MODELING INTERACTIONS OF PYRITE AND MONOCHLOROPHENOLS

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The overall aims of this research were to examine the ability of pyrite in the destruction of selected chloro-phenols found in drinking water and the interfacial properties of pyrite-water suspensions. The selected monochlorophenol (MCP) isomers were 2-chlorophenol (2-CP), 3-chlorophenol (3-CP), and 4-chlorophenol (4-CP). The adsorption density values on pyrite increased in the order, 2-CP < 3-CP < 4-CP at 298 K. The MCP adsorption data were always in accordance with the Langmuir model. According to the calculated thermodynamic parameters, in most cases, $\Delta H^{\#} < -T\Delta S^{\#}$, indicating that the adsorption step was largely entropy-controlled. The optimal pH of the MCP adsorption onto pyrite was ranged pH between 5 and 6.

The mechanism of adsorption of 4-CP onto pyrite was identified by IR spectroscopic data. The pyrite oxidation had occurred both at ≡Fe(II) and $\equiv S_2$ sites forming FeOOH and $S_2O_3^{2-}$ on pyrite surface. The ≡Fe(III) at sulfur-deficient defect sites can split adsorbed water molecules into hydroxyl radicals ($OH^{\bullet}_{ads}$), ≡Fe(II) and surface bound H^{+}. The spectroscopic evidence showed the formation of ≡FeOOH on pyrite surface by confirming the formation of $OH^{\bullet}_{ads}$ and H_2O_2. The 4-chlorophenolate anionic intermediate was formed at the production of inner-sphere surface complexes with ≡FeOOH on pyrite surface. The ≡SS-H groups on pyrite produced weak physical bonding with 4-CP. The IR bands observed at 1170, 1203 and 1145 cm^{-1} evidenced for the presence of HSO_4^- and $FeSO_4^0$ species in the vicinity. The most dominant sulfur oxy-anions are SO_3^{2-} and HSO_4^-.

The mechanistic pathway of the adsorptive degradation of 4-CP on pyrite was postulated as: