Potential Energy and Molecular Dynamics Simulation of Gold(I) solutions

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Potential energy functions for Au(I)-nitromethane (NM, CH_3NO_2) and NM-NM interactions were calculated by fitting analytical expressions to quantum chemically derived energies. These functions were then used in a molecular dynamics simulation of one Au(I) cation in 499 nitromethane molecules in the NVT ensemble at room temperature. A comparative simulation with a generic NM-NM potential energy function was also performed for comparison and gave the same results with respect to the calculated properties. It was found that the first solvation shell around the gold ion contains 9-10 nitromethane molecules in a flexible environment with no strong symmetry. Complementary, cluster calculations on $AuNM_n^+$ were performed. The especially strong binding of nitromethane in $AuNM_2^+$ and the validity of the pair approximation are discussed. Similar calculations on $Au(CN)_2^-$ are presented as well.