentation

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Abstract

Previously obtained

The data previously obtained with the use of *ab initio* quantum chemical methods in relation to the given statistical sums on the states of isotopic forms (β -factors) for the hydrated chloride ion and crystalline halite have been used for theoretical modeling of the process of fractionation chlorine isotopes during sedimentation of NaCl from saturated solution. It has been shown that during precipitation of halite in the process of evaporation of natural water reservoirs, appreciable separation of isotopes of chlorine may take place, wherein the thermodynamic component of isotope effect being dominant.