Enthalpy of Ionization for Isomeric Chlorophenols in Water

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Chlorophenols are introduced into the environment as a part of common pesticides and from various industrial processes such as pulp bleaching. Due to their toxicity and relatively high bioaccumulation potential, chlorophenols have been classified as priority water pollutants. The design of technologies for their effective removal from wastewaters requires reliable knowledge of their partition and reaction properties, namely of their standard chemical potential and ionization constant in aqueous solution in a range of environmentally relevant temperatures. Convenient method of modeling the temperature dependence for these properties is based on using their derivatives, which are the enthalpy of hydration or ionization, in simple thermodynamic integration.

We have measured the enthalpy of dissolution for *o*-, *m*-, and *p*-chlorophenol in water and the enthalpy of neutralization of these substances with stock sodium hydroxide solutions in the temperature range 15–45°C and at atmospheric pressure. The experimental enthalpy of dissolution and enthalpy of neutralization obtained at several finite concentrations were extrapolated to infinite dilution for the corresponding standard molar properties.

The enthalpy of hydration for chlorophenols can be determined from the standard molar enthalpy of solution and the enthalpy of sublimation or vaporization, obtained from the literature. Finally, the enthalpy of ionization of aqueous *o*-, *m*-, and *p*-chlorophenol was computed combining the standard molar enthalpy of solution, standard molar enthalpy of neutralization, and the enthalpy of water ionization taken from the literature.

Resulting temperature evolution of hydration and ionization enthalpy of chlorophenols can be applied in the construction of a temperature-dependent thermodynamic model for standard molar properties and ionization properties for these solutes. Combined with other literature results, the new data are also useful for the development of a group contribution scheme for aqueous chloro-substituted aromatics.

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