Contribution ID: **104** Type: **Poster**

Selectivity for Actinides with N,N’-Diethyl-N,N’ -Ditolyl-2,9-Diamide-1,10- Phenanthroline Ligand: A Hard-Soft Donor Combined Strategy

Thursday, 15 May 2014 17:30 (1h 15m)

Selectivity for Actinides with N,N’-Diethyl-N,N’-Ditolyl-2,9-Diamide-1,10-
Phenanthroline Ligand: A Hard-Soft Donor Combined Strategy

Wei-Qun Shi*, Cheng-Liang Xiao, Li-Yong Yuan, Yu-Liang Zhao, Zhi-Fang Chai,
Key Laboratory of Nuclear Radiation and Nuclear Energy Technology, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China
* Corresponding author: shiwq@ihep.ac.cn

MA(III) and Ln(III) have similar physicochemical properties, such as oxidation state, ionic radii, hydration, and complexation mode. Extractants containing soft sulfur or nitrogen atoms are preferred to recognize MA(III) over Ln(III). R-BTP, R-BTBP, and R-BTPhen ligands are the successful representatives for Ln(III)/MA(III) in the last 20 years [1-2]. However, light actinides (U, Np, Pu) normally favor ligands (alkylamide or alkylphosphate) containing hard oxygen atoms [3]. If we make sure the selectivity for light actinides using hard-atoms ligands, the separation of MA(III) from Ln(III) is difficult to achieve. To separate all the actinides from lanthanides, the synthesis, solvent extraction, and complexation behaviors of actinides and lanthanides by a novel phenanthroline-based tetradentate ligand with combined hard-soft atoms, N,N’-diethyl-N,N’-ditolyl-2,9-diamide-1,10-phenanthroline (Et-Tol-DAPhen, 1), are described in this work. The ligand exhibits excellent extraction ability and high selectivity of actinides over lanthanides from highly acidic solution. X-ray crystallographic structures of Et-Tol-DAPhen with thorium and uranyl ions are showed to be 1:1 complexation. The stability constants for some actinides and lanthanides complexes with Et-Tol-DAPhen are also determined in methanol by UV-Vis spectrometry. The results of density functional theory (DFT) calculation reveal that the An-N bonds have more covalent characters than that of Eu-N, which may dominate the selectivity of Et-Tol-DAPhen towards actinides. This work can shed light on the design of new ligands with combined soft-hard atoms for group separation of actinides from highly acidic nuclear waste.

[1] J. H. Lan, W. Q. Shi, Z. F. Chai , et al., Coord. Chem. Rev., 256, 1406 (2012).
[2] C. Z. Wang, J. H. Lan, W. Q. Shi, et al., Inorg. Chem. 52, 196 (2013).
[3]C.L. Xiao, C.Z. Wang, W. Q. Shi, et al., Inorg. Chem.2014, Submitted

This work was supported by NSFC (Grants 91026007, 21201166, and 21101157) and the “Strategic Priority Research Program” of the Chinese Academy of Sciences (Grant XDA030104).

Primary author: Prof. SHI, Weiqun (Institute of High Energy Physics,Chinese Academy of Sciences)

Co-authors: Dr XIAO, Chengliang (Institute of High Energy Physics,Chinese Academy of Sciences); Dr YUAN, Liyong (Institute of High Energy Physics,Chinese Academy of Sciences); Prof. ZHAO, Yuliang (Institute of High Energy Physics,Chinese Academy of Sciences); Prof. CHAI, Zhifang (Institute of High Energy Physics,Chinese Academy of Sciences)

Presenter: Prof. SHI, Weiqun (Institute of High Energy Physics,Chinese Academy of Sciences)

Session Classification: Poster Session - Chemistry of Nuclear Fuel Cycle / 1st ASGARD International Workshop

Track Classification: Chemistry of Nuclear Fuel Cycle / 1st ASGARD International Workshop