Title : Using the Markov model to study the chemical kinetics of Magnesium ion in aqueous solution

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ABSTRACT

The kinetics of water exchange around Mg^{2+} ions in aqueous solutions can be elucidated using molecular dynamics (MD) simulations, time-independent component analysis (tICA), and Markov State Modeling (MSM) to explore the underlying mechanisms. Well-Tempered Metadynamics (WT-MTD) simulations were used to sample different states of the system, including Contact Ion Pair (CIP), Transition State (TS), and Solvent-Separated Ion Pair (SSIP). From these, 30 representative structures were selected for tICA, which reduces the complexity of the data and identifies the slowest-changing features. The results show that the slowest motion is mainly determined by the distance between Mg^{2+} and oxygen in water molecules (dMgO), while the second slowest motion is linked to the distance between Mg^{2+} and a randomly chosen water molecule (dMgO,2). MSM provides a more accurate estimate of the timescales for water exchange, showing that these processes take much longer than suggested by tICA alone, as expected for rare and slow events. The Chapman-Kolmogorov (CK) test confirms that the MSM correctly describes the system's behavior over time. This study highlights the effectiveness of combining tICA and MSM to analyze slow molecular processes and identify key factors in ion exchange dynamics. The approach provides a strong foundation for future research on ion solvation, ligand exchange reactions, and other rare events in chemical and biological systems.

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