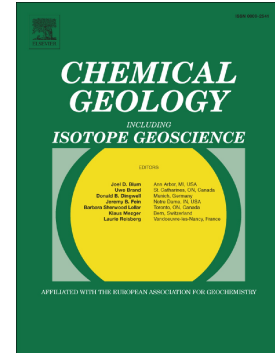


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Complexation of copper in acetate-rich low-temperature hydrothermal fluids: evidence from ab initio molecular dynamics simulations

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Abstract: Acetate ions are widely distributed in various geo-fluids and can be enriched in metamorphic brines under saturated vapor pressure in the temperature range of 80 to 200 °C. To examine the potential role of acetate in transporting metals, we conducted a series of ab initio molecular dynamics (MD) simulations to investigate the complexation of Cu⁺ with Cl⁻, HS⁻ and acetate ions. All the ab initio MD simulations were conducted at the temperature of 150 °C and pressures of 10 bar or 1000 bar. The ionic compositions of aqueous solutions for the simulations include four groups: (1) Cu⁺ and CH₃COO⁻; (2) Cu⁺, CH₃COO⁻ and Cl⁻; (3) Cu⁺, CH₃COO⁻, Cl⁻ and HS⁻; and (4) Cu⁺, CH₃COO⁻ and HS⁻. The simulation results demonstrated some important regularities for complexation of copper with acetate. The static computation results suggest that Cu⁺ forms linear complexes with one or two acetate ions, rather than with one acetate ion in a nearly symmetric bidentate structure,. The stoichiometry of the complexes, which can be represented by [Cu(CH₃COO)(H₂O)], [(CH₃COO)₂Cu]⁻ and [Cu(CH₃COO)Cl]⁻, depends on the fluid composition, environmental pressure and solvated structures of the acetate ligands in these complexes. Compared with Cl⁻, the acetate ion is a ligand of higher affinity for Cu⁺,

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