

# A Computational Simulation Spectral Analyses of Lanthanide and Actinide Complexes

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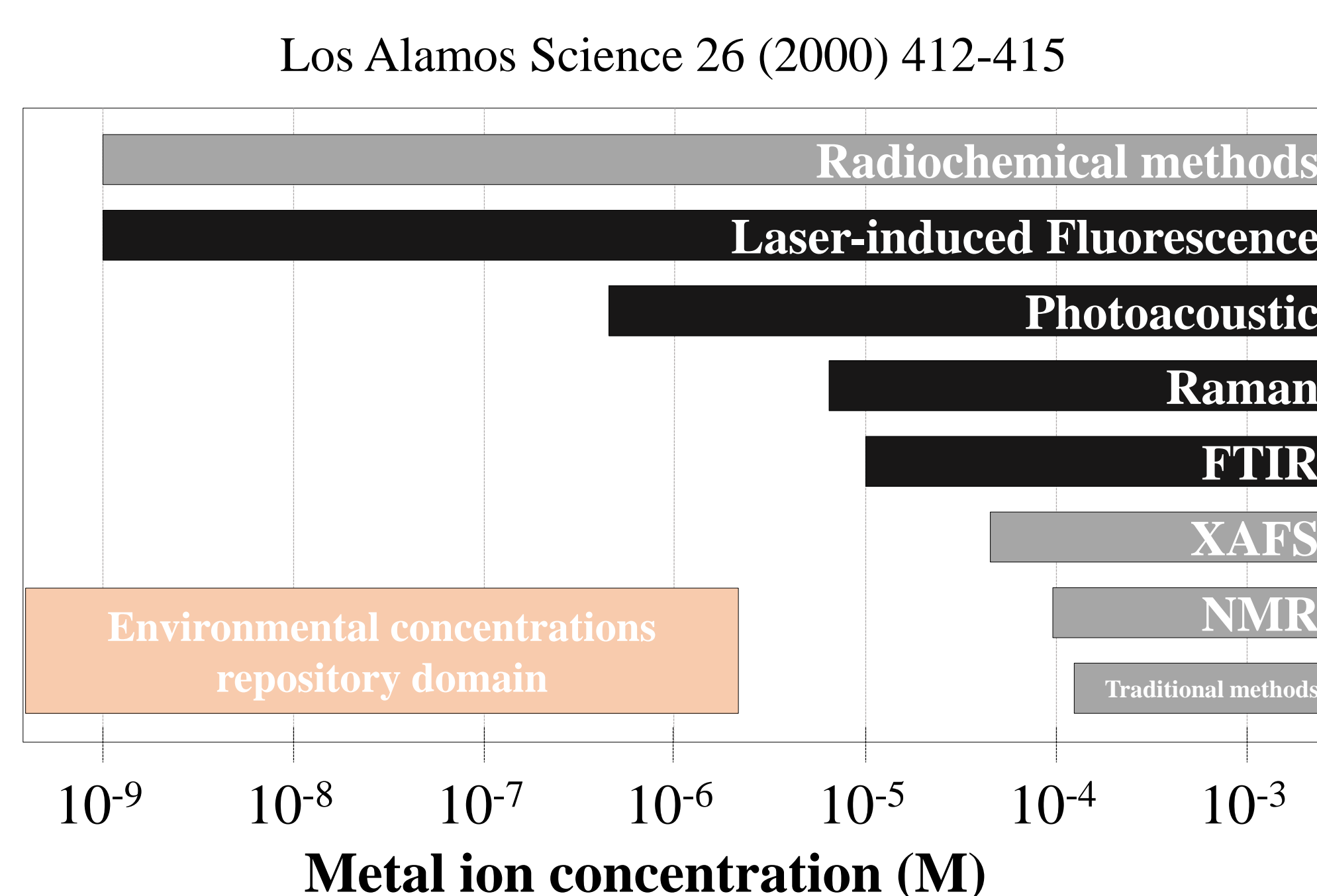
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## Abstract

Spectral analyses of the lanthanide and actinide complexes are essential part for the remote detection of leaking of radioactive stream. However, there is riskiness that caused radioactivity during experimental approaches to obtain radioisotope spectra especially in actinide complexes cases, therefore the virtual screening using advanced simulation techniques has been proposed and extensively used to reduce the chance of exposure to radioactive materials. Here, we perform the computational investigations for the complexes, especially samarium chloride complexes. All of simulations are accomplished using Gaussian 09 program package with B3LYP, and CAM-B3LYP functional and the levels of basis set are 6-311++G(3df,3pd) for ligand and the Wood-Boring quasi-relativistic method(MWB) for center metal atom. We optimized some complex structures, and simulated their UV-Vis spectra. Through the natural transition orbital(NTO) research, we could assign their peaks on the spectra to their electronic transition.

## Introduction



## Method

Gaussian 09 Program Package

Functional: B3LYP (CAM-B3LYP for UV-Vis)

Basis Set: 6-311++G(3df,3pd) for ligands

MWB28, MWB60 for center metals

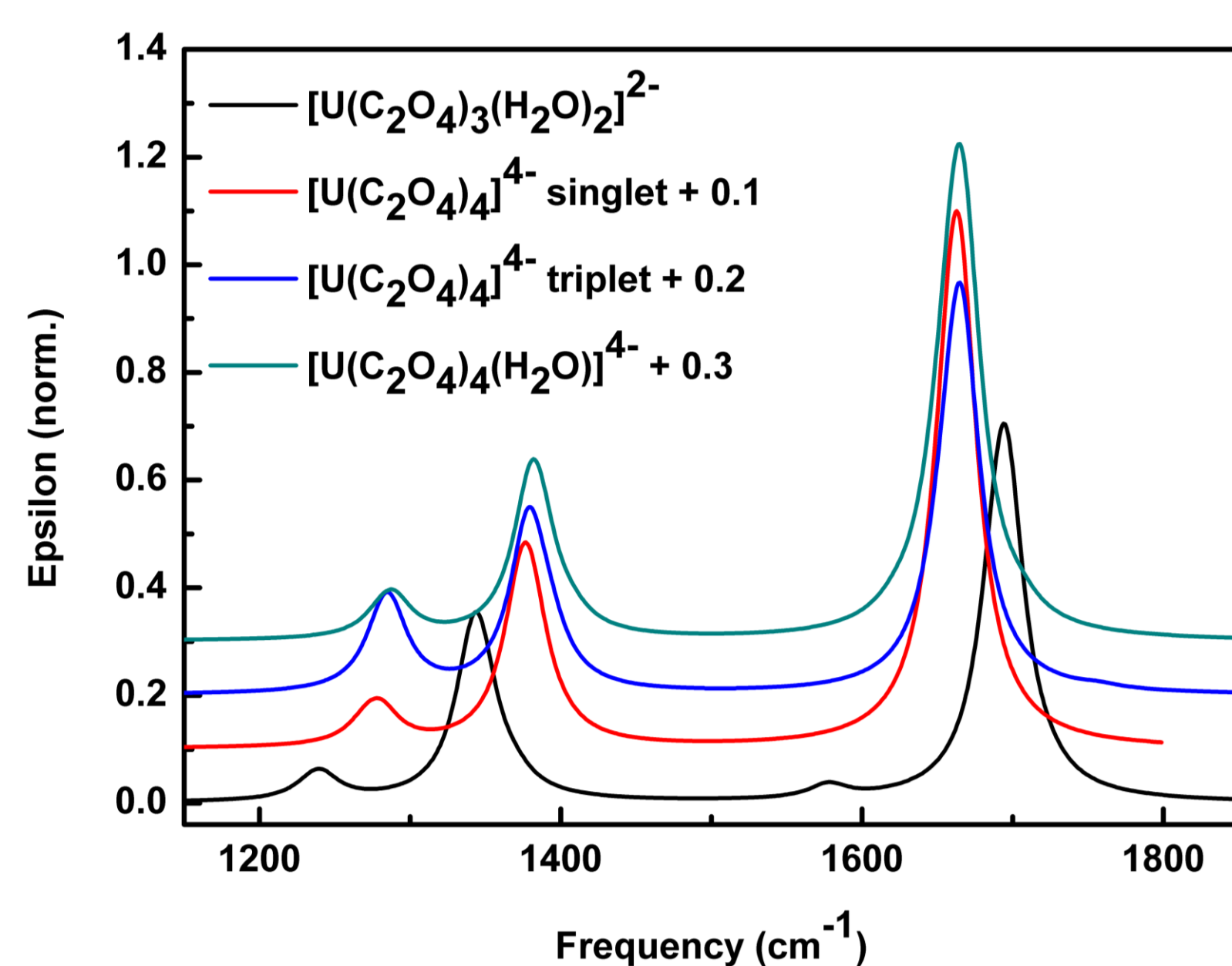
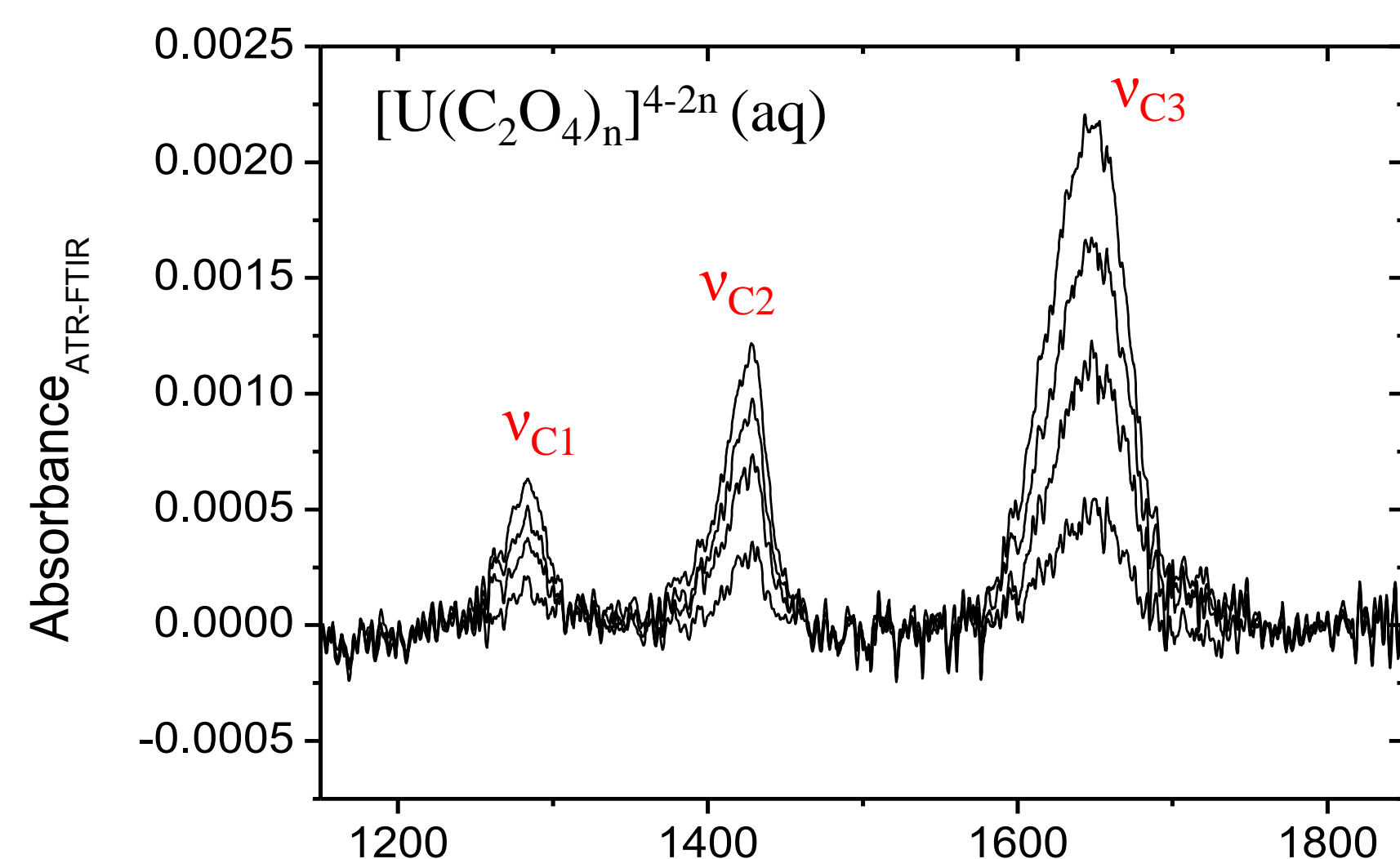
Natural Bonding Orbital, Natural Transition Orbital

\*MWB; Wood-Boring quasi-relativistic method for multi-valence electron system

## Results (U-Ox)

	Spin State	Coordination Number	U-O bond distance (Å)	
			Calc.	Ref.
[U(C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sup>2-</sup>	Singlet	8	2.407	
[U(C <sub>2</sub> O <sub>4</sub> ) <sub>4</sub> ] <sup>4-</sup>	Singlet	8	2.393	~2.41
	Triplet	8	2.397	
[U(C <sub>2</sub> O <sub>4</sub> ) <sub>4</sub> (H <sub>2</sub> O)] <sup>4-</sup>	Triplet	9	2.455	~2.47

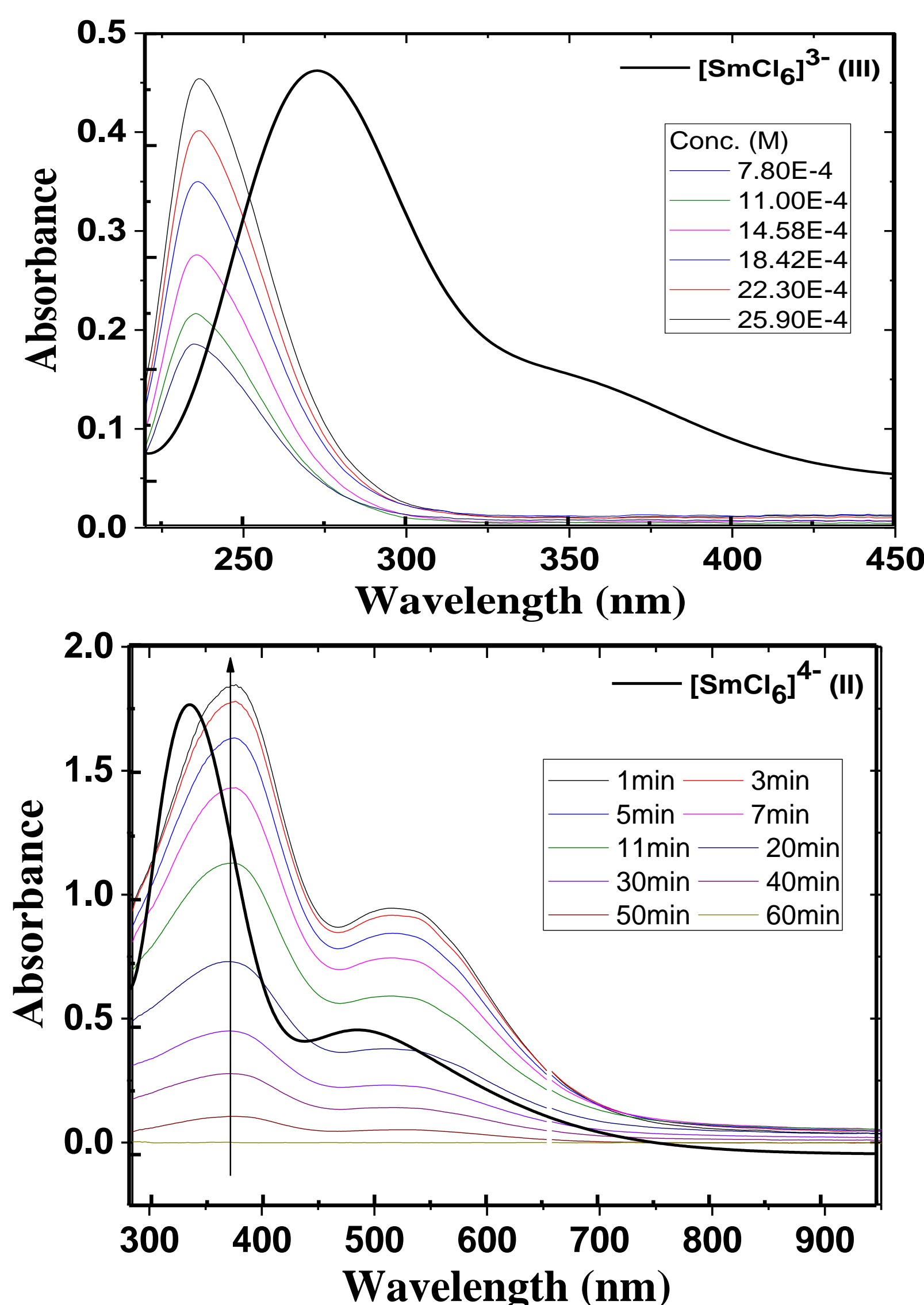
L. Duvieubourg-Garela et al. Journal of Solid State Chemistry 181 (2008) 1899-1908



## Results (Sm-Cl)

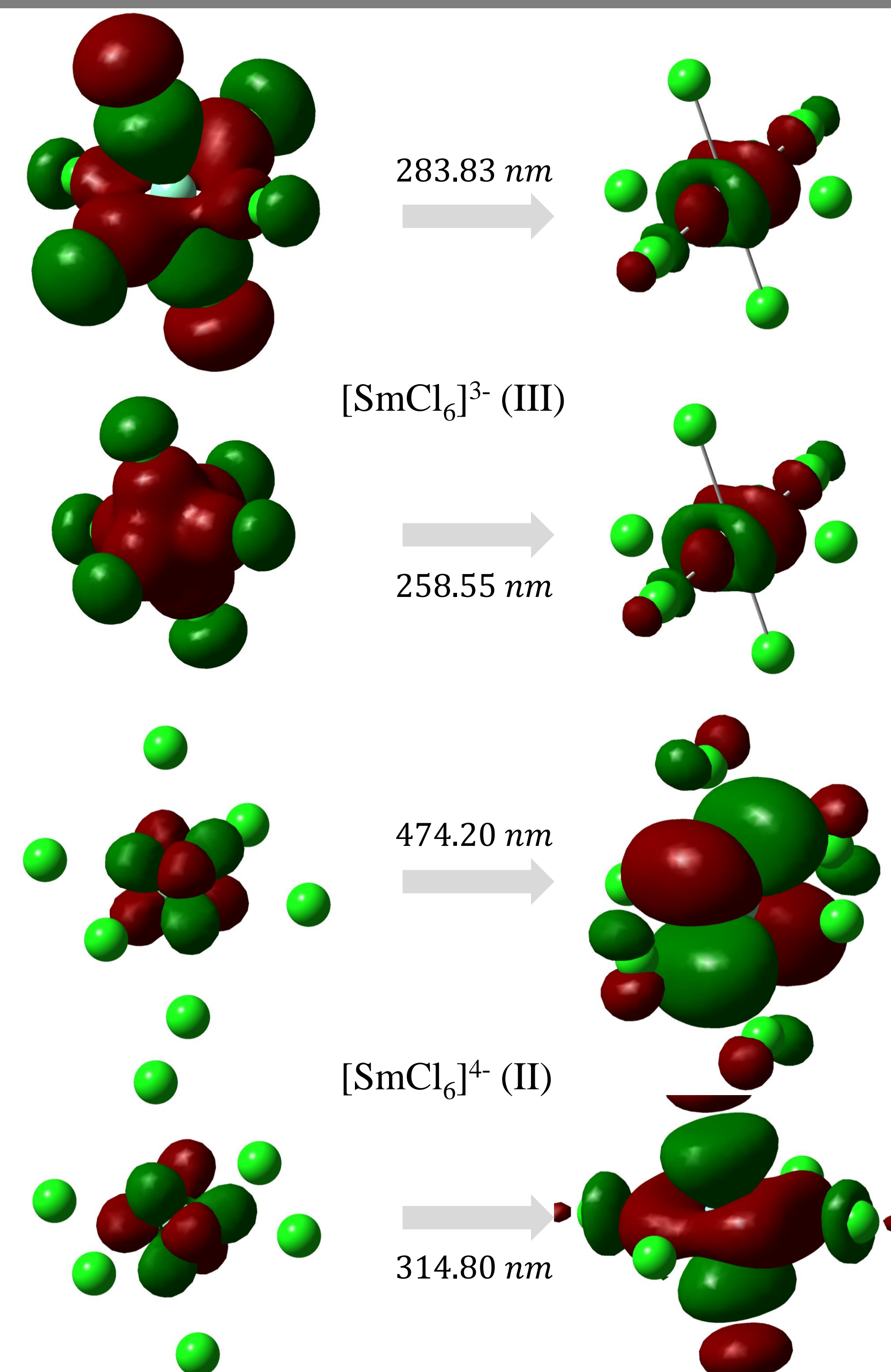
Sm-Cl bond length (Å)	
[SmCl <sub>6</sub> ] <sup>4-</sup> (II)	3.026
[SmCl <sub>6</sub> ] <sup>3-</sup> (III)	2.761

Electronic configuration:  
Sm(II): [Xe]4f<sup>6</sup>, Sm(III): [Xe]4f<sup>5</sup>  
Spin multiplicity 2S+1  
[SmCl<sub>6</sub>]<sup>3-</sup> (III): Sextet [SmCl<sub>6</sub>]<sup>4-</sup> (II): Septet



Wavelength (nm)	235 nm	380 nm	530 nm
Sm(III)	778	-	-
Sm(II)	-	1465	810

## Results (Sm-Cl NTO)



## Acknowledgment

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