

Effects of the uranyl association in aqueous solutions

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In our investigation we explored a complexation behavior of uranyl in aqueous solutions. For this purpose we performed a set of all-atom molecular dynamics simulations. During the simulation the fractions of uranyl ions being involved in dimer and trimer formations were monitored. To accompany fraction statistics we also collected distributions characterizing bound times of dimer and trimer complexes. Two factors influencing uranyl complexation were considered: temperature and pH level. As one can expect the increase of the temperature decreases uranyl ability to form associates lowering bound times/fractions and vice versa. The influence of pH level was modeled by adding H^+ or OH^- groups to a “neutral” solution. The addition of OH^- groups favors formation of complexes increasing the bound times and fractions. The extra H^+ ions in the solution make an opposite effect lowering uranyl association ability. For all the observed complexes we also made a structural analysis to reveal the mutual orientation of uranyl ions.