

CURRICULUM VITAE

- Name** Dr. Al Mokhtar Lamsabhi
- Birth date** August 05, 1971 (Marrakesh, Morocco)
- Researcher ID** **A-5659-2010**
- Professional Address** Química, C-IX, Ciencias. Universidad Autónoma de Madrid
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- Qualifications**
- PhD Thesis, in Theoretical Chemistry (University Cadi Ayyad Marrakech) **(01-07-2001)**
(Tutors: Profs. Widad Bouab and M'hamed Esseffar)
- Post-doctoral, Universidad Autónoma de Madrid **(10/2002 to 07/2004)**
(Advisor: Prof. Otilia Mó)
- Post-doctoral, Universidad Andrés bello, Santiago de Chile, Chile **(09/2004 to 07/2005)**
(Advisor: Dr. Patricia Pérez)
- Post-doctoral Contract (Juan de la Cierva) Universidad Autónoma de Madrid **(07/2005 to 05/2008)**
(Advisor: Prof. Manuel Yáñez)
- Visiting Post-Doc, Department of Chemistry, Dalhousie University, Halifax, NS Canada **(09/2007 to 01/2008)**
(Advisor: Prof. Russell J. Boyd)
- Present Position:** Permanent Lecturer at the Department of Chemistry at Universidad Autonoma de Madrid since **2008**
- Scientific research stays**
- Compagnie Minière de Guemassa (marrakech) (2 months 1994)
Instituto Rocasolano CSIC, Madrid (2 months 1998)
Universidad Autónoma de Madrid (3 months 1998, 1999, 2000)
Université Evry val d'Essones, Paris (2 weeks, 2003, 2004)
Universidad de Chile, Santiago, Chile (2 weeks, 2005, 2006 and 2007)
- Present Research** Gas-phase and in solution reactivity of some biological and pharmaceutical compounds.
- Keywords** Theoretical modelling, *Ab-initio* methods, Density functional theory, Acidity, Basicity, Charge Transfer complex, Donor, Acceptor, Excited states, Transition metals.
- Foreign languages** Arabic, French, Spanish, English
- Awards and Grants**
- Best Phd thesis in region Houz-Tensift (Marrakech) **2001**
Grant from the Ministry of Science of Spain for Foreign Scientist: **2002-2004**
Grant of Millennium from the Chilean government **2004-2005**
Grant Juan de la Cierva **2005-2008**
Grant José Castillejo for mobility to Young Scientist **2007**

<i>Publications</i>

- 39- **A. M. Lamsabhi**, S. Guttierrez-Oliva, A. Toro-Labbe, O. Mó, M. Yáñez
“*Uracil tautomerism, New View*”
Chem. Eur. J., (2011)
- 38- **A. M. Lamsabhi**, I. Corral, P. Pérez, O. Tapia and M. Yáñez
“*Oxygenation of the Phenylhalocarbenes. Are spin allowed or spin forbidden reactions?*”
Journal of Molecular Modeling, (2011) (In press)
- 37- M. Hurtado, **A. M. Lamsabhi**, O. Mó, M. Yáñez and J-C. Guillemin
“*Stability trends and tautomerization of chalcocyclopentadienes. The role of aromaticity?*”
New Journal of Chemistry, (2011) In Press
- 36- **A. M. Lamsabhi**, M. Yáñez, O. Mó, C. Trujillo, F. Blanco^b, I. Alkorta, J. Elguero, S. Rodriguez, C. Claessens and T. Torres.
“*TDDFT study of the UV-vis spectra of subporphyrins and subphthalocyanines*”
Journal of Porphyrins and Phthalocyanines, (2011) In Press
- 35- I. Corral, A. M. Lamsabhi, Otilia Mó and Manuel Yáñez
“*Infrared spectra of charge-solvated vs. salt-bridge conformations of glycine-, serine- and cysteine-Ca²⁺ complexes*”
International Journal of Quantum Chemistry, (2011) DOI: 10.1002/qua.23169, (In press)
- 34- C. Trujillo, **A. M. Lamsabhi**, O. Mó, M. Yáñez and J. Y. Salpin
“*Unimolecular Reactivity of Uracil–Ca²⁺ Complexes in the Gas Phase*”
International Journal of Mass Spectrometry, 306(1), 27-36, **2011**
- 33- A. Eizaguirre, **A. M. Lamsabhi**, O. Mó, M. Yáñez
“*double transfer in the uracil dimmer complex with Calcium*”
Theoretical Chemistry Accounts, 128:457-464, **2011**
- 32- M. M. Montero-Campillo, N. Mora-Diez and **A. M. Lamsabhi**,
“*The Thermodynamic Stability of Neutral and anionic PFOS: A Gas Phase, n-Octanol and Water Theoretical Study?*”
Journal of Physical Chemistry A, 114 (37), pp 10148-10155, **2010**
- 31- M. Hurtado, **A. M. Lamsabhi**, O. Mó, M. Yáñez and J-C. Guillemin
“*Are cyclopentadienberyllium, magnesium and calcium hydrides carbonic or metal acids in the gas phase?*”
Dalton Transactions, 39, 4593 – 4601, **2010**
- 30- **A. M. Lamsabhi**, O. Mó, M. Yáñez,
“*Serine-Ca²⁺ vs. Serine-Cu²⁺ complexes: A theoretical perspective*”
Canadian Journal of Chemistry, 88, 759-768, **2010**
- 29- S. Zaki and **A. M. Lamsabhi**

“A Theoretical Density Functional Study of Association of Zn^{2+} with Oxazolidine and its Thio Derivatives in Gas Phase”

Journal of Physical Organic Chemistry, 23, 751-758, **2010**

28- A. Guermoune, **A. M. Lamsabhi**, D. Cherqaoui, A. Jarid, H. Anane, G. Merino
“The tri- μ -hydrido-bis[(_5-C5Me5)aluminum(III)] Theoretical Study, The Assets of Sandwiched M_2H_3 (M of 13th group elements) stability.”

Journal of Molecular Modeling, 16(3), 551-557, **2010**

27- H. Zettergren, Y. Wang, **A. M. Lamsabhi**, M. Alcamí, F. Martín

“Density functional Theory study of multiply ionized van der Waals fullerenes dimers”

Journal of Chemical Physics, 130, 224302, **2009**

26- AUTORES (p.o. de firma): **A. M. Lamsabhi**, J-Y, Salpin, J. Tortajada, M. Yáñez

TITULO: “Gas-phase Chemistry of Organo-Copper Compounds”

The Chemistry of Organocopper Compounds, **2009**

Editors: Z. Rappoport and I. Marek, John Wiley & Sons,

25- J. Y. Salpin, S. Guillaumont, J. Tortajada, **A. M. Lamsabhi**

“Experimental and computational study of the gas-phase interactions between Lead(II) ions and thiouracil nucleobases”

Journal of the American Society for Mass spectrometry, 20, 359-369, **2009**

24- **A. M. Lamsabhi**, P. Pérez, S. Gutiérrez-Oliva, A. Toro-Labbé, O. Mó, M. Yáñez

“The Mechanism of Double Proton Transfer in Dimers of Uracil and 2-Thiouracil: The Reaction Force Perspective?”

Journal of Computational Chemistry, 30, 589-598, **2009**

23- **A. M. Lamsabhi**, O. Mó, M. Yáñez, J.-Y. Salpin, V. Haldys, J. Tortajada, J.-C. Guillemin

“ Ni^+ reactions with aminoacrylonitrile, a species of astrochemical relevance”

Journal of Physical Chemistry A, 112, 10509-10515, **2008**

22- C. Trujillo, **A. M. Lamsabhi**, O. Mó, M. Yáñez and J. Y. Salpin

“Interaction of Ca^{2+} with Uracil and its Thio Derivatives in the Gas Phase”

Organic & Biomolecular Chemistry, 6, 3695-3702, **2008**

21- **A. M. Lamsabhi**, O. Mó, M. Yáñez and R. J Boyd

“Gas-Phase Interaction of Calcium (Ca^{2+}) with Seleno Derivatives of Uracil”

Journal of Chemical Theory and Computation, 4, 1002-1011, **2008**

20- C. Trujillo, **A. M. Lamsabhi**, O. Mó, M. Yáñez

“The importance of the oxidative character of doubly charged metal cations in binding neutral bases. $[Urea-M]^{2+}$ and $[thiourea-M]^{2+}$ ($M = Mg, Ca, Cu$)”

Physical Chemistry Chemical Physics, 10, 3229-3235, **2008**

19- A. Medina, C. G. Claessens, G. M. A. Rahman, **A. M. Lamsabhi**, O. Mó, M. Yáñez, D. M. Guldi and T. Torres,

“Accelerating charge transfer in a triphenylamine-subphthalocyanine donor-acceptor system”

Chemical Communications, 1759-1761 **2008**

(*Synfacts* 2008, 6, 0584-0584)

18- **A. M. Lamsabhi**,

“*Specific hydration effects on Oxo-Thio triazepine derivatives*”

Journal of Physical Chemistry A, 112, 1791-1797, **2008**

17- **A. M. Lamsabhi**, O. M6, M. Y6ñez, V. Haldys, J.-Y. Salpin J. Tortajada, J.-C. Guillemin

“*Ni+ reactions with aminoacetonitrile, a potential pre-biological precursor of glycine*”

Journal of Mass Spectrometry, 43, 317-326, **2008**

16- S. Zaki, **A. M. Lamsabhi**,

“*Gas-Phase Reactivity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives towards Cu⁺ Cation: A DFT Study*”

Journal of Physical Chemistry A, 111, 2213-2219, **2007**

15- **A. M. Lamsabhi**, M. Alcam6, O. M6, J.-Y. Salpin, J. Tortajada, M. Y6ñez.

“*Unimolecular Reactivity of Uracil-Cu²⁺ Complexes in the Gas Phase*”,

ChemPhysChem, 8, 181-187, **2007**.

14- C. Trujillo, **A. M. Lamsabhi**, O. M6, M. Y6ñez

“*The reactions of F⁺(³P) and F⁺(¹D) with silicon oxide. Possibility of spin-forbidden process*”

Journal of Physical Chemistry A, 110, 7130-7135, **2006**.

13- **A. M. Lamsabhi**, M. Alcam6, O. M6, M. Y6ñez, J. Tortajada

“*Gas-phase deprotonation of Uracil-Cu²⁺ and Thiouracil-Cu²⁺ Complexes.*”

Journal of Physical Chemistry A, 106, 1943-1950, **2006**

12- C. C6rdenas, **A. M. Lamsabhi**, P. Fuentealba.

“*Nuclear Reactivity Index in the Context of Spin Polarized Density Functional Theory*”

Chemical Physics, 322, 303-310, **2006**

11- **A. M. Lamsabhi**, C. A. Escobar, P. P6rez

“*Do substituents make any contribution to the formation of systems where the electronic effects seem to be neutralized? The case of the indigo dye formation*”

Journal of Physical Organic Chemistry, 18, 1161-1168, **2005**

10- S. Guillaumont, J. Tortajada, J.-Y. Salpin, **A. M. Lamsabhi**

“*Experimental and computational study of the gas-phase interactions between lead(II) ions and two pyrimidic nucleobases: Uracil and thymine*”

International Journal of Mass Spectrometry, 243, 279-293, **2005**

9- **A. M. Lamsabhi**, M. Alcam6, O. M6, M. Y6ñez and J. Tortajada

“*Association of Cu²⁺ with uracil and its thio derivatives: A theoretical study*”

ChemPhysChem, 5, 1871-1877, **2005**.

8- A. El Guerraze, H. Anane, C. Serrar, A. Es-sofi, **A. M. Lamsabhi**, A. Jarid

“*Is the Lewis-acid behavior of GaH₃ comparable to that of BH₃ and AlH₃? a DFT comparison study of H₃AXH₃ (A=B, Al, Ga and X=N, P, As) donor-acceptor complexes*”

Journal of Molecular Structure (Theochem), 709, 117-122, **2004**

- 7- A. El Firdoussi, M. Esseffar, W. Bouab, **A.M. Lamsabhi**, J. L. M. Abboud, O. M6, M. Yáñez
“*Basicity of Lactones and Cyclic ketones toward I2 and ICl. An experimental and theoretical study*”
New Journal of Chemistry 27: 1741-1747, **2003**
- 6- **A. M. Lamsabhi**, M. Alcamí, O. M6, M. Yáñez
“*Gas- phase Reactivity of Uracil, 2-thiouracil, 4-thiouracil and 2,4-dithiouracil towards Cu+. Density Functional Theory Study*”.
ChemPhysChem, 4 (9): 1011-1016, **2003**
- 5- **A. M. Lamsabhi**, M. Esseffar, W. Bouab, T. El Messaoudi, M. El Messaoudi, J. L. -M. Abboud, M. Alcamí, M. Yáñez
“*The Gas-Phase Basicity of 2,7-dimethyl-[1,2,4] Triazepine Thio Derivatives*”
Journal of Physical Chemistry A 106 (32): 7383-7389 **2002**
- 4- **A. M. Lamsabhi**, M. Esseffar, T. El Messaoudi, M. Alcamí, M. Yáñez
“*Prototropic tautomerism of thioxo(oxo)- oxo(thioxo)-5 2,7-dimethyle-1,2,4-triazepine*”
New Journal of Chemistry 26 (6): 711-719, **2002**
- 3- **A. M. Lamsabhi**, W. Bouab, M. Esseffar, M. Alcamí, M. Yáñez, J. L.M. Abboud
“*Basicity of some carbonyl compounds towards iodine monochloride: experimental and theoretical study*”
New Journal of Chemistry, 25, 509-517, **2001**
- 2- **A. M. Lamsabhi**, M. Alcamí, O. M6, W. Bouab, M. Esseffar, J. L. M. Abboud, M. Yáñez
“*Are Thiouracils sulfur Bases in the gas-phase ?*”
Journal of Physical Chemistry A, 104, 5122-5130, **2000**
- 1- M. Esseffar, W. Bouab, **A. M. Lamsabhi**, J.L.M. Abboud, R. Notario, M. Yáñez
“*An Experimental and Theoretical study on some thiocarbonyl-I2 molecular complexes*”
Journal of American Chemical Society, 122, 2300-2308, **2000**

<i>Conferences and Seminars</i>

- 26- **A. M. Lamsabhi**, O. M6 and M. Y6ñez “*Serine-Ca²⁺ vs. Serine-Cu²⁺ complexes. A theoretical perspective.*”
36^{me} Congr6s des chimistes th6oriciens d'expression latine, 19-24 September, **2010**, Anglet, France
- 25- M. Monte, **A.M. Lamsabhi**, O. M6, M. Y6ñez and J.-Y. Salpin “*An Experimental and Theoretical Study of Gas Phase reactions of Ca²⁺ with Cysteine*”
7th Congress on Electronic Structure: Principles and Applications (ESPA 2010), 29 June-4 July, **2010**, Oviedo, Spain
- 24- **A. M. Lamsabhi**, P. P6rez, O. Tapia and M. Y6ñez “*Oxygenation of the Phenylhalocarbenes. Are spin allowed or spin forbidden reactions?*”
13th Edition of the International Conference on the Applications of Density Functional Theory in Chemistry and Physics, 1-4 September, **2009**, Lyon, France
- 23- **A. M. Lamsabhi**, P. P6rez, S. Guti6rrez-Oliva, A. Toro-Labb6, O. M6, M. Y6ñez, “*The Mechanism of Double Proton Transfer in Dimers of Uracil and 2-Thiouracil: The Reaction Force Perspective?*”
The Seventh Computational Chemistry Canadian Conference (CCCC)
20-26 July, **2009**, Halifax, NS, Canada
- 22- AUTORES: **A. M. Lamsabhi**, O. M6, V. Haldys, J.-Y. Salpin, J.-C. Guillemin, J. Tortajada, M. Y6ñez “*Ni⁺ reactions with aminoacrylonitrile, a species of astrochemical relevance*”
Electronic Structure: Principles and Applications (ESPA08),
2-5 September, **2008**, Palma de Mallorca, Spain
- 21- C. Trujillo, **A. M. Lamsabhi**, O. M6, M. Y6ñez, “*The Importance of the oxidative character of doubly charged metal cations in binding neutral bases*”
Electronic Structure: Principles and Applications (ESPA08),
2-5 September, **2008**, Palma de Mallorca, Spain
- 20- **A. M. Lamsabhi**, O. M6, M. Y6ñez, R. J. Boyd, “*Gas-phase Interaction of Calcium (Ca²⁺) with Seleno Derivatives of Uracil*”
Isolated Biomolecules and Biomolecular Interactions (IBBI08), 13-18 April **2008**, Valladolid, Spain.
- 19- **A. M. Lamsabhi**, O. M6, P. P6rez, S. Gutierrez-Oliva, A. Toro-Labb6 and M. Y6ñez “*On the Mechanism of Double Hydrogen Transfer in Uracil Dimers and Derivatives*”
Isolated Biomolecules and Biomolecular Interactions (IBBI08), 13-18 April, **2008**, Valladolid, Spain.
- 18- J-Y Salpin, J. Tortajada, C. Trujillo, **A. M. Lamsabhi**, O. M6., M.Y6ñez “*Interactions between Ca²⁺ ions and uracil derivatives. A combined experimental and theoretical study*”
24^{emes} journ6es Fran6aises de Spectrom6trie de Mass, 17-20 septembre, **2007** Pau, Francia,

17- Z. Safi, **A. M. Lamsabhi** “*Reactividad en fase gas del Cu⁺ con los Tio derivados del 2,7-dimetilotriazepina*”

XXXI reunión Bienal de la real Sociedad Española de Química, 9-14 Septiembre **2007**
Toledo, Spain

16- **A. M. Lamsabhi**, O. Mó, M. Yáñez, V. Haldys, J.-Y. Salpin J. Tortajada, J.-C. Guillemin
“*Gas-phase aminoacetonitrile reactivity with Nickel*”

The 12th International Conference on the Applications of Density Functional Theory (DFT07), 26-30 agosto, **2007** Amsterdam, Holland

15- **A. M. Lamsabhi**, “*Water interaction with oxo-thione derivatives of 2,7-dimethyl-1,2,4-triazepines*”,

11th European Symposium on organic reactivity, ESOR2007, 1-6 Julio, **2007**, Faro, Portugal

14- **A. M. Lamsabhi**, M. Alcamí, O. Mó, J. Tortajada and M. Yáñez “*Reactivity of Uracil-Cu²⁺ Complex: Experimental and theoretical Study*”

Electronic Structure: Principles and Applications (ESPA 2006) 18-21 July, **2006** Santiago de Compostela, España.

13- **A. M. Lamsabhi**, O. Mó, V. Haldys, J-Y Salpin, J. Tortajada, J. Guillemin and M. Yáñez
“*Ni⁺ Reactions with aminoacetonitrile, A potential pre-biological precursor of Glycine*”

Electronic Structure: Principles and Applications (ESPA 2006) 18-21 July **2006** Santiago de Compostela, Spain

12- **A. M. Lamsabhi**, M. Alcamí, O. Mó, J. Tortajada and M. Yáñez “*Experimental and DFT-Study of the Gas-Phase Deprotonation and Reactivity of Uracil-Cu²⁺ Complex and its Thio derivatives*”

The XIIth International Congress of Quantum Chemistry (ICQC), 21-26 May **2006**, Kyoto, Japan.

11- **A. M. Lamsabhi**, C. A. Escobar, P. Pérez “*Substituent Effects on the Mechanism of Indigo Dyes Formation: Time Dependent Density Functional Theory Study*”

The 11th International Conference on the Applications of Density Functional Theory (DFT) in Chemistry and Physics. 11-15 September **2005**, Geneva, Switzerland

10- **A. M. Lamsabhi**, M. Alcamí, O. Mó, M. Yáñez and J. Tortajada “*Cu²⁺ association to uracil and its thio-derivatives. A theoretical study*”

Electronic Structure Principles and Applications (ESPA2004), 15-17 September **2004**
Valladolid, Spain

9- A. El Guerraze, A. Jarid, H. Anane, C. Serrar, A. Es-sofi, **A. M. Lamsabhi** “*Etude théorique des complexes donneur-accepteur H3AXH3 (A=B, Al, Ga et X=N, P, As) comparaison du borane de l’alane et du gallane*”

29ème Congrès des chimistes théoriciens d'expression latine 07-12 September 2003
Marrakech, Morocco.

8- A. El Guerraze, A. Jarid, H. Anane, C. Serrar, A. Es-sofi, **A. M. Lamsabhi** “*Etude Comparative des modes de coordination des ligands BH₄⁻ et B₃H₈⁻, application aux complexes Ln Cu(BH₄) et LnCu(B₃H₈) n=1, 2, 3*”

29ème Congrès des chimistes théoriciens d'expression latine, 07-12 September **2003**
Marrakech, Morocco.

- 7- **A. M. Lamsabhi**, O. M6, J. Tortajada, M. Alcamí, M. Yáñez, “*Deprotonation de l’uracile et de ses dérivés thio sous l’effet de l’association avec le Cuivre (II)*”
29ème Congrès des chimistes théoriciens d’expression latine, 07-12 September **2003**
Marrakech, Morocco.
- 6- **A.M. Lamsabhi**, O. M6, M. Alcamí, M. Yáñez, “*Gas-Phase Reactivity of Uracil, 2-thiouracil, 4-thiouracil and 2,4-dithiouracil towards Cu+. Density Functional Theory Study*”
XIth International Congress of Quantum Chemistry “ICQC” 19-26 July **2003** Bonn, Germany.
- 5- **A.M. Lamsabhi**, M. Esseffar, W. Bouab, T. El Messaoudi, M. El Messaoudi, M. Alcamí, M. Yáñez, J. L. –M. Abboud “*Etude Comparative de la basicité des dérivés thio de l’uracile et de la 1,2,4-triazépine*”
27ème Congrès des Chimistes Théoriciens d’expression Latine 3-8 September CHITEL **2001**
Toulouse, France
- 4- **A. M. Lamsabhi**, M. Esseffar, W. Bouab, M. Alcamí, M. Yáñez, J. L. –M. Abboud, “*Basicité de quelques composés carbonylés vis-à-vis du Monochlorure d’iode: étude expérimentale et théorique*”
XXVI Congresso dos Químicos Teóricos de Expressão latina Qtel 2000, 3-9 september **2000**,
Caxambo, MG- Brasil
- 3- M. Esseffar, **A. M. Lamsabhi**, W. Bouab, R. Notario, J. L. M. Abboud, M. Yáñez “*Are thiouraciles sulfur Bases*”
International Symposium On Physical Organical Chemistry, In honor of Professor J. Elguero
8-10 July **1999**, Miraflores de la sierra Madrid, España
- 2- M. Esseffar, W. Bouab, **A. M. Lamsabhi**, R. Notario, J. L. M. Abboud, M. Yáñez
“*Complexation des composés thiocarbonylés avec l’iode moléculaire*”
XXV Congresso, Internazionale dei Chimici Teorici di Expressione Latina (CHITEL99) 13-
18 september **1999**, Napoles, Italy
- 1- **A. M. Lamsabhi**, W. Bouab, M. Esseffar, R. Notario, J. L. –M. Abboud “*Spectroscopic and theoretical study on the basicity of uracil thio derivatives in association with proton and iodine*”
XVI Reunión Nacional de Espectroscopia, 20-25 September **1998**, Sevilla, Spain.