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239th ACS National Meeting, San Francisco, CA

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Program Area: NUCL: Division of Nuclear Chemistry and Technology

Symposium Title: Separation for application to the nuclear fuel cycle, in Memory of Dr. Charles Madic

INSTITUTIONS

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Reason for Abstract Submission: I am contributing this paper in response to the Call for Papers.

Invitation from: No response indicated

Email of Inviter: No response indicated

Criteria are met: Are met by at least one author

Presenting author will register: Yes

Abstract will be withdrawn if author cannot attend: Yes, I agree

Abstract submitted only once: Yes, I agree

Equipment Needs: No response indicated

Comments to Organizers: Submission for the Division of Nuclear Chemistry & Technology (NUCL)

This abstract is sent following the call for papers for the ACS symposium in memory of Charles Madic. I am a member of the ACSEPT integrated project of the European Community headed by the CEA (and by Charles Madic before his death). This abstract is sent at the CEA invitation.

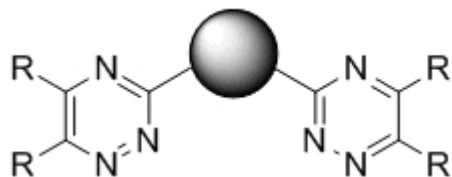
Preferred Presentation Method: Oral Preferred

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Undergraduate Student No

Title: NMR investigation of the lanthanide complexes with bis-triazine ligands: solution structure and extraction properties

Abstract Body: Bis-triazine ligands are remarkably selective extracting agents for the actinides/lanthanides separation. However, their effectiveness decreases on going from a central pyridine ring (BTP) to a bipyridine (BTBP) and finally to a terpyridine unit (BTTP). Nuclear magnetic relaxation dispersion and 1- and 2-dimensional NMR techniques have been used to unravel the solution structure of the complexes thanks to the dipolar paramagnetic shifts induced by Yb(III). The complexes stoichiometries and solvation have been deduced from the relaxivity changes caused by Gd(III). This analysis has been combined with molecular modeling and extraction data. BTP forms highly symmetric tris-complexes that are so compact that solvent molecules and anions are unable to penetrate the coordination sphere. Aliphatic substituents are rigidified on the NMR time frame, a phenomenon that has never been observed so far. These highly hydrophobic structures are very well extracted. Less crowded bis-complexes are formed by BTBP with enough room for a solvent molecule or a nitrate ion and for allowing linear and cyclic aliphatic substituents to rotate freely or invert their conformation. Finally, BTTP forms a bis-capped square-antiprismatic bis-complex with the two terpyridine units in intertwined coil geometries. Substituents are again rigidified in this highly crowded arrangement but nitrate ions easily compete with the ligands to form poorly extractable 1:1 species.



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