

## Accepted Manuscript

Uranyl solvation by a reference interaction site model

Bo Li, Alexei V. Matveev, Sven Krüger, Notker Rösch

PII: S2210-271X(14)00488-5

DOI: <http://dx.doi.org/10.1016/j.comptc.2014.10.032>

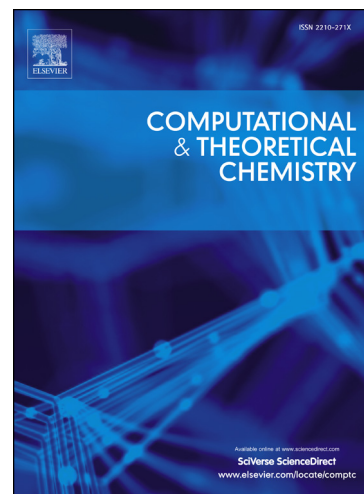
Reference: COMPTC 1656

To appear in: *Computational & Theoretical Chemistry*

Received Date: 5 September 2014

Revised Date: 23 October 2014

Accepted Date: 26 October 2014



Please cite this article as: B. Li, A.V. Matveev, S. Krüger, N. Rösch, Uranyl solvation by a reference interaction site model, *Computational & Theoretical Chemistry* (2014), doi: <http://dx.doi.org/10.1016/j.comptc.2014.10.032>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## Uranyl solvation by a reference interaction site model

Bo Li,<sup>a</sup> Alexei V. Matveev,<sup>a†</sup> Sven Krüger,<sup>a</sup> Notker Rösch<sup>a,b,\*</sup>

<sup>a</sup> Department Chemie and Catalysis Research Center, Technische Universität München, 85747 Garching, Germany

<sup>b</sup> Institute of High Performance Computing, Agency for Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore

### Abstract

We apply the one-dimensional reference interaction site model (RISM) to the solvation of uranyl in water. Uranyl aqua complexes with 4–6 explicit water ligands and an implicit water solvent, modeled by RISM to represent the further solvent environment, have been examined. The interaction of explicitly represented atoms of the aqua complexes are treated either by molecular mechanics or density functional theory, to build the free energy functional. A comparison of solvation energies and geometries of the aqua complexes for different numbers of explicit water ligands at the local minimum of the free energy surface indicate the interchangeability of explicit and implicit solvent models. Consequently the solvation energy is rather independent of the number of aqua ligands of the uranyl complex used as solute model, in contrast to results of a polarizable continuum model of solvation. For uranyl with four and five explicit water ligands in the first solvation shell we determined only a minor preference for the latter, in agreement with experiment. Other computational approaches tend to overestimate this preference.

### Keywords

Reference interaction site model, aqueous environment, uranyl, solvation

<sup>†</sup> Email: matveev@theochem.tu-muenchen.de

\* Corresponding author. Email: roesch@mytum.de

Download English Version:

<https://daneshyari.com/en/article/5393387>

Download Persian Version:

<https://daneshyari.com/article/5393387>

[Daneshyari.com](https://daneshyari.com)