

Chimie théorique des actinides

Pierre Vitorge^{1,2}

¹CEA Saclay DPC

²LAMBE (= UMR 8587)

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Chimie des actinides

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M.Duvail,³ B.Siboulet,³ C.Marsden,⁴

A.Cadi-Essadek,¹ A.Quemet,¹ T.Ha Duong,² M.Masella,⁵ D.Borgis,⁶ J.-F.Dufrêche,³

R.Spezia,² R.Vuilleumier,⁶ F.Martelli,² S.Abadie,^{2,6} P.D'Angelo,⁷ A.Zitolo, V.Migliorati,⁷ G.Chillemi,⁸

³ICSMarcoule UMR 5257, ⁴LPQ Toulouse UMR 5626, ⁵CEA DSV IBITEC-S, ⁶ENS UMR Pasteur

⁷Université de Rome "La Sapienza", ⁸CASPUR (Rome)

Publications 2011 dans le cadre de PARIS

Covalence dans des composés d'éléments f

Modélisations d'un actinide extrait en phase organique

Inorg. Chem., 50 (10), (2011) 4572–4579. doi: 10.1021/ic200260r

Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution

Paola D'Angelo,^{*,†} Andrea Zitolo,[†] Valentina Migliorati,[†] Giovanni Chillemi,[‡] Magali Duvail,[§] Pierre Vitorge,^{§,||} Sacha Abadie,^{†,§} and Riccardo Spezia[§]

[†]Department of Chemistry, University of Rome "La Sapienza", P. le A. Moro 5, 00185 Roma, Italy

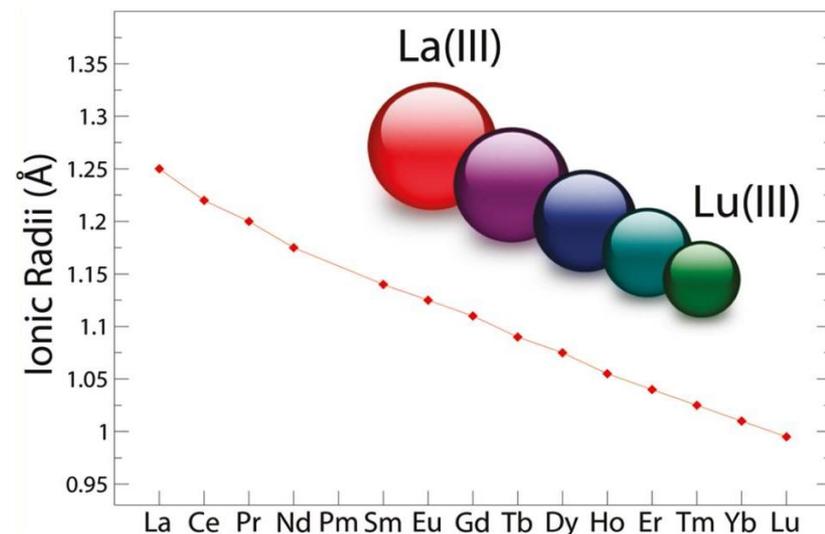
[‡]CASPUR, Inter-University Consortium for Supercomputing in Research, via dei Tizii 6b, 00185 Roma, Italy

[§]Laboratoire Analyse et Modelisation pour la Biologie et l'Environnement, UMR 8587 CNRS-CEA-UEVE, Université d'Evry Val d'Essonne, Bd F. Mitterrand, 91025 Evry Cedex, France

^{||}Laboratoire de Speciation des Radionucléides et des Molecules, CEA, DEN, F-91191 Gif-sur-Yvette, France

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AIP | The Journal of Chemical Physics

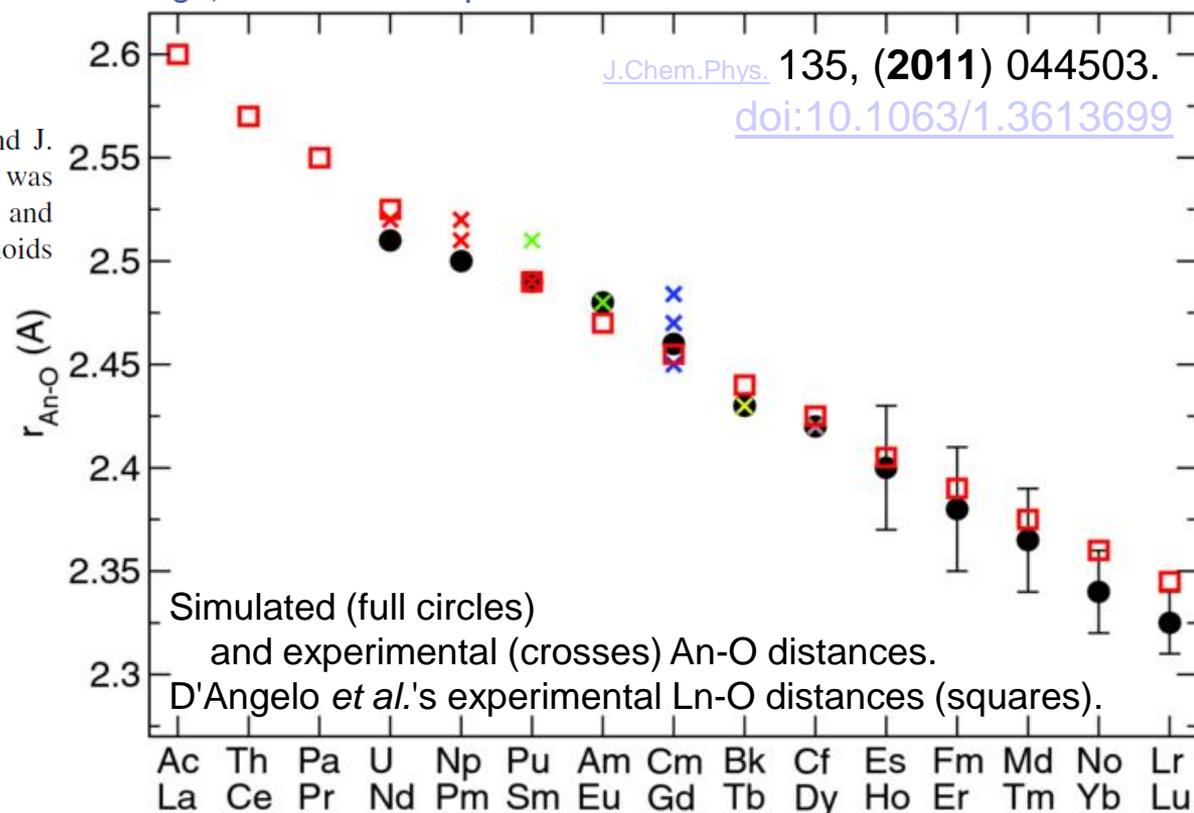
Polarizable interaction potential for molecular dynamics simulations of actinoids(III) in liquid water

UMR8587 : Magali Duvail, Fausto Martelli, Pierre Vitorge, and Riccardo Spezia



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J. Phys. Chem. B (2011) 115 (13), pp 3560–3570. [doi:10.1021/jp111726b](https://doi.org/10.1021/jp111726b)



énergie atomique • énergies altern

UMR8587 :



Stability and Instability of the Isoelectronic UO_2^{2+} and PaO_2^+ Actinyl Oxo-Cations in Aqueous Solution from Density Functional Theory Based Molecular Dynamics

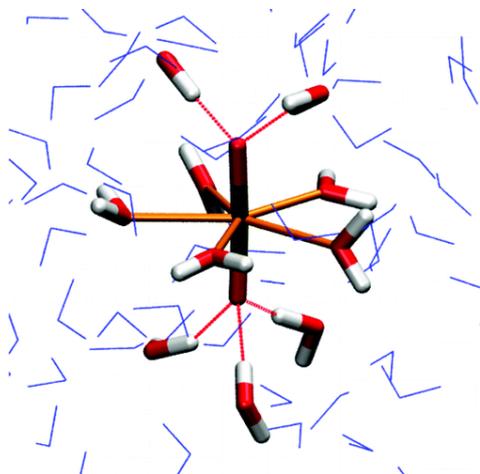
Riccardo Spezia,^{*,†} Bertrand Siboulet,[‡] Sacha Abadie,^{†,§} Rodolphe Vuilleumier,[§] and Pierre Vitorge^{*,†,⊥}

[†]Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement, UMR 8587, CNRS, CEA, UEVE, Université d'Evry Val d'Essonne, Boulevard F. Mitterrand, F-91025 Evry Cedex, France

[‡]CEA, DEN, DRCP, F-30207 Bagnols-sur-Cèze, France

[§]Ecole Normale Supérieure, Département de Chimie, 24, rue Lhomond, 75005 Paris, France, and UPMC Univ Paris 06, 4, Place Jussieu, 75005 Paris, UMR 8640 CNRS-ENS-UPMC, France

[⊥]CEA, DEN, Laboratoire de Spéciation des Radionucléides et des Molécules, F-91991 Gif-sur-Yvette, France



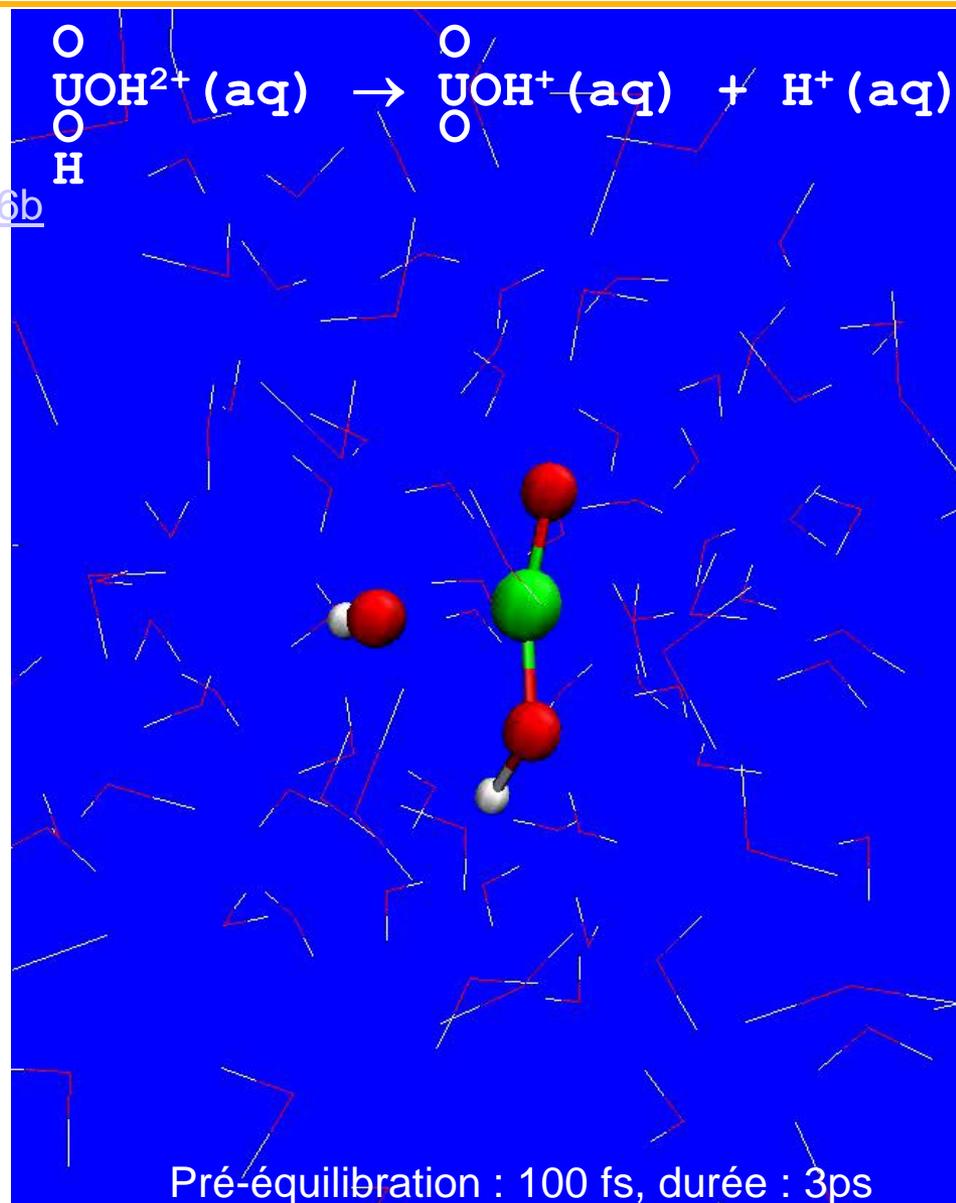
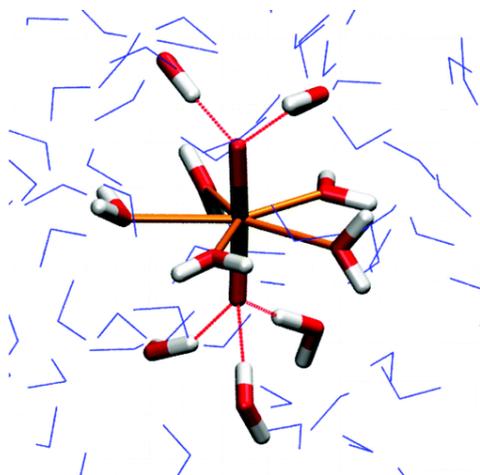
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J. Phys. Chem. B (2011) 115 (13),
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Riccardo Spezia,^{*,†} Bertrand Siboulet,
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and Pierre Vitorge



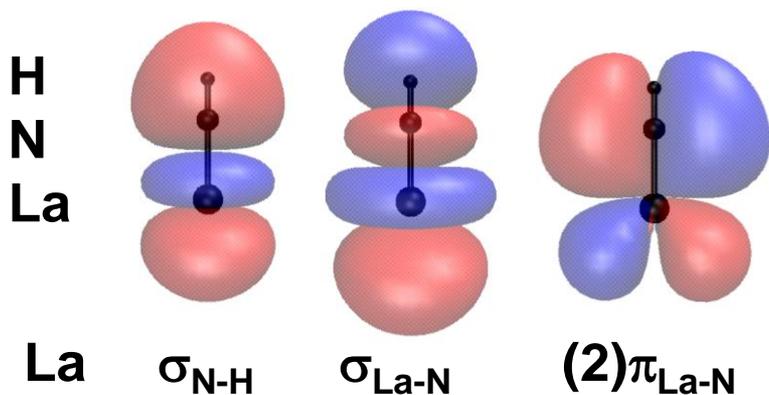
Covalence dans des composés d'éléments f

Explication et prévision de la réactivité chimique en phase gazeuse, utilisée en spectrométrie de masse pour le dosage de combustible nucléaire irradié.



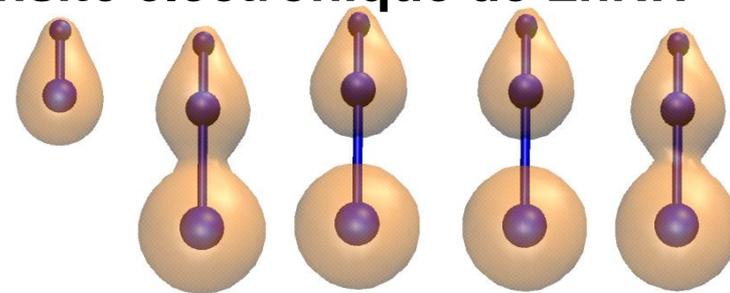
Alexandre Quemet, thèse en cours

La \equiv N-H⁺



La	6s 5p _z	6s 5p _z 5d _{z²}	5d _{(x ou y)z}
N	2s 2p _z	2s 2p _z	2p _{x ou y}
H	1s	1s	

Densité électronique de LnNH⁺

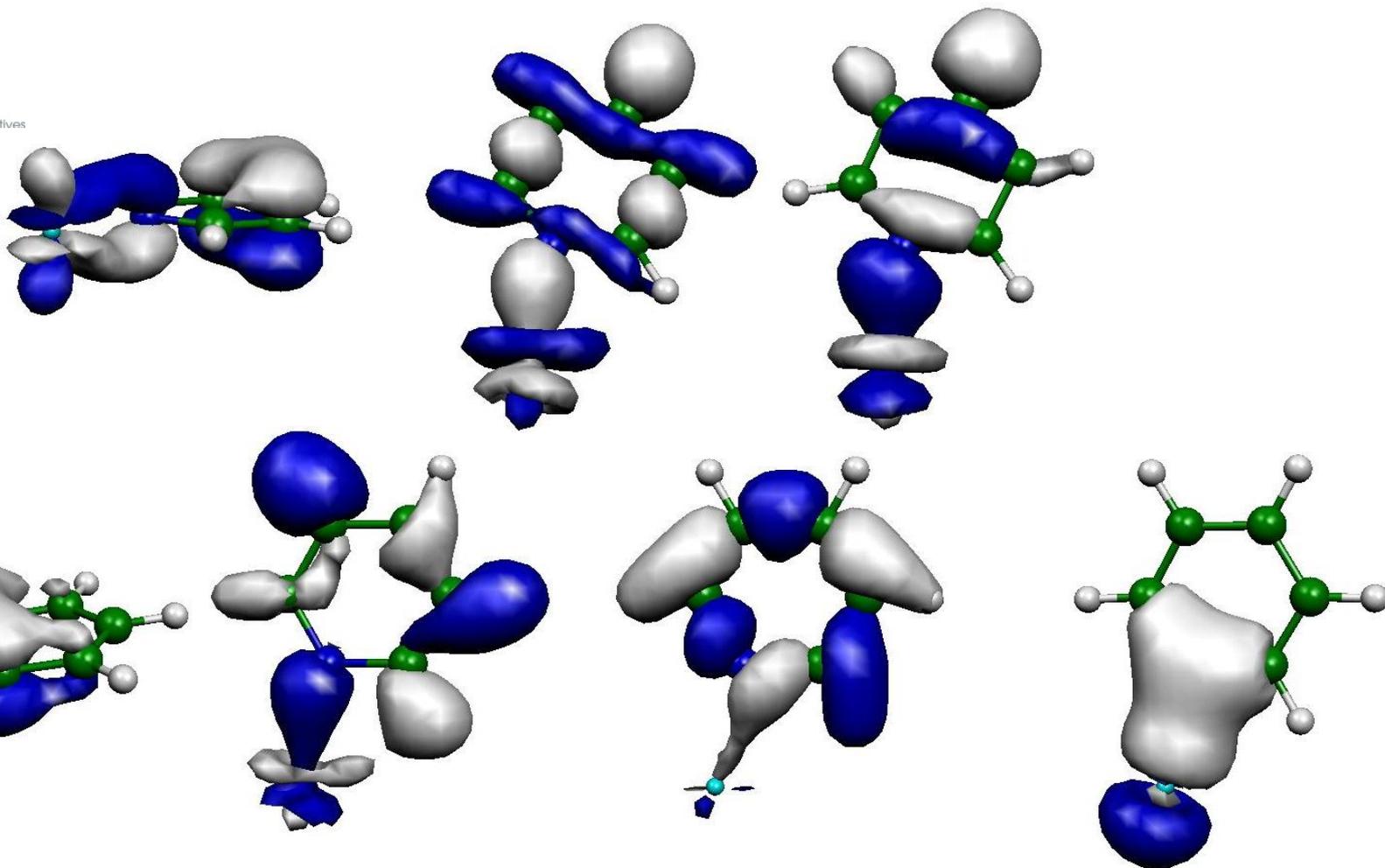


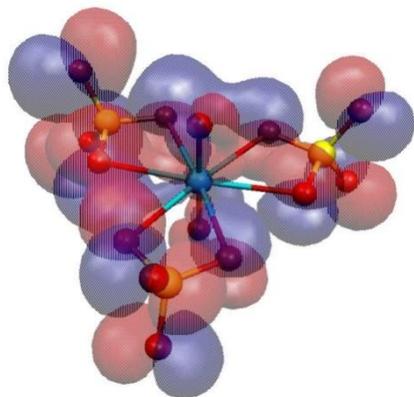
Ln La Sm Eu Gd

Covalence dans des composés d'éléments f

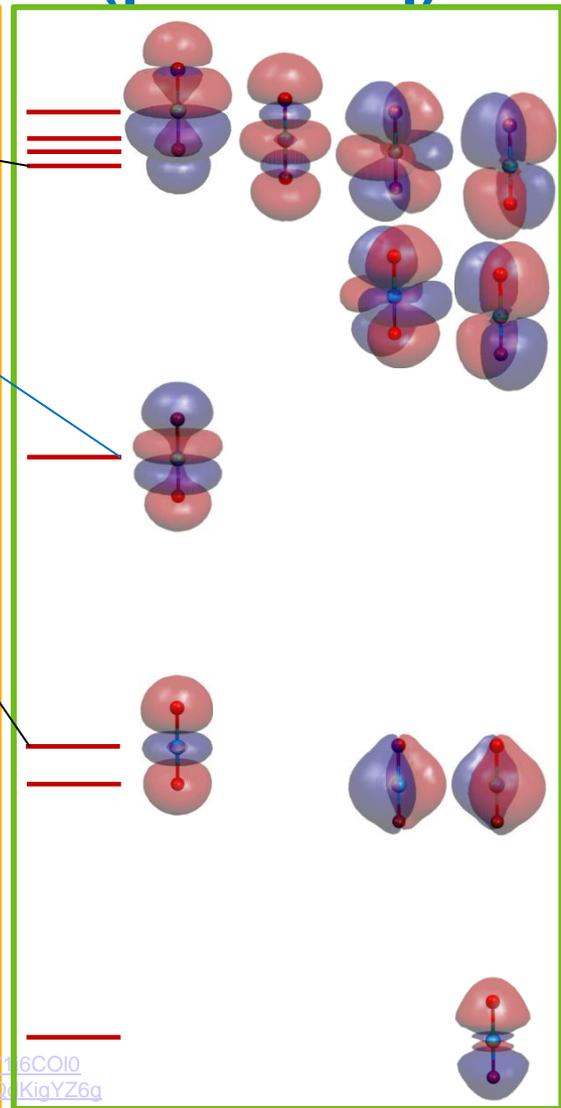
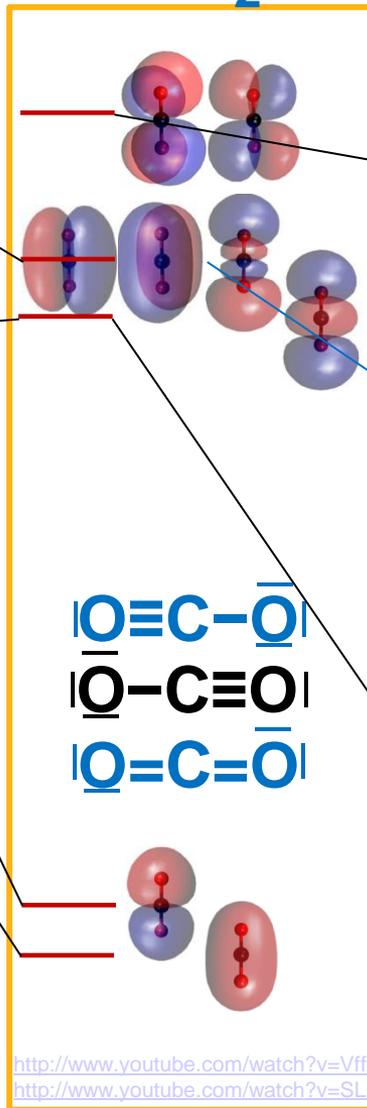
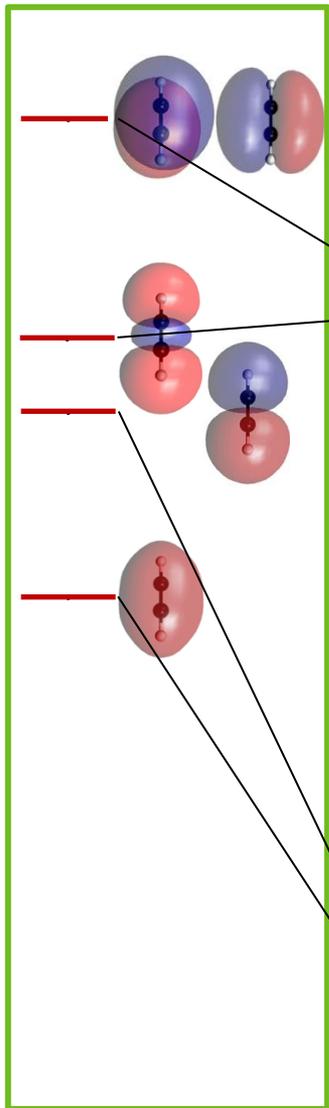
Liaison entre cation f et N (ou O) de ligands

(séparation des $\alpha...$).



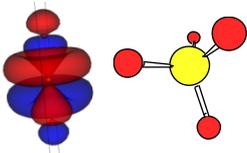


Abdelaziz
Cadi-Essadek,
stage ENSCBP



<http://www.youtube.com/watch?v=Vff716COI0>
<http://www.youtube.com/watch?v=SL0KiqYZ6g>

T.Ha Duong,
M.Masella,
D.Borgis,
J.-F.Dufrêche...



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