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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: Analytical Chemistry in Nuclear Technology

INSTITUTIONS

1. University of Liege, Coordination and radiochemistry, Sart Tilman B16, Liege, Liege, B4000, Belgium

AUTHORS

1. [Jean F. Desreux](#)¹, University of Liege, Coordination and Radiochemistry, Sart Tilman B16, Liege, Liege, B4000, Belgium , 3243663501, 3243664736, jf.desreux@ulg.ac.be
2. Geoffrey Vidick¹ ,
3. Nouri Bouslimani¹ ,

Reason for Abstract Submission: I was specifically invited to submit this paper.

Invitation from: Herman Cho, Pacific Northwest National Laboratories

Email of Inviter: hm.cho@pnl.gov

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Abstract will be withdrawn if author cannot attend: Yes, I agree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: Submitted at the invitation of Herman Cho, Pacific Northwest National Laboratories for the session on Advances in Magnetic Resonance Techniques in the Symposium on Analytical Chemistry in Nuclear Technology

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Undergraduate Student No

Title: NMR Spectroscopy and relaxivity of the actinide ions and of their complexes: In search of covalency effects

Abstract Body: Nuclear magnetic resonance has very rarely been used for investigating actinide ions and their complexes not only because of the lack of dedicated spectrometers but also because it is often assumed that paramagnetism cause excessive line broadenings. It will be shown that well-resolved NMR spectra of actinide complexes (U-Cm) can be obtained for stable, symmetric and rigid species. The induced paramagnetic shifts originate from both a through space dipolar contribution and a through bonds contact contribution. The latter gives access to delocalized unpaired electron densities that are directly related to the covalency of the actinide-ligand bonds. However, electron densities can only be obtained after separation of the two contributions. This has been accomplished thanks to variable temperature studies. In another approach, new ligands with rigid aliphatic substituents have been synthesized and contact contributions were deduced with the assumption that delocalization does not proceed to the ^1H nuclei most removed from the metal center. Covalency effects in lanthanide and actinide complexes will be compared and it will be shown that Cm(III) induces particularly large contact shifts

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