

Gold solubility in ammonia-rich alkaline hydrothermal fluids: insights from *ab initio* molecular dynamics simulations

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Gold is transported as aqueous complexes in chloride and sulfur rich hydrothermal fluids in its reduced oxidation state (Au(I)) with major ligands (Cl⁻ and HS⁻, and recently S₃⁻), which has been investigated by considerable theoretical and experimental studies (see reviews by Williams-Jones et al., 2009; Pokrovski et al., 2014; Brugger et al., 2016). However, ammonia-rich alkaline hydrothermal fluids may play an important role in some gold deposits, yet the solubility of gold and complexation of Au(I) with hydroxyl and ammine ligands in sulfur- and chloride-poor fluids received limited attention so far.

In this study, we use *ab initio* molecular dynamics (MD) simulations to calculate the coordination structures of Au(I)-OH and Au(I)-NH₃ complexes, and use thermodynamic integration to determine the formation constants of these species at temperatures up to 350 °C and at water-saturated pressures. Our simulations showed linear structures of Au(I) complexes with two bonded ligands (OH/NH₃/H₂O), consistent with previous experimental and theoretical studies of Au(I) complexation (e.g., Liu et al., 2014). The derived formation constants show that the stability of Au(I)-OH and Au(I)-NH₃ complexes decreases progressively with increasing temperature. These new data enable better understanding and quantitative modelling of gold mobility in alkaline and ammonia-rich hydrothermal fluids.

References:

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