Thermodynamics of monochlorophenol isomers and pyrite interfacial interactions in the activation state

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Abstract

Thermodynamic parameters of the activation state for phenol and three monochlorophenol (MCP) isomer–pyrite complexes, i.e., MCP isomers used were 2-chlorophenol (2-CP), 3-chlorophenol (3-CP), 4-chlorophenol (4-CP), have been derived from the temperature-dependent kinetic data. Both the initial rate and adsorption density values increased in the order phenol < 2-CP < 3-CP < 4-CP. This suggests that the presence of chlorine substituent on the aromatic ring results in enhanced CP adsorption on pyrite. The activation energy (E_a), Gibbs free energy ($\Delta G^{\#}$), entropy ($\Delta S^{\#}$), and enthalpy ($\Delta H^{\#}$) of the activation stage for MCP adsorption on pyrite were calculated by Arrhenius and Eyring models. Always $\Delta S^{\#}$ values approximate to zero and $-T\Delta S^{\#}$ values are positive, which indicates that the activation state of MCP adsorption process is entropy-controlled, and the observed linear dependence of $\Delta H^{\#}$ on $-T\Delta S^{\#}$ signals an entropy–enthalpy compensation effect of the MCP adsorption process. The Γ_{MCP} data were quantified well both by $1 - \mathrm{p}K$ diffused double layer ($1 - \mathrm{p}K$ DLM) and Langmuir models.

Keywords: Pyrite; Monochlorophenol isomers; Phenol; Activation state; Electrical double layer; Langmuir model

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