

Curriculum Vitae Manuel Yáñez

Last Name: Yáñez

First Name: Manuel

SEX: Male

Born: in Lugo (Spain)

Address: Departamento de Química, C-9
Universidad Autónoma de Madrid
Cantoblanco, 28049-Madrid. Spain

Secondary Education: Instituto de Bachillerato de Lugo (1958-1965)

Tertiary Education: Universidad de Santiago de Compostela (1965-1970)

Degrees Held:

B.Sc. in Chemistry (1st class honours) 1970 (Universidad de Santiago de Compostela)

M.Sc. In Chemistry 1970 (Universidad de Santiago de Compostela)

Ph.D. , 1973 (Universidad Autónoma de Madrid)

Awards

1. Premio Extraordinario de Licenciatura en Ciencias Químicas.
Universidad de Santiago de Compostela.
Julio de 1970.
2. Premio Nacional Fin de Carrera. Sección de Químicas.
Marzo de 1971.
3. Ingreso en la Orden Civil de Alfonso X el Sabio, con categoría de Cruz.
Julio de 1971.
4. Premio Extraordinario de Doctorado.
Universidad Autónoma de Madrid.
Enero de 1974.
5. Research Prize of Fundación de la U. A. M.
Mayo de 1993.
6. Research Prize in Physical Chemistry of the Spanish Royal Society of Chemistry
November 2002
7. Bettancourt-Perronet Research Prize of the French Ministry of Foreign Affairs
March 2003

Professional Societies:

American Chemical Society since 1976.

European Physical Society since 1987.

Real Sociedad Española de Física since 1988.

Grupo Especializado de Física Atómica y Molecular since 1988

Committees and academic positions:

Faculty Board. Universidad Autónoma de Madrid. 1984-1988, 1993-1997

Secretary of the Grupo Especializado de Física Atómica y Molecular 1988-199

Head of the Department of Chemistry. Universidad Autónoma de Madrid. 1993-1997

Head of the Scientific Computational Center of the Universidad Autónoma de Madrid. 1998-2002

Member of the Committee for the Evaluation of the Portuguese Universities. 1998-2003

Member of the Management Committee of the COST Action D26 Integrative Computational Chemistry of the European Community.

Vice-chairman of the Management Committee of the European Division of Computational Chemistry (EUCCO-CC)

Member of the Board of the World Association of Theoretically Oriented Chemists (WATOC)

Member of the Editorial Board of Mass Spectrometry Reviews

Associate Editor of the Journal of Molecular Structure THEOCHEM

Conference organization:

Committee Member First Europhysics Summer School on Chemical Physics: Atomic and Molecular Physics. Santander (Spain), July, 1996.

Chairman of the Third Europhysics Summer School on Chemical Physics: Ion Chemistry. Santander (Spain), July 1988.

Committee Member. III Congress on Atomic and Molecular Physics, Toledo (Spain), 1991

Chairman of the Workshop on Computational Chemistry. Miraflores de la Sierra (Madrid, Spain). June 1998.

Chairman of the International Symposium on Physical Organic Chemistry in the Honour of Prof. José Elguero. Miraflores de la Sierra (Madrid, Spain). July 1998.

Graduate Research:

Physical Chemistry. Professor M.A. Ríos. Universidad de Santiago de Compostela (1969-70)

Physical Chemistry. Professor J.I. Fernández Alonso. Universidad de Valencia (1970-71) y Universidad Autónoma de Madrid (1971-73)

Postdoctoral Research

Theoretical Chemistry. Postdoctoral Research Associate with **Prof. J.A. Pople**, Department of Chemistry, Carnegie Mellon University, Pittsburgh (USA) (1974-76).

Previous Positions

1976-77	Prof. Adjunto Interino	Univ. Autónoma de Madrid
1978-80	Prof. Adjunto Numerario	Univ. Autónoma de Madrid
1980-83	Prof. Agregado Numerario	Univ. Autónoma de Madrid

Current Position:

Professor of Physical Chemistry. Department of Chemistry. Universidad Autónoma de Madrid

PUBLICATIONS

Approximately 320, See attached List:

1. M. Yáñez y J.I. Fernández Alonso.
Contribución al estudio teórico de la reactividad química por el método de Klopman.
Afinidad **38**, 1123 (1971).
2. M. Yáñez, A. Macías and J.I. Fernández-Alonso.
Study of the influence of the attacking-ion on the reactivity of conjugated systems.
Chem. Phys. Lett., **17**, 63 (1972).
3. M. Yáñez and J.I. Fernández Alonso.
Study of the influence of attacking-ions and dipoles on the reactivity of conjugated systems.
Chemical and Biochemical Reactivity, **VI**, 431 (1974).

4. O. Mó, M. Yáñez and J.I. Fernández Alonso.
Theoretical study of charge-transfer complexes.
J. Phys. Chem., **79**, 137 (1975).
5. M. Yáñez, O. Mó and J.I. Fernández Alonso.
A theoretical study of the electrophilic substitution on aminophenols and aminobenzenethiols.
Tetrahedron, **31**, 245 (1977).
6. J. Catalán, A. Macías, O. Mó and M. Yáñez.
Calculations on the inversion of anhydrous and hydrated aziridine.
Mol. Phys., **34**, 1429 (1977).
7. O. Mó and M. Yáñez.
Influence of polarization functions on molecular electrostatic potentials.
Theoret. Chim. Acta, **47**, 263 (1978).
8. J. Catalán, O. Mó and M. Yáñez.
Theoretical study of the structure of azetidione.
J. Mol. Struct. **43**, 251 (1978).
9. J. Catalán and M. Yáñez.
A theoretical study of proton addition to oxirane, aziridine and 2-azirene.
J. Am. Chem. Soc., **100**, 1398 (1978).
10. M. Yáñez, R.F. Stewart and J.A. Pople.
The projection of molecular charge density into spherical atoms. I. Density basis functions for first row atoms.
Acta Cryst. **A34**, 641 (1978).
11. M. Yáñez and R.F. Stewart.
The projection of molecular charge density into spherical atoms. II. An Application to X-Ray Diffraction Data.
Acta Cryst. **A34**, 648 (1978).
12. V. López, A. Macías, R.D. Piacentini, A. Riera and M. Yáñez.
Molecular treatment of elastic and double charge-exchange He^{2+} -He collisions.
Phys. B, Atom. Molec. Phys., **11**, 2889 (1978).
13. J. Catalán, M. Yáñez and J.I. Fernández Alonso.
A theoretical study of hydrogen bonding in malonaldehyde.
J. Am. Chem. Soc., **100**, 6917 (1978).
14. J. Catalán and M. Yáñez.
Correlation between ring-proton affinities and C_{1s} binding energies. Application to monosubstituted benzenes.
Chem. Phys. Lett., **60**, 499 (1979).
15. J. Catalán and M. Yáñez.
Protonation and Proton Affinities of monosubstituted benzenes. A theoretical study.
J. Chem. Soc. Perkin Trans. II, 741 (1979).
16. J. Catalán and M. Yáñez.
Protonation and proton affinity of anisole. A theoretical study.
J. Am. Chem. Soc., **101**, 3490 (1979).
17. J. Catalán and M. Yáñez.
Prediction of proton affinities and preferred protonation sites in benzene derivatives, from $1s$ orbital energies.
J. Chem. Soc. Perkin Trans. II, 1627 (1979)
18. O. Mó and M. Yáñez.
Structure and charge distribution of some alkynoyl cations. A theoretical study.
Theoret. Chim. Acta, **53**, 337, (1979).
19. J. Catalán, O. Mó, P. Pérez and M. Yáñez.

- Proton affinities and preferred protonation sites in 3- and 4- substituted pyridines. Prediction from 1s orbital energies.*
 J. Am. Chem. Soc. **101**, 6520 (1979).
20. M. Dorado, O. Mó and M. Yáñez.
A theoretical study of the structure and charge distribution of some alkynylcarbenium ions.
 J. Am. Chem. Soc., **102**, 947 (1980)
21. J. Catalán and M. Yáñez.
A theoretical study of the protonation of benzamide.
 Tetrahedron, **36**, 665 (1980).
22. J. Catalán, F. Escudero, J. Laso, O. Mó and M. Yáñez.
The effect of substituents on the structure of dioxirane.
 J. Mol. Struct., **69**, 217 (1980).
23. A. Macías, A. Riera and M. Yáñez.
Molecular treatment of the He⁺ + H collisions.
 Phys. Rev., **A23**, 2941 (1981).
24. F. Escudero and M. Yáñez.
Atoms in molecules. Density basis functions for second row atoms.
 Mol. Phys., **45**, 617 (1982).
25. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
Prediction of proton affinities and protonation sites using a multivariate linear correlation.
 J. Chem. Soc. Perkin Trans. II, 1409 (1982).
26. J. Catalán, P. Pérez and M. Yáñez.
A theoretical study of the protonation of methylindole derivatives.
 Tetrahedron, **38**, 3693 (1982).
27. A. Macías, A. Riera and M. Yáñez.
Molecular states of HeH⁺. Energies and dynamical couplings.
 Phys. Rev., **A27**, 206 (1983).
28. A. Macías, A. Riera and M. Yáñez.
Excitation and charge transfer in He⁺ - H collisions. A study of the origin dependence of calculated cross sections.
 Phys. Rev., **A27**, 213 (1983).
29. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
A theoretical study of the structure, charge distribution and gas-phase basicity of 1H-indazole and its N-methyl derivatives.
 J. Mol. Struct., **94**, 143 (1983).
30. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
A theoretical study of the structure, charge distribution and gas-phase basicity of azaindoles.
 Tetrahedron, **39**, 2851 (1983).
31. F. Escudero, O. Mó and M. Yáñez.
A theoretical study of the charge distribution of aminopyridines, aminopyrimidines and some diazine N-oxides.
 J. Chem. Soc. Perkin Trans. II, 1735 (1983).
32. J.L.G. de Paz and M. Yáñez.
Ring functions, as polarization functions, for ab initio calculations of small rings. Dioxirane.
 Theoret. Chim. Acta, **64**, 57 (1983).
33. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
Theoretical study on the stable conformers of 1,3-diazetidene.
 J. Mol. Struct. THEOCHEM, **106**, 251 (1984).

34. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
Conformation of four-membered rings. Comparison between azetidione and 1,3-diazetidione.
J. Mol. Struct. THEOCHEM, **107**, 269 (1984).
35. J. Catalán, O. Mó, P. Pérez and M. Yáñez.
Influence of the tautomeric forms of azaindoles on their basicity in solution.
J. Mol. Struct. THEOCHEM, **107**, 263 (1984).
36. J. Catalán, J.L.G. de Paz and M. Yáñez.
Very strong bases. A theoretical determination of their gas-phase proton- affinities.
J. Mol. Struct. THEOCHEM., **107**, 257 (1984).
37. J.L.G. de Paz and M. Yáñez.
On the use of bond functions, as polarization functions, in ab initio calculations.
J. Mol. Struct. THEOCHEM., **107**, 59 (1984).
38. A. Macías, R. Mendizábal, F. Pelayo, A. Riera and M. Yáñez.
A stabilization treatment of an infinitely excited quasimolecule. $LiHe^{3+}$.
J. Mol. Struct. THEOCHEM., **107**, 245 (1984).
39. J. Catalán and M. Yáñez.
Alfa vs. beta protonation of pyrrole and indole.
J. Am. Chem. Soc., **106**, 421 (1984).
40. J. Catalán, O. Mó, P. Pérez, M. Yáñez and F. Amat-Guerri.
Comparative study of the structure and properties of 1-methyl-7-azaindole and 7-methyl-7H-pyrrolo(2,3-b)pyridine, in their ground states.
Nouv. J. Chim., **8**, 87 (1984).
41. J. Catalán, J.L.G. de Paz, M. Yáñez and J. Elguero.
The problem of the relationship between proton affinity (intrinsic basicity) and the charge on the basic centre.
J. Mol. Struct. THEOCHEM., **108**, 161 (1984).
42. J. Catalán, O. Mó, J.L.G. de Paz, P. Pérez and M. Yáñez.
Protonation of azanaphthalenes, azaindoles and purine bases. The "lone-pair charge" approach.
Nucleic Acid Symposium Series, **14**, 105 (1984).
43. J. Catalán, O. Mó, J.L.G. de Paz, P. Pérez and M. Yáñez.
A theoretical study on the tautomer preference for 4(5)-substituted imidazoles.
Nucleic Acid Symposium Series, **14**, 161 (1984).
44. J. Catalán, J.L.G. de Paz, M. Yáñez and J. Elguero.
The Azoles. A theoretical study.
Chemica Scripta, **24**, 84 (1984).
45. J. Catalán, J.L.G. de Paz, M. Yáñez and J. Elguero.
The relationship between substituent-induced energy and charge effects in proton transfer equilibria involving heteroaromatic nitrogen systems. The "lone-pair charge" approach.
J. Am. Chem. Soc., **106**, 6552 (1984).
46. J. Catalán, O. Mó, J.L.G. de Paz, P. Pérez, M. Yáñez and J. Elguero.
Basicity of azoles. Part 6. Calculated intrinsic basicities for methyl-substituted pyrazoles and imidazoles. Comparison to aqueous solution data: N-methylation effect.
J. Org. Chem., **49**, 4379 (1984).
47. F. Escudero, O. Mó, J.L.G. de Paz and M. Yáñez.
Structure and charge distribution of 4-substituted benzenediazonium ions.
J. Mol. Struct. THEOCHEM., **120**, 377 (1985).
48. O. Mó, A. Riera and M. Yáñez.
Calculation of radial couplings in the model potential and pseudopotential approaches. The NaH

- quasimolecule.*
 Phys. Rev., **A31**, 3977 (1985).
49. L.F. Errea, L. Méndez, A. Riera, M. Yáñez, J. Hanssen, C. Harel and A. Salin.
The LiH^{2+} quasimolecule. A comparison between the configuration interaction and the OEDM approaches.
 J. Physique, **46**, 709 (1985).
50. L.F. Errea, L. Méndez, A. Riera, M. Yáñez, J. Hanssen, C. Harel and A. Salin.
Charge exchange in $Li^{2+} (1s) + H (1s)$ collisions. A molecular approach including two-electron translation factors.
 J. Physique, **46**, 719 (1985).
51. F. Martín, A. Riera and M. Yáñez.
Calcul de sections de choc entre particules lourdes avec des fonctions d'onde moléculaires obtenues par la méthode de Feshbach.
 "11^{ème} Colloque Col. At. et Elect. Vol. 2 (Conferences)", pag. 68.
 Ed. U.E.R. Sciences Exactes et Naturelles (Metz) (1986).
52. A. Macías, R. Mendizábal, F. Pelayo, A. Riera and M. Yáñez.
Application of the stabilization method to the molecular states of $LiHe^{3+}$. Energies and radial couplings.
 Phys. Rev., **A33**, 242 (1986).
53. F. Martín, A. Riera and M. Yáñez.
Molecular (Feshbach) treatment of charge exchange $Li^{3+} + He$ collisions. I. Energies and couplings.
 J. Chem. Phys., **84**, 5412 (1986).
54. L.F. Errea, F. Martín, L. Méndez, A. Riera and M. Yáñez.
Molecular (Feshbach) treatment of charge exchange $Li^{3+} + He$ collisions. II. Cross sections.
 J. Chem. Phys., **84**, 5422 (1986).
55. J.L.G. de Paz and M. Yáñez.
Polarization effects in small rings containing sulfur. A theoretical study of the structure of thiete.
 J. Mol. Struct. THEOCHEM, **138**, 311 (1986).
56. A. del Pozo, A. Riera and M. Yáñez.
Galilean invariance in the exponential model of atomic collisions.
 Phys. Rev. **A34**, 3723 (1986).
57. O. Mó, J.L.G. de Paz, and M. Yáñez.
Protonation energies and tautomerism of azoles. Basis set effects.
 J. Phys. Chem. **90**, 5597 (1986).
58. F. Martín, A. Riera and M. Yáñez.
Single and double charge exchange transfer in $Be^{4+} + He$ collisions. A molecular (Feshbach) approach.
 Phys. Rev. A **34**, 4675 (1986)
59. O. Mó, J.L.G. de Paz, and M. Yáñez.
Protonation of azines. An ab initio molecular orbital study.
 J. Mol. Struct. THEOCHEM., **150**, 135 (1987).
60. F. Borondo, F. Martín and M. Yáñez.
Molecular treatment of the ion-pair formation reaction in $H(1s) + H(1s)$ collisions.
 Phys. Rev. A, **35**, 60 (1987).
61. R. Mendizábal, O. Mó, A. Riera and M. Yáñez.
Energies and radial couplings for the $^1\Sigma$ and $^3\Sigma$ states of $NaHe^+$ quasimolecule.
 J. Mol. Struct. THEOCHEM., **150**, 345 (1987).
62. O. Mó, M. Yáñez and J. Elguero.
Binding of NH_4^+ to azoles in the gas phase. A theoretical study of the $N...H^+ \dots N$ Ionic hydrogen bond.
 J. Org. Chem., **52**, 1713 (1987).
63. F. Borondo, F. Martín and M. Yáñez.

- Adiabatic energies and radial couplings of the $^3\Sigma_u^+$ states of H_2 .*
J. Chem. Phys. **86**, 4982 (1987).
64. F. Martín, A. Riera and M. Yáñez.
Feshbach-type calculation of autoionizing states of the $BeHe^{4+}$ quasimolecule.
J. Chem. Phys., **86**, 6927 (1987).
65. M. Attinà, F. Cacace and M. Yáñez.
Electrophilic aromatic nitration in the gas phase.
J. Am. Chem. Soc. **109**, 5092 (1987).
66. F. Martín, O. Mó, A. Riera and M. Yáñez.
Feshbach resonant energies and widths in a pseudopotential approach.
Europhys. Lett. **4**, 799 (1987).
67. F. Martín, O. Mó, A. Riera and M. Yáñez.
Feshbach and pseudopotential theories. A useful analogy.
J. Chem. Phys. **87**, 6635 (1987).
68. F. Borondo, F. Martín and M. Yáñez.
A molecular mechanism for hydrogen-hydrogen excitation collisions.
Phys. Rev. A, **36**, 3630 (1987).
69. A. Macías, F. Martín, A. Riera and M. Yáñez.
Simple discretization method for autoionization widths. I. Theory.
Phys. Rev. A **36**, 4179 (1987).
70. A. Macías, F. Martín, A. Riera and M. Yáñez.
Simple discretization method for autoionization widths. II. Atoms.
Phys. Rev. A **36**, 4187 (1987).
71. A. Macías, F. Martín, A. Riera and M. Yáñez.
Simple discretization method for autoionization widths. III. Molecules.
Phys. Rev. A **36**, 4203 (1987).
72. O. Mó, J.L.G. de Paz and M. Yáñez.
Protonation of three membered ring heterocycles. An ab initio molecular orbital study.
J. Phys. Chem. **91**, 6484 (1987).
73. O. Mó, J.L.G. de Paz and M. Yáñez.
Counterpoise estimates of the BSSE in the evaluation of protonation energies.
Theoret. Chim. Acta **73**, 307 (1988).
74. M. Alcamí, J.L.G. de Paz and M. Yáñez.
Study of polarization effects in three-membered ring heterocycles.
J. Mol. Struct. THEOCHEM., **165**, 99 (1988).
75. A. Macías, F. Martín, A. Riera and M. Yáñez.
A practical solution to the "Unknown normalization" problem.
Int. J. Quant. Chem. **XXXIII**, 279 (1988).
76. J. Catalán, J.L.G. de Paz, M. Yáñez, F. Amat-Guerri, R. Houriet, E. Rolli, R. Zehring, P. Oelhafen, R.W. Taft, F. Anvia and J.H. Qian.
Study of the gas-phase basicity of 1-methyl-azaindole, 7-methyl-7H-pyrrolo(2,3-b) pyridine and related compounds.
J. Am. Chem. Soc. **110**, 2699 (1988).
77. F. Martín, A. Riera, M. Yáñez and H. Bachau.
Comparison of the conventional and pseudopotential Feshbach methods: $N^{5+}(3l,3l')^1S^e$ and $^{1,3}P^o$ resonances.
J. Phys. B **21**, 2261 (1988).
78. F. Martín, O. Mó, A. Riera and M. Yáñez.
Energies and widths of $(1s^23l3l')$ resonant states of C^{2+} , N^{5+} , O^{4+} and N^{6+} .
Phys. Rev. A **38**, 1094 (1988).

79. F. Martín, A. Riera and M. Yáñez.
Continuum vs. discretized wavefunctions. The importance of being well normalized.
Chem. Phys. Lett. **149**, 85 (1988).
80. A. Macías, F. Martín y M. Yáñez.
El continuo electrónico. Estados resonantes.
Capítulo del Libro: "Nuevas Tendencias de la Química Teórica",
Vol II, pag. 19, Ed. S. Fraga, C.S.I.C (Madrid), 1989.
81. M. Yáñez.
Clusters en fase gaseosa.
Capítulo del Libro: "Modelos teóricos e informáticos en la Química actual".
Ed. A. Riera. Editorial Centro de Estudios Ramón Areces, Madrid (1989).
82. *Ion Chemistry.*
Editor: M. Yáñez.
Editorial de la Universidad Autónoma de Madrid. Madrid. (1989).
83. A. Macías, F. Martín, O. Mó, A. Riera and M. Yáñez.
Atomic and molecular autoionizing states. A theoretical approach.
J. Physique **50**, C1-37 (1989).
84. A. Macías, O. Mó, A. Riera, M. Yáñez, H. Bachau, P. Galán and F. Martín.
Extension of the conventional and pseudopotential Feshbach methods to the study of "two active electrons + core" resonance states. Application to $C^{2+} (1s^2 3131')$ and $Ne^{6+} (1s^2 3131')$ systems.
J. Physique **50**, C1-99 (1989).
85. M. Boudjema, P. Moretto-Capelle, A. Bordenave-Montesquieu, P. Benoit-Cattin, A. Gleizes, H. Bachau, P. Galan, F. Martín, A. Riera and M. Yáñez.
Double capture into $1s^2 3131'$ configurations in collisions between He-like ions ($Z= 7, 8$ and 10) and helium target at 10 qKeV, 10° .
J. Phys. B **22**, L121 (1989).
86. M. Alcamí, O. Mó and M. Yáñez.
A molecular orbital study of azole- Li^+ complexes.
J. Phys. Chem. **93**, 3929 (1989).
87. F. Fernández-Lázaro, J. Mendoza, O. Mó, S. Rodríguez-Morgade, T. Torres, M. Yáñez, and J. Elguero.
Phtalocyanine analogues. Part I. Synthesis, spectroscopy and theoretical study of 9,20-Dihydro-5,24:12,17-Diimino-7,10:19,22-dinitrilobenz (f,p)[1,2,4,9,11,12,14,19] octaazacycloeicosine and MNDO calculations on its related Hückel heteroannulene.
J. Chem. Soc. Perkin 2, 797 (1989).
88. M. Alcamí, J.L.G. de Paz and M. Yáñez.
Nitrogen inversion barriers in three-membered rings. An ab initio molecular orbital study.
J. Comput. Chem. **10**, 468 (1989).
89. F. Martín, A. Riera and M. Yáñez.
Core effects in atomic resonances. A comparison between $^{1,3}P^o (3131')$ states of He-like and Be-like systems.
J. Chem. Phys. **91**, 376 (1989).
90. O. Mó, M. Yáñez and J. Elguero.
A MO analysis of the aromaticity of some nitrogen heterocyclic compounds.
J. Mol. Struct. THEOCHEM., **201**, 17 (1989).
91. A. Macías, F. Martín, O. Mó, A. Riera and M. Yáñez.
A new method to calculate lifetimes of atomic and molecular autoionizing states.
J. Mol. Struct. THEOCHEM., **202**, 235 (1989).
92. O. Mó, J.L.G. de Paz, M. Yáñez, I. Alkorta, J. Elguero, P. Goya and I. Rozas.
A molecular orbital study of the conformation (inversion and rotational barriers) and electronic properties of

- sulfamide*.
Can. J. Chem. **67**, 2227 (1989).
93. F. Martín, O. Mó, A. Riera and M. Yáñez.
A study of core effects in quasimolecular structure.
J. Mol. Struct. THEOCHEM., **205**, 43 (1990).
94. M. Alcamí, O. Mó, J.L.G. de Paz and M. Yáñez.
Enhanced Li^+ binding energies of some azines: a molecular orbital study.
Theoret. Chim. Acta **77**, 1,(1990).
95. J. Elguero, P. Goya, A. Martínez, I. Rozas, O. Mó, J.L.G. de Paz and M. Yáñez.
On the problem of the aromaticity of 1,2,6-Thiadiazine 1,1-Dioxides.
J. Phys. Org. Chem. **3**, 470 (1990).
96. J. Catalán, J.L.G. de Paz, M. Yáñez, R.M. Claramunt, C. López, J. Elguero, F. Anvia, J.H. Quian, M. Taagepera and R.W. Taft.
An intrinsic basicity scale based on azoles: Theoretical and experimental study of methyldiazoles basicity.
J. Am. Chem. Soc. **112**, 1303 (1990).
97. H. Bachau, P. Galán, F. Martín, A. Riera and M. Yáñez.
Resonance parameters and properties of berylliumlike doubly excited states: $4 \leq Z \leq 10$.
At. Data and Nuc. Data Tables **44**, 305, (1990).
98. M. Alcamí, O. Mó, M. Yáñez, F. Anvia and R.W. Taft.
An experimental and theoretical study of Li^+ affinities of methyldiazoles.
J. Phys. Chem. **94**, 4796, (1990).
99. M. Alcamí, O. Mó, M. Yáñez, J.L.M. Abboud and J. Elguero.
Bond Activation by protonation in the gas phase.
Chem. Phys. Lett. **172**, 471 (1990).
100. H. Bachau, P. Galán, F. Martín, A. Riera and M. Yáñez.
Comment on "Calculations of energies of intra-shell doubly excited states of beryllium-like ions"
J. Phys. B. **23**, L83, (1990).
101. M. Alcamí, A. Luna, O. Mó and M. Yáñez.
A topological analysis of the bond activation in $N_2H_4X^+$ and $H_2O_2X^+$ ($X=H, Li, Na, Al$) complexes.
Chem. Phys. Res. **1**, 119, (1990).
102. *Trends In Atomic and Molecular Physics*.
Editor: M. Yáñez
Editorial de la Universidad Autónoma de Madrid. (1991)
103. M. Alcamí, O. Mó, M. Yáñez and J.L.M. Abboud.
Ab initio MO study of the halogen cation basicities of some organic bases.
J. Phys. Org. Chem. **4**, 177, (1991).
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Lido di Ostia (Italy), 1982

Symposium on the Chemistry of Heterocyclic Compounds (VIIIth) and of Nucleic Acid Components

Prague (Czechoslovakia), 1984

11^{ème} Colloque sur la Physique des Collisions Atomiques et Electroniques.

Metz (France), 1986

International Conference on the Physics of Multicharged Ions

Grenoble (France), 1988

XIX Congreso Internacional dei Chimici Teorici dei Paesi di Espressione Latina.

Roma (Italy), 1990

I South European Conference of the Atomic and Molecular Physics.

Gandia (Spain), 1992

XX Congreso de Químicos Teóricos de los Países de expresión Latina.

Mérida (Venezuela), 1992

First Iberian Meeting on Atomic and Molecular Physics.

Lisboa (Portugal), 1993

The 5th European Symposium on Organic Reactivity. ESOR-V

Santiago de Compostela (Spain), 1995

Workshop on Weakly Bonded Species in ionic gas-phase Reactions

Palaiseau (France), 1996

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Cáceres (Spain), 1996

International Meeting on Localization and Transfer of Hydrogen

Madrid (Spain), 1996

Fourth European Workshop on FTMS

Pont-à-Mousson (France), 1997

Recent Theoretical and Experimental Advances in Hydrogen-Bonded Clusters

Elounda, Crete, 1997

Sixth European Symposium on Organic Reactivity ESOR VI

Louvain-la Neuve (Belgium), 1997

Hydrogen Transfer: Experiment and Theory

Berlin (Germany), 1997

International Symposium on Gas-Phase Ion Chemistry and Physics

Rome (Italy), 1998

2da. Escuela Iberoamericana de Química Computacional y Diseño Molecular

La Habana (Cuba), 1998

International Conference in Honor John A. Pople.

Amelia Island Florida (USA), 1999

Energetique et Reactivite des Ions en Phase Gazeuse: Experience et Théorie. (ERIG99)

Gif sur Yvette (France), 1999

15th International Mass Spectrometry Conference.

Barcelona (España), 2000

Third European Conference on Computational Chemistry EUCCO-CC3.

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International Conference on: Electronic Structure: Prediction and Applications.

San Sebastián (España), 2000

8th European Symposium on Organic Reactivity.

Cavtat (Dubrovnik) (Croatia), 2001
9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics.
S. Lorenzo del Escorial (España), 2001
4th European Conference on Computational Chemistry.
Assisi (Italia), 2002
HALCHEM Internacional Meeting
Cerdeña (Italia), 2002
Gordon Research Conference: Gaseous Ions: Structures, Energetics & Reactions
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Molecular Quantum Mechanics: The No Nonsense Path to Progress
Cambridge (Inglaterra), 2004
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Valladolid (España), 2004
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Ciudad del Cabo (Sudáfrica), 2005
Symposium in Honor of J.A. Pople. 229th ACS National Meeting
San Diego, CA (USA), 2005
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