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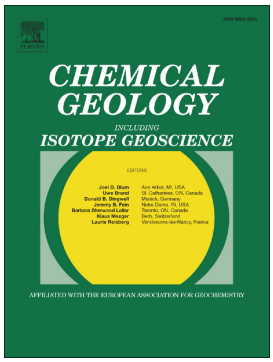

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Complexation of copper in acetate-rich low-temperature hydrothermal fluids: evidence from ab initio molecular dynamics simulations

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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 ℃. 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 ℃ and pressures of 10 bar or 1000 bar. The ionic compositions of aqueous solutions for the simulations include four groups: (1) Cu^+ and CH_3COO^-; (2) Cu^+, CH_3COO^- and Cl^-; (3) Cu^+, CH_3COO^-, Cl^- and HS^-; and (4) Cu^+, CH_3COO^- 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 $[Cu(CH_3COO)(H_2O)]$, $[(CH_3COO)_2Cu]^-$ and $[Cu(CH_3COO)Cl]^-$, 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^+,