Theoretical study on the mechanism of the removal of Mo from seawater in oxic environment

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There are still some arguments and disagreements remaining for the mechanism of Mo removal from the seawater under oxic environment [1-5]. There is a 1.7-2.0‰ (in terms of $^{97}Mo/^{95}Mo$) Mo isotopic composition offset between the seawater and the oxic sediments. To explain this offset, we should have the knowledge of the fractionations between the dominant $MoO_4^{2-}(aq)$ species and other possible aqueous Mo species and also the absorption complexes at the surface of (Fe,Mn)-oxyhydroxides. This study will show the results of these Mo fractionations especially including in the solvation effects of various aqueous Mo species.

Urey model or Bigeleisen-Mayer equation based theoretical method and the super-molecule clusters are used to precisely evaluate the solvation effects. The decent B3LYP/(6-311+G(2df,p),LANL2DZ) level method is used for frequencies calculation. Twenty-four water molecules are used to form the supermolecues surrounding the Mo species. At least 4 different conformers for each supermolecule are used to prevent the errors from the diversity of configurations in solution.

Our results show that the solvation effects can dramatically change the fractionation numbers from the ones in gas-phase. For example, the MoO_4^{2-} $Mo(OH)_6$ fractionation at 25°C is 0.8‰ for gas-phase but it is changed to 2.0‰ in solution. Our new results provide a base for discussing the mechanism of Mo removal from the seawater.

[1] Barling & Anbar (2004) *EPSL* **217**, 315-329. [2] Tossell (2005) *GCA* **69,** 2981-2993.

Bio-facies and organic geochemical features of the Jurassic organic-rich mudstone source rocks in the northern Qaidam Basin, NW China

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Through a comprehensive and sophisticated microscopic observation on organic petrologic macerals of the Jurassic mudstone source rocks in the northern Qaidam Basin, it is identified that algae, cutinites and sporophytes are the main organic macerals. Their content varies largely in different kinds of mudstones. Thus, according to different abundance of these organic macerals, four bio-facies types of mudstone source rocks were divided as type-A (algae-bed), type-B (dense convey-deposit algae), type-C (sparse convey-deposit algae) and type-D (algae-bits). From the type-A to type-D, the abundance of organic macerals become less and less.

In order to know how such bio-faies is related to quality of source rocks, a comparative correlation between bio-facies and organic geochemical parameters of source rocks was carried out. The result showed that the type-A source rock has a high TOC content higher than 4.0% and relatively good quality kerogen types as I-α_1. In contrast, the other three type source rocks have lower and lower TOC contents, as well as worse and worse kerogen type accordingly from the type-B to C, and to D. Therefore, it can be concluded that bio-facies is the main factor controlling the quality of source rocks. Specifically, the type-A source rock clearly has the best hydrocarbon generative potential and is the key object of petroleum geologic research and exploration. Analysis on the section of source sequences indicate that the type-A source rocks are only developed in parts (ca. several-tens of meters) of the Lower Jurassic, showing the heterogeneity of source rocks. Organic-rich source sequences tend to deposit in lagoon environments of lake-deltaic sedimentary systems. Therefore, it is showed that in the northern Qaidam Basin, the quality of mudstone source rocks was well differentiated and appraised based on bio-facies.