



María Carmen Barrientos Benito

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Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

I have a degree in Chemical Sciences (June 1982) and a Ph.D. in Chemical Sciences (February 1986) from the University of Valladolid (with extraordinary award). In 1986 the Higher Council for Scientific Research awarded me a postdoctoral fellowship to the University of Kent (UK). I remained as a Postdoctoral Fellow and Visiting Research fellow during 1987. I have made stays in various foreign institutions: in the Radio Astronomy Laboratory of the Ecole Normale Supérieure (Paris) and in the Department of Chemistry and Materials of the University of L'Aquila (Italy).

I started teaching with the position of Assistant Professor in the Department of Physical Chemistry at the University of Valladolid in October 1983. In February 1993 I reached a position as Titular University Professor of the University at the University of Oviedo. I returned to the University of Valladolid in 1995 as Titular University Professor. Since 2011 I have been a Full Professor at University of Valladolid.

My research activity has developed through three lines of research. The first line is methodological and within it I have participated in the development of the quantum defect orbital method that was initially applied mainly to the study of photoexcitation processes. The second line of research is structural and has focused on the study of the structure and properties of new interstellar molecules. The third field of research corresponds to studies on reactivity and has basically focused on reactions with implications in atmospheric and interstellar chemistry. In this field we have actively collaborated with Profs. J. Ugalde (San Sebastián) and Y. Ellinger (Paris). In recent years I have maintained an active collaboration with Professor José Luis Alonso of the Molecular Spectroscopy Group (GEM) of the University of Valladolid, Professor José Cernicharo of the Institute of Fundamental Physics of the IFF, CSIC, Group of Molecular Astrophysics (Madrid, Spain), Professor Jean-Claude Guillemin of the Ecole Nationale Supérieure de Chimie (Rennes, France) and Professor Arnaud Belloche of the Max-Planck-Institut für Radioastronomie (Bonn, Germany). Through the collaboration with spectroscopists, it has been intended to seek an even closer synergy with experimental studies. We intend to extend this collaboration to the experimental observation of new molecules that may eventually be present in space, increasing the knowledge about the composition of the interstellar medium.

I am the Responsible Research of the recognized research group (GIR) of the University of Valladolid "Theoretical and Computational Chemistry, as well as the Consolidated Research Unit of the Junta de Castilla y León (UIC 139) and the Associated Unit CSIC formed together with the Molecular Spectroscopy Group of the University of Valladolid. This collaboration has made possible the study of natural sweeteners. The HELIOS SA consortium, one of the



leading companies in the food sector in Spain collaborates with our research through project VA244P20.

I am the author of 143 publications in scientific journals and 3 book chapters. I have presented 120 communications at international scientific conferences. I have directed 4 Ph.D. Thesis. Two of the doctors to whom I have directed their thesis are currently permanent professors, C. Lavin (Universidad of Valladolid) and A. Cimas (Evry, France). I am currently directing a PhD entitled "From interstellar systems to terrestrial organic and biomolecules: a synergetic theoretical and experimental rotational study" in collaboration with Prof. Alonso. The dissertation will be presented in January 2022.

I have participated in 25 Research Projects and Integrated Actions financed continuously by the corresponding Spanish Ministry or by the Autonomous Government in various public calls. In the last 10 years I have participated in 8 Research Projects. Currently, I am the Responsible Research of 2 Research Projects. I participate, regularly, in the evaluation and revision of R&D projects and papers. I am Assistant of the gas-phase chemistry panel at Barcelona Supercomputing Center. I was invited by the Nobel Committee for Chemistry, on behalf of the Royal Swedish Academy of Sciences, to nominate candidates for the award of The Nobel Prize in Chemistry for 2014.

General Quality Indicators:

Total Publications: 143 Sum of Times Cited: 1890

Average citations per year (citations/year): 85/2010, 60/2011, 108/2012, 81/2013, 88/2014, 65/2015, 74/2016, 57/2017, 44/2018, 71/2019, 60/2020

h-index: 24.

Q1 Publications: 74.

Periods of Research Activity: 6.



General quality indicators of scientific research

This section describes briefly the main quality indicators of scientific production (periods of research activity, experience in supervising doctoral theses, total citations, articles in journals of the first quartile, H index...). It also includes other important aspects or peculiarities.

Total Publications: 143 Sum of Times Cited: 1890

Average citations per year (citations/year): 85/2010, 60/2011, 108/2012, 81/2013, 88/2014, 65/2015, 74/2016, 57/2017, 44/2018, 71/2019, 60/2020

h-index: 24.

Q1 Publications: 74.

María Carmen Barrientos Benito

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Name: **María Carmen**
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ScopusID: **56235679300**
ResearcherID: **K-9698-2014**
Gender: **Female**
Nationality: **Spain**
Country of birth: **Spain**
Aut. region/reg. of birth: **Castile and León**
Contact province: **Valladolid**
City of birth: **Valladolid**
Contact address: **Departamento de Química Física y Química Inorgánica.
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Contact country:
Contact aut. region/reg.:
Contact city:
Land line phone:
Email:

Current professional situation

Employing entity: Universidad de Valladolid
Department: Química Física y Química Inorgánica, Facultad de Ciencias
Professional category: Catedrática de Universidad
Start date: 11/11/2011
Type of contract: Civil servant **Dedication regime:** Full time
Primary (UNESCO code): 230700 - Physical chemistry
Secondary (UNESCO code): 210000 - Astronomy & Astrophysics; 230700 - Physical chemistry
Tertiary (UNESCO code): 210000 - Astronomy & Astrophysics; 220608 - Molecular structure; 230000 - Chemistry
Identify key words: Density functional theory; Electronic correlation; Microwaves

Previous positions and activities

	Employing entity	Professional category	Start date
1	Universidad de Valladolid	Profesora Titular de Universidad	16/05/1995
2	Universidad de Oviedo	Profesora Titular de Universidad	03/04/1993
3	Universidad de Oviedo	Profesora Titular de Universidad Interina	01/10/1989
4	Universidad de Valladolid	Profesora Ayudante de Universidad	01/10/1983
5	University of Kent	Visiting Research Fellow y Becaria Postdoctoral del CSIC	01/01/1987



- 1** **Employing entity:** Universidad de Valladolid **Type of entity:** University
Professional category: Profesora Titular de Universidad
Start-End date: 16/05/1995 - 10/11/2011 **Duration:** 16 years - 5 months - 25 days
- 2** **Employing entity:** Universidad de Oviedo **Type of entity:** University
Professional category: Profesora Titular de Universidad
Start-End date: 03/04/1993 - 15/05/1995 **Duration:** 2 years - 1 month - 12 days
- 3** **Employing entity:** Universidad de Oviedo **Type of entity:** University
Professional category: Profesora Titular de Universidad Interina
Start-End date: 01/10/1989 - 02/04/1993 **Duration:** 3 years - 6 months - 1 day
- 4** **Employing entity:** Universidad de Valladolid **Type of entity:** University
Professional category: Profesora Ayudante de Universidad
Start-End date: 01/10/1983 - 30/09/1989 **Duration:** 6 years
- 5** **Employing entity:** University of Kent **Type of entity:** University
Professional category: Visiting Research Fellow y Becaria Postdoctoral del CSIC
Start-End date: 01/01/1987 - 31/12/1987 **Duration:** 1 year



Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

1 University degree: Doctorate

Name of qualification: Doctora en Ciencias Químicas

Degree awarding entity: Universidad de Valladolid **Type of entity:** University

Date of qualification: 09/04/1986

2 University degree: Higher degree

Name of qualification: Licenciada en Ciencias Químicas

Degree awarding entity: Universidad de Valladolid **Type of entity:** University

Date of qualification: 01/06/1982

Doctorates

Doctorate programme: Doctorado en Química

Degree awarding entity: Universidad de Valladolid **Type of entity:** University

Date of degree: 09/04/1986

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
French		C1	A1	A1	A1
English		C1	C1	C1	C1

Teaching experience

General teaching experience

1 Type of teaching: Official teaching

Name of the course: Química Física I

University degree: Química

Start date: 01/09/2011

End date: 31/07/2014

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

2 Name of the course: Química Experimental II

University degree: Química

Start date: 01/09/2011

End date: 31/07/2014



Entity: Universidad de Valladolid
Faculty, institute or centre: Facultad de Ciencias

Type of entity: University

3 Type of teaching: Official teaching

Name of the course: Físico-Química de la atmósfera

Type of programme: Master's degree

University degree: Master en Técnicas Avanzadas en Química

Start date: 01/09/2010

End date: 31/07/2013

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

4 Type of teaching: Official teaching

Name of the course: Química de la atmósfera

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Químicas

Start date: 01/09/2000

End date: 31/07/2013

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

5 Type of teaching: Official teaching

Name of the course: Introducción a la Experimentación Química y a las Técnicas Instrumentales II

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Químicas

Start date: 01/09/2000

End date: 31/07/2012

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

6 Type of teaching: International teaching

Name of the course: Computational Techniques and Numerical calculus

Type of programme: Master's degree

University degree: European Master in Theoretical Chemistry and Computational Modelling

Start date: 01/09/2010

End date: 31/07/2011

Entity: Universidad de las Islas Baleares

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

Subject language: English

7 Type of teaching: Official teaching

Name of the course: Química Física II

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Químicas

Start date: 01/09/2000

End date: 31/07/2011

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

8 Type of teaching: Official teaching

Name of the course: Fundamentos y aplicaciones de la Química Computacional

Type of programme: Doctorate

University degree: Doctorado en Ciencias Químicas

Start date: 01/09/2008

End date: 31/07/2009

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias



- 9** **Type of teaching:** Official teaching
Name of the course: Métodos de la Química Cuántica
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas
Start date: 01/09/2006 **End date:** 31/07/2008
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 10** **Type of teaching:** Official teaching
Name of the course: Métodos de la Química Cuántica
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas
Start date: 01/09/2006 **End date:** 31/07/2008
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 11** **Type of teaching:** Official teaching
Name of the course: Técnicas Computacionales. Métodos Numéricos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas (Doctorado Interuniversitario en Química Teórica y Computacional)
Start date: 01/09/2005 **End date:** 31/07/2006
Entity: Universitat Rovira i Virgili **Type of entity:** University
Faculty, institute or centre: Facultat de Química
- 12** **Type of teaching:** Official teaching
Name of the course: Técnicas Computacionales. Métodos Numéricos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas (Doctorado Interuniversitario en Química Teórica y Computacional)
Start date: 01/09/2004 **End date:** 31/07/2005
Entity: Universidad de Extremadura **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 13** **Type of teaching:** Official teaching
Name of the course: Técnicas Computacionales. Métodos Numéricos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas (Doctorado Interuniversitario en Química Teórica y Computacional)
Start date: 01/09/2003 **End date:** 31/07/2004
Entity: Universitat de Girona **Type of entity:** University
Faculty, institute or centre: Facultat de Ciències
- 14** **Type of teaching:** Official teaching
Name of the course: Química Computacional
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/2000 **End date:** 31/07/2004
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias



- 15** **Type of teaching:** Official teaching
Name of the course: Determinación Teórica de Parámetros Espectroscópicos Moleculares. Fundamentos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas
Start date: 01/09/2000 **End date:** 31/07/2003
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 16** **Type of teaching:** Official teaching
Name of the course: Determinación Teórica de Parámetros Espectroscópicos Moleculares. Fundamentos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas-1
Start date: 01/09/2000 **End date:** 31/07/2003
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 17** **Type of teaching:** Official teaching
Name of the course: Laboratorio Integrado II
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1999 **End date:** 31/07/2000
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 18** **Type of teaching:** Official teaching
Name of the course: Cinética y Dinámica Molecular
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1998 **End date:** 31/07/2000
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 19** **Type of teaching:** Official teaching
Name of the course: Cinética y Mecanismos de Reacciones
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1996 **End date:** 31/07/2000
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 20** **Type of teaching:** Official teaching
Name of the course: Métodos Numéricos y Programación en Química
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas
Start date: 01/09/1995 **End date:** 31/07/2000
Entity: Universidad de Valladolid **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias



- 21** **Type of teaching:** Official teaching
Name of the course: Química Cuántica
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1998
Entity: Universidad de Valladolid
Faculty, institute or centre: Facultad de Ciencias
End date: 31/07/1999
Type of entity: University
- 22** **Type of teaching:** Official teaching
Name of the course: Ampliación de Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1995
Entity: Universidad de Valladolid
Faculty, institute or centre: Facultad de Ciencias
End date: 31/07/1998
Type of entity: University
- 23** **Type of teaching:** Official teaching
Name of the course: Ampliación de Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas-1
Start date: 01/09/1995
Entity: Universidad de Valladolid
Faculty, institute or centre: Facultad de Ciencias
End date: 31/07/1998
Type of entity: University
- 24** **Type of teaching:** Official teaching
Name of the course: Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1995
Entity: Universidad de Valladolid
Faculty, institute or centre: Facultad de Ciencias
End date: 31/07/1998
Type of entity: University
- 25** **Type of teaching:** Official teaching
Name of the course: Ampliación de Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1994
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química
End date: 31/07/1995
Type of entity: University
- 26** **Type of teaching:** Official teaching
Name of the course: Termodinámica Química
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1994
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química
End date: 31/07/1995
Type of entity: University
- 27** **Type of teaching:** Official teaching
Name of the course: Determinación teórica de parámetros espectroscopicos moleculares: Aplicaciones
Type of programme: Doctorate



University degree: Doctorado en Ciencias Químicas
Start date: 01/09/1991
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química

End date: 31/07/1995
Type of entity: University

28 **Type of teaching:** Official teaching
Name of the course: Cinética Química
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1991
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química

End date: 31/07/1994
Type of entity: University

29 **Type of teaching:** Official teaching
Name of the course: Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1991
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química

End date: 31/07/1994
Type of entity: University

30 **Type of teaching:** Official teaching
Name of the course: Determinación teórica de parámetros espectroscopicos moleculares: Fundamentos
Type of programme: Doctorate
University degree: Doctorado en Ciencias Químicas
Start date: 01/09/1990
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química

End date: 31/07/1994
Type of entity: University

31 **Type of teaching:** Official teaching
Name of the course: Cálculo y Programación en Química Física
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1989
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Biología

End date: 31/07/1991
Type of entity: University

32 **Type of teaching:** Official teaching
Name of the course: Química General
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/01/1989
Entity: Universidad de Oviedo
Faculty, institute or centre: Facultad de Química

End date: 31/07/1991
Type of entity: University

33 **Type of teaching:** Official teaching
Name of the course: Química Cuántica y Espectroscopía
Type of programme: Bachelor's degree
University degree: Licenciatura en Ciencias Químicas
Start date: 01/09/1986
Entity: Universidad de Valladolid

End date: 31/07/1989
Type of entity: University



Faculty, institute or centre: Facultad de Ciencias

34 Type of teaching: Official teaching

Name of the course: Ampliación de Química Física

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Químicas

Start date: 01/09/1985

End date: 31/07/1989

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

35 Type of teaching: Official teaching

Name of the course: Química General

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Físicas

Start date: 01/09/1983

End date: 31/07/1989

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

36 Type of teaching: Official teaching

Name of the course: Química General

Type of programme: Bachelor's degree

University degree: Licenciatura en Ciencias Químicas

Start date: 01/09/1983

End date: 31/07/1989

Entity: Universidad de Valladolid

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias

Experience supervising doctoral thesis and/or final year projects

1 Project title: Síntesis de precursores de glicina en el medio interestelar: Estudio teórico

Type of project: Doctoral thesis

Co-director of thesis: Pilar Redondo Cristóbal

Entity: Universidad de Valladolid

Type of entity: University

Student: Laura Largo Escudero

Obtained qualification: Sobresaliente "Cum Laude" Numérica: 10

Date of reading: 17/06/2011

2 Project title: Estudio teórico de estructura y propiedades de especies TiCn (n=1-8)

Type of project: Minor thesis

Entity: Universidad de Valladolid

Type of entity: University

Student: Laura Largo Escudero

Date of reading: 2006

3 Project title: Estudio teórico de procesos de interés en Química Atmosférica: reacciones de nitrógeno atómico con derivados halocarbonados

Type of project: Doctoral thesis

Co-director of thesis: Antonio Largo Cabrerizo

Entity: Universidad de Valladolid

Type of entity: University

Student: Álvaro Cimas Samaniego

Obtained qualification: Sobresaliente cum laude por unanimidad. Numérica: 10

Date of reading: 14/07/2005



- 4** **Project title:** Estudio teórico de las especies CnCl , CnCl^+ , CnCl^- ($n=1-7$)
Type of project: Minor thesis
Co-director of thesis: Antonio Largo Cabrerizo
Entity: Universidad de Valladolid **Type of entity:** University
Student: Álvaro Cimas Samaniego
Date of reading: 2000
- 5** **Project title:** Formación de compuestos policarbonados de fósforo en el medio interestelar: estudio teórico
Type of project: Minor thesis
Co-director of thesis: Antonio Largo Cabrerizo
Entity: Universidad de Oviedo **Type of entity:** University
Student: Emma del Río Redondo
Date of reading: 1995
- 6** **Project title:** Análisis de series espectrales principal y subordinadas en sistemas con dos electrones de valencia
Type of project: Doctoral thesis
Entity: Universidad de Valladolid **Type of entity:** University
Student: Francisco Javier Virumbrales Gutiérrez
Obtained qualification: Apto Cum Laude
Date of reading: 10/04/1992
- 7** **Project title:** Análisis teórico de tendencias sistemáticas y efectos de polarización del core en fuerzas de oscilador
Type of project: Doctoral thesis
Entity: Universidad de Valladolid **Type of entity:** University
Student: Carmen Lavín Puente
Obtained qualification: Apto Cum Laude
Date of reading: 21/07/1989
- 8** **Project title:** Estudio de regularidades en las transiciones electrónicas correspondientes a la serie isoelectrónica del MgI
Type of project: Minor thesis
Entity: Universidad de Valladolid **Type of entity:** University
Student: Inmaculada Gútiez Antolín
Date of reading: 1988
- 9** **Project title:** Formulaciones alternativas de la integral de transición y regularidades en series isoelectrónicas
Type of project: Minor thesis
Entity: Universidad de Valladolid **Type of entity:** University
Student: Elena Charro Huerga
Date of reading: 1988
- 10** **Project title:** Efectos de polarización del core en las transiciones electrónicas
Type of project: Minor thesis
Entity: Universidad de Valladolid **Type of entity:** University
Student: Jesús Mazón Nieto de Cossio
Date of reading: 1986



Student tutorials

- 1** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.011
- 2** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.012
- 3** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.013
- 4** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.014
- 5** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.015
- 6** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.016
- 7** **Name of the programme:** Programa Orienta. Tutoría de alumnos Grado en Química
Entity: Universidad de Valladolid **Type of entity:** University
Frequency of the activity: 2.017

Educational or pedagogical publications, books, articles, etc.

- 1** Juan J. Novoa Vide; Antonio Largo Cabrerizo; Carmen Barrientos Benito; Emili Besalú. Computational Techniques and Numerical calculus, Theoretical and Computational Chemistry: Foundations, Methods and techniques (ISBN: 978-84-8021-615-9). pp. 279 - 384. Universitat Jaume I Castellón.
Name of the materials: Capítulo de Libro para la docencia del Master Europeo en Theoretical Chemistry and Computational Modelling
Date of drafting: 2007
Format: Chapters of books
- 2** Antonio Largo Cabrerizo; Carmen Barrientos Benito. Técnicas Computacionales, Química Teórica y Computacional (ISBN: 84-8021-312-4).. pp. 143 - 215. Universitat Jaume I Castellón.
Name of the materials: Capítulo de Libro para la docencia del Master Interuniversitario en Química Teórica y Computacional
Date of drafting: 2000
Format: Chapters of books

Participation in innovative teaching projects

- 1** **Project title:** Desarrollo e implementación de nuevas metodologías docentes en la Química Física y Química Analítica dentro del marco de la convergencia europea
Type of participation: Team member
Time of working relationship: For a limited time
Funding entity: Universidad de Valladolid
Start-End date: 01/10/2008 - 30/09/2017
Type of entity: University
Duration: 1 year
- 2** **Project title:** Ayuda para la elaboración de recursos de apoyo y experiencias innovadoras en torno a la Convergencia Europea: Desarrollo de competencias para el trabajo en grupo en el ámbito de la Química.
Type of participation: Others
Time of working relationship: For a limited time
Funding entity: Agencia para la Calidad del Sistema Universitario. Castilla y León
Start-End date: 08/10/2004 - 07/10/2005
Duration: 1 year
- 3** **Project title:** Ayuda para la elaboración de recursos de apoyo y experiencias innovadoras en torno a la Convergencia Europea: Desarrollo de competencias para el trabajo en grupo en el ámbito de la Química.
Type of participation: Others
Time of working relationship: For a limited time
Funding entity: Consejería de Educación, Junta de Castilla y León
Start-End date: 08/10/2004 - 07/10/2005
Duration: 1 year

Participation in conferences with talks focused on teacher training

- 1** **Name of the event:** I Jornadas sobre Convergencia Europea en los estudios de Química
Type of event: Workshop
City of event: Valencia, Spain
Date of presentation: 29/06/2005
Organising entity: Universitat de València
Type of entity: University
Experiencias docentes sobre el desarrollo de competencias en el ámbito de la Química.
- 2** **Name of the event:** Organización de las jornadas sobre: "Espacio Europeo de Educación Superior"
Type of event: Workshop
City of event: Valladolid, Spain
Date of presentation: 05/2005
Organising entity: Universidad de Valladolid
Type of entity: University
- 3** **Name of the event:** Jornada de Intercambio de Experiencias Innovadoras en Torno a la Convergencia Europea
Type of event: Workshop
City of event: Valladolid, Spain
Date of presentation: 17/06/2005
Organising entity: Universidad de Valladolid
Type of entity: University
Desarrollo de competencias para el trabajo en grupo en el ámbito de la Química.

Other activities/achievements not included above

- 1** **Description of the activity:** Tramo Docente 6 desde 01/10/08 hasta 30/09/13
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/2013
- 2** **Description of the activity:** Tramo Docente 5 desde 01/10/03 hasta 30/09/08
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/2008
- 3** **Description of the activity:** Tramo Docente 4 desde 01/10/98 hasta 30/09/03
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/2003
- 4** **Description of the activity:** Tramo Docente 3 desde 01/10/93 hasta 30/09/98
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/1998
- 5** **Description of the activity:** Tramo Docente 2 desde 01/10/88 hasta 30/09/93
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/1993
- 6** **Description of the activity:** Tramo Docente 1 desde 01/10/83 hasta 30/09/88
Organising entity: Universidad de Valladolid **Type of entity:** University
End date: 30/09/1988

Scientific and technological experience

Research and development groups/teams

Name of the group: Química Teórica y Computacional (GIR reconocido)
Aims of the group: Investigación
Type of collaboration: Co-authorship of publications
Affiliation entity: Universidad de Valladolid **Type of entity:** University
Start date: 2003 **Duration:** 10 years

Scientific or technological activities

R&D projects funded through competitive calls of public or private entities

- 1** **Name of the project:** Simulaciones Computacionales en Astroquímica: Propiedades Espectroscópicas y Reactividad de Moléculas Interestelares - PID2020-117742GB-I00
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Nº of researchers: 6
Type of participation: Principal investigator
Start-End date: 01/09/2021 - 31/08/2025
Total amount: 64.130 €
- 2** **Name of the project:** Laser Abaltion Spectroscopic Techniques: from buiding blocks and sweeteners to interstellar molecules VA244P20
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito
Nº of researchers: 7
Funding entity or bodies: Junta de Castilla y León **Type of entity:** Autonómica
City funding entity: Valladolid, Castile and León, Spain
Type of participation: Principal investigator
Code according to the funding entity: VA244P20
Start-End date: 01/09/2020 - 31/08/2023 **Duration:** 3 years
Total amount: 172.000 €
Dedication regime: Full time
- 3** **Name of the project:** Astroquímica computacional: formación de moléculas prebióticas y predicción de parámetros espectroscópicos de nuevas moléculas (VA010G18)
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito
Nº of researchers: 7
Funding entity or bodies: Junta de Castilla y León **Type of entity:** Autonómica
City funding entity: Valladolid, Castile and León, Spain
Type of participation: Principal investigator



Code according to the funding entity: VA010G18

Start-End date: 01/09/2018 - 31/08/2021

Duration: 3 years

Total amount: 12.000 €

Dedication regime: Full time

- 4** **Name of the project:** Astroquímica Computacional: formación de moléculas prebióticas y predicción de parámetros espectroscópicos de moléculas relevantes(VA077U13).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo; Carmen Barrientos Benito; Pilar Redondo Cristóbal; Víctor Manuel Rayón Rico; Henar Martínez García

Nº of researchers: 5

Funding entity or bodies:

Ministerio de Ciencia, Innovación y Universidades

Type of entity: State agency

City funding entity: Madrid, Spain

Type of participation: Team member

Code according to the funding entity: AYA2017-87515-P

Start-End date: 01/01/2018 - 31/12/2020

Duration: 3 years

Total amount: 30.000 €

Sub-project amount: 30.000 €

Dedication regime: Full time

- 5** **Name of the project:** Procesos ion-molécula en fase gas: síntesis interestelar de biomoléculas y reactividad de derivados halocarbonados (VA077U13).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito

Nº of researchers: 7

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómica

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Principal investigator

Code according to the funding entity: VA077U13

Start-End date: 03/09/2013 - 02/09/2016

Duration: 3 years

Total amount: 30.000 €

Dedication regime: Full time

- 6** **Name of the project:** Estudio mecano-cuántico y cinético de sistemas y procesos ion-molécula de interés en Astroquímica y química sintética (CTQ2010-16864).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: Universidad de Valladolid

Type of entity: University



City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito
Funding entity or bodies:
Ministerio de Ciencia e Innovación.

Type of participation: Principal investigator
Code according to the funding entity: CTQ2010-16864
Start-End date: 01/01/2011 - 01/01/2014 **Duration:** 3 years
Total amount: 71.390 €
Dedication regime: Full time

7 Name of the project: Reacciones ion-molécula en fase gas. Implicaciones en Química sintética y Astroquímica (VA040A09)

Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: Universidad de Valladolid **Type of entity:** University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómica

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Principal investigator
Code according to the funding entity: VA040A09
Start-End date: 01/01/2009 - 01/01/2012 **Duration:** 3 years
Total amount: 42.100 €
Dedication regime: Full time

8 Name of the project: Reactividad en fase gas de cationes metálicos con CH₃X (X=H,F,Cl). La importancia de la formación de intermediatos en reactividad química (CTQ2007-67234-C02-02).

Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: Universidad de Valladolid **Type of entity:** University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito

Funding entity or bodies:

Ministerio de Educación y Ciencia. Dirección General de Investigación.

Type of participation: Principal investigator
Code according to the funding entity: CTQ2007-67234-C02-02
Start-End date: 13/12/2007 - 12/12/2010 **Duration:** 3 years
Total amount: 77.440 €
Dedication regime: Full time

9 Name of the project: Estudio de la estructura y síntesis de compuestos de interés en química atmosférica y en el medio interestelar (VA077A06)

Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional

Degree of contribution: Coordinator of total project, network or consortium



Entity where project took place: Universidad de Valladolid **Type of entity:** University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómico

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Co-ordinator

Code according to the funding entity: VA077A06

Start-End date: 01/01/2006 - 01/01/2009

Duration: 3 years

Total amount: 13.300 €

Dedication regime: Full time

- 10** **Name of the project:** Estudio mecanístico de reacciones de interés en química atmosférica y astroquímica (CTQ2004-07405-C02-01).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo; Carmen Barrientos Benito

Funding entity or bodies:

Ministerio de Educación y Ciencia. Dirección General de Investigación.

Type of participation: Others

Code according to the funding entity: CTQ2004-07405-C02-01

Start-End date: 13/12/2004 - 13/12/2007

Duration: 3 years

Total amount: 52.000 €

Dedication regime: Full time

- 11** **Name of the project:** Estructura y procesos de síntesis de compuestos policarbonados: estudio teórico (VA085/03)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Carmen Barrientos Benito

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómico

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Co-ordinator

Code according to the funding entity: VA085/03

Start-End date: 01/01/2003 - 01/01/2006

Duration: 3 years

Participating entity/entities: Universidad de Valladolid

Total amount: 13.500 €

Dedication regime: Full time

- 12** **Name of the project:** Reacciones de interés en química medioambiental e interestelar: importancia de los procesos prohibidos por el spin . Acción Integrada Hispano-Italiana (HI2002-0025)
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** European Union
Degree of contribution: Researcher
Entity where project took place: Universidad de Valladolid - Università de L'Aquila (Italia)
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo; Carmen Barrientos Benito
Funding entity or bodies: Ministerio de Ciencia y Tecnología
Type of participation: Others
Name of the programme: Acción Integrada Hispano - Italiana
Code according to the funding entity: HI2002-0025
Start-End date: 01/01/2003 - 01/01/2005 **Duration:** 2 years
Participating entity/entities: Universidad de Valladolid-Università de L'Aquila (Italia)
Total amount: 10.400 €
Dedication regime: Full time
- 13** **Name of the project:** Red de Excelencia en Química Teórica y Computacional (BQU2001-5037-E)
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** European Union
Degree of contribution: Researcher
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Manuel Yáñez Montero (Universidad Autónoma de Madrid) - IP
Nº of researchers: 18
Funding entity or bodies: Ministerio de Ciencia y Tecnología
Type of participation: Others
Code according to the funding entity: BQU2001-5037-E)
Start-End date: 01/01/2003 - 01/01/2005 **Duration:** 2 years
Participating entity/entities: Distintos grupos de investigación de 18 Universidades
Dedication regime: Full time
- 14** **Name of the project:** Reacciones de interés en química medioambiental, atmosférica e interestelar: importancia del cruce entre sistemas y de los complejos pre-reactivos (BQU2001-3660-C02-02).
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo
Funding entity or bodies: Ministerio de Ciencia y Tecnología. Dirección General de Investigación.
Type of participation: Others
Code according to the funding entity: BQU2001-3660-C02-02
Start-End date: 01/01/2002 - 31/12/2004 **Duration:** 3 years
Total amount: 43.873,88 €



Dedication regime: Full time

- 15 Name of the project:** Equipamiento multidisciplinar en estructura molecular. Proyecto de adquisición de infraestructura científica (Fondos FEDER) Subvención concedida: 48.6 Mptas. (Petición conjunta de cuatro grupos de investigación del Departamento de Química Física).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo, José L. Alonso, Inmaculada Martín (IPs)

Type of participation: Others

Start-End date: 01/01/2000 - 01/01/2003

Duration: 3 years

Dedication regime: Full time

- 16 Name of the project:** Estudio teórico de reacciones ion-molécula en fase gas. Aplicaciones en Química Interestelar (VA 18/00B)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómico

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Others

Code according to the funding entity: VA 18/00B

Start-End date: 01/01/2000 - 01/01/2003

Duration: 3 years

Participating entity/entities: Universidad de Valladolid

Dedication regime: Full time

- 17 Name of the project:** Estudio teórico de la estructura, reactividad y espectroscopía de especies atómicas y moleculares de interés en astroquímica.(PB97-0399-C03-01)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo

Type of entity: University

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Inmaculada Martín García (IP)

Funding entity or bodies:

DGICYT

Type of participation: Others

Code according to the funding entity: PB97-0399-C03-01

Start-End date: 01/07/1998 - 01/07/2001

Duration: 3 years

Participating entity/entities: Universidad de Oviedo; Universidad de Valladolid

Dedication regime: Full time

- 18** **Name of the project:** Medio ambiente y fuentes de energía alternativas. Efectos de las impurezas en la fusión nuclear termocontrolada.

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Inmaculada Martín García

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Autonómico

City funding entity: Valladolid, Castile and León, Spain

Type of participation: Others

Code according to the funding entity: VA 21/97

Start-End date: 01/01/1997 - 01/01/2000

Duration: 3 years

Participating entity/entities: Universidad de Valladolid

Dedication regime: Full time

- 19** **Name of the project:** Estudio teórico ab initio y semiempírico de la química interestelar y de las llamas.(PB94-1314-C03-02)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo

Type of entity: University

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

DGICYT

Type of participation: Others

Code according to the funding entity: PB94-1314-C03-02

Start-End date: 01/07/1995 - 01/07/1998

Duration: 3 years

Participating entity/entities: Universidad de Oviedo; Universidad de Valladolid

Dedication regime: Full time

- 20** **Name of the project:** Estudio teórico mediante métodos ab initio y semiempíricos, de propiedades espectrales y químicas de interés astrofísico. (PB91-0207-C02-02)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo

Type of entity: University

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

DGICYT

Type of participation: Others

Code according to the funding entity: PB91-0207-C02-02)

Start-End date: 15/06/1992 - 15/06/1995

Duration: 3 years



Participating entity/entities: Universidad de Oviedo; Universidad de Valladolid

Dedication regime: Full time

21 Name of the project: Estudio teórico de moléculas y procesos químicos interestelares. Acción Integrada Hispano-Francesa (Conv 1991 HF-304)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: European Union

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo - Ecole Normale Supérieure (Paris)

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

DGICYT (Subdirec. Gener. Coop. Inter.).

Type of participation: Others

Name of the programme: Acción Integrada Hispano - Francesa

Code according to the funding entity: 1991 HF-304

Start-End date: 01/01/1992 - 01/01/1993

Duration: 1 year

Participating entity/entities: Universidad de Oviedo-Ecole Normale Supérieure (Paris)

Dedication regime: Full time

22 Name of the project: Estudio teórico de procesos físicos y químicos en el medio interestelar (PB88-0343).

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): Inmaculada Martín García (IP)

Funding entity or bodies:

Ministerio de Educación y Ciencia. DGICYT

Type of participation: Others

Code according to the funding entity: PB88-0343

Start-End date: 22/09/1989 - 22/09/1992

Duration: 3 years

Participating entity/entities: Universidad de Valladolid

Dedication regime: Full time

23 Name of the project: Estudio teórico de moléculas y procesos químicos interestelares. Acción Integrada Hispano-Francesa (Conv 1990 HF-316)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: European Union

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo - Ecole Normale Supérieure (Paris)

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

DGICYT (Subdirec. Gener. Coop. Inter.).

Type of participation: Others

Name of the programme: Acción Integrada Hispano - Francesa

Code according to the funding entity: 1990 HF-316

Start-End date: 01/01/1991 - 01/01/1992

Duration: 1 year



Participating entity/entities: Universidad de Oviedo-Ecole Normale Supérieure (Paris)

Dedication regime: Full time

- 24** **Name of the project:** Estudio teórico de moléculas y procesos químicos de interés en Astrofísica.(DF90/2194)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo

Type of entity: University

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo (IP)

Funding entity or bodies:

Universidad de Oviedo

Type of entity: University

City funding entity: Oviedo, Principality of Asturias, Spain

Type of participation: Others

Code according to the funding entity: DF90/2194

Start-End date: 01/01/1990 - 01/01/1991

Duration: 1 year

Participating entity/entities: Universidad de Oviedo

Dedication regime: Full time

- 25** **Name of the project:** Estudio teórico de moléculas y procesos químicos interestelares. Acción Integrada Hispano-Francesa (Conv 1989 HF-236)

Type of project: Basic research (including archaeological digs, etc)

Geographical area: European Union

Degree of contribution: Researcher

Entity where project took place: Universidad de Oviedo - Ecole Normale Supérieure (Paris)

City of entity: Oviedo, Principality of Asturias, Spain

Name principal investigator (PI, Co-PI....): Antonio Largo Cabrerizo

Funding entity or bodies:

DGICYT (Subdirec. Gener. Coop. Inter.).

Type of participation: Others

Name of the programme: Acción Integrada Hispano - Francesa

Code according to the funding entity: 1989 HF-236

Start-End date: 01/01/1990 - 01/01/1991

Duration: 1 year

Participating entity/entities: Universidad de Oviedo-Ecole Normale Supérieure (Paris)

Dedication regime: Full time



Scientific and technological activities

Scientific production

H index: 24

Date of application: 21/05/2020

Publications, scientific and technical documents

- 1** Miguel Sanz-Novio; Iker León; José Luis Alonso; Antonio Largo; Carmen Barrientos. Formation of interstellar cyanoacetamide: a rotational and computational study. *Astronomy and Astrophysics*. 644 - A3, pp. 1 - 10. 22/09/2020.
Type of production: Scientific paper **Format:** Journal
- 2** Pilar Redondo; Antonio Largo; Carmen Barrientos. Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules. *THE ASTROPHYSICAL JOURNAL*. 899 - 135, pp. 1 - 9. 01/09/2020.
Type of production: Scientific paper **Format:** Journal
- 3** Pilar Redondo; Miguel Sanz-Novio; Antonio Largo; Carmen Barrientos. Amino acetaldehyde conformers: structure and spectroscopic properties. *Monthly Notices of the Royal Astronomical Society*. 492 - 2, pp. 1827 - 1833. 01/02/2020.
Type of production: Scientific paper **Format:** Journal
- 4** Carlos Cabezas; Carmen Barrientos; Antonio Largo; Jean-Claude Guillemin; José Cernicharo; José L. Alonso. Alkaline and alkaline-earth cyanoacetylides: A combined theoretical and rotational spectroscopic investigation. *JOURNAL OF CHEMICAL PHYSICS*. 151 - 5, pp. 054312-1. 07/08/2019.
Type of production: Scientific paper **Format:** Journal
- 5** Miguel Sanz-Novio; Antonio Largo; Pilar Redondo; Carmen Barrientos. Formation of Protonated Glycine Isomers in the interstellar Medium. *ACS EARTH AND SPACE CHEMISTRY*. 3 - 7, pp. 170 - 181. 01/07/2019.
Type of production: Scientific paper **Format:** Journal
- 6** Pilar Redondo; Carmen Barrientos; Antonio Largo. Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest. *THE ASTROPHYSICAL JOURNAL*. 871 - 2, pp. 180. 01/02/2019.
Type of production: Scientific paper **Format:** Journal
- 7** Pilar Redondo; Antonio Largo; Carmen Barrientos. Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. *Monthly Notices of the Royal Astronomical Society*. 478 - 3, pp. 3042 - 3048. 04/05/2018. ISSN 0004-6361
Type of production: Scientific paper **Format:** Journal
- 8** Pilar Redondo; Víctor Manuel Rayón; Carmen Barrientos; Antonio Largo. Structural Trends in Monoboronyl Compounds: Analysis of the Interaction of Second-Row Elements with BO. *JOURNAL OF PHYSICAL CHEMISTRY A*. 122 - 1, pp. 398 - 409. 11/01/2018.
Type of production: Scientific paper **Format:** Journal

- 9** Pilar Redondo; Henar Martínez; Antonio Largo; Carmen Barrientos. Prebiotic molecules formation through the gas-phase reaction between azanone and protonated vinyl alcohol. ASTRONOMY & ASTROPHYSICS. 603, 13/06/2017. ISSN 0004-6361
Type of production: Scientific paper **Format:** Journal
- 10** Alvaro Vega-Vega; Antonio Largo; Pilar Redondo; Carmen Barrientos. Structure and Spectroscopic Properties of [Mg,C,N,O] Isomers: Plausible Astronomical Molecules. ACS EARTH AND SPACE CHEMISTRY. 1, pp. 158 - 167. 01/05/2017.
Type of production: Scientific paper **Format:** Journal
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- 96** E delRio; C Barrientos; A Largo. Theoretical studies of possible processes for the interstellar production of phosphorus compounds: The reaction of P^+ with C_3H_2 . JOURNAL OF PHYSICAL CHEMISTRY. 100 - 35, pp. 14643 - 14650. 08/1996. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 97** VM Rayon; C Barrientos; A Largo. Reaction of carbon atoms with H_2Cl^+ : An ab initio study of a possible interstellar process. THEOCHEM-JOURNAL OF MOLECULAR STRUCTURE. 363 - 3, pp. 319 - 331. 04/1996. ISSN 0166-1280
Type of production: Scientific paper **Format:** Journal
- 98** A Largo; C Barrientos. Theoretical studies of simple organoboron compounds: Structures and stabilities of BC_2H_4 isomers. APPLIED ORGANOMETALLIC CHEMISTRY. 10 - 3-4, pp. 283 - 295. 04/1996. ISSN 0268-2605
Type of production: Scientific paper **Format:** Journal
- 99** E delRio; C Barrientos; A Largo. Theoretical study of the C_3P radical and its cation. JOURNAL OF PHYSICAL CHEMISTRY. 100 - 2, pp. 585 - 593. 01/1996. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal

- 100** C BARRIENTOS; A LARGO. IONIZATION AND PROTONATION OF (MGCN) - AN AB-INITIO STUDY OF SOME GAS-PHASE PROPERTIES OF THE FIRST MAGNESIUM COMPOUND IN-SPACE. THEOCHEM-JOURNAL OF MOLECULAR STRUCTURE. 336 - 1, pp. 29 - 37. 06/1995. ISSN 0166-1280
Type of production: Scientific paper **Format:** Journal
- 101** A LARGO; C BARRIENTOS; X LOPEZ; FP COSSIO; JM UGALDE. THEORETICAL-STUDIES OF POSSIBLE PROCESSES FOR THE INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - THE REACTION OF P+ WITH ACETYLENE. JOURNAL OF PHYSICAL CHEMISTRY. 99 - 17, pp. 6432 - 6440. 04/1995. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 102** FJ VIRUMBRALES; I MARTIN; C BARRIENTOS. ISOELECTRONIC SMOOTHING OF ENERGY-LEVELS AND CALCULATIONS ON THE 2SNS S-1-]2SMP P-1(0) TRANSITIONS IN THE BERYLLIUM ISOELECTRONIC SEQUENCE. ZEITSCHRIFT FUR PHYSIK D-ATOMS MOLECULES AND CLUSTERS. 32 - 3, pp. 179 - 185. 12/1994. ISSN 0178-7683
Type of production: Scientific paper **Format:** Journal
- 103** C LAVIN; C BARRIENTOS; I MARTIN. RELATIVISTIC QUANTUM-DEFECT CALCULATIONS ON THE COPPER ISOELECTRONIC SEQUENCE. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 50 - 6, pp. 411 - 428. 06/1994. ISSN 0020-7608
Type of production: Scientific paper **Format:** Journal
- 104** A LARGO; C BARRIENTOS; X LOPEZ; JM UGALDE. THEORETICAL-STUDY OF THE C2P RADICAL AND (C2P)(+) SPECIES. JOURNAL OF PHYSICAL CHEMISTRY. 98 - 15, pp. 3985 - 3988. 04/1994. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 105** A LARGO; C BARRIENTOS. THEORETICAL-STUDY OF THE STRUCTURES AND STABILITIES OF (SiC2H2)(+) SPECIES - THE REACTION OF Si+ WITH ACETYLENE. JOURNAL OF PHYSICAL CHEMISTRY. 98 - 15, pp. 3978 - 3984. 04/1994. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 106** X LOPEZ; FP COSSIO; JM UGALDE; C BARRIENTOS; A LARGO. AB-INITIO CHARACTERIZATION OF GASEOUS (CO2P)(+) SPECIES. JOURNAL OF PHYSICAL CHEMISTRY. 98 - 9, pp. 2294 - 2297. 03/1994. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 107** X LOPEZ; JM UGALDE; FP COSSIO; A LARGO; C BARRIENTOS. TOPOLOGICAL ANALYSIS OF THE CHARGE-DENSITY FOR PHOSPHORUS ION-MOLECULE COMPLEXES BOUND TO WATER AND AMMONIA MOLECULES. JOURNAL OF PHYSICAL CHEMISTRY. 98 - 12, pp. 3148 - 3153. 03/1994. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 108** JR FLORES; C BARRIENTOS; A LARGO. REACTIONS OF CH3+ WITH 2ND-ROW ATOMS - AN AB-INITIO STUDY. JOURNAL OF PHYSICAL CHEMISTRY. 98 - 4, pp. 1090 - 1099. 01/1994. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 109** X LOPEZ; JM UGALDE; FP COSSIO; B LECEA; A LARGO; C BARRIENTOS. AB-INITIO STUDY OF PHOSPHORUS ION COMPLEXES OF AMMONIA AND WATER. JOURNAL OF PHYSICAL CHEMISTRY. 97 - 37, pp. 9337 - 9340. 09/1993. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 110** I MARTIN; J KARWOWSKI; GHF DIERCKSEN; C BARRIENTOS. TRANSITION-PROBABILITIES IN THE LITHIUM SEQUENCE. ASTRONOMY & ASTROPHYSICS SUPPLEMENT SERIES. 100 - 3, pp. 595 - 605. 09/1993. ISSN 0365-0138

Type of production: Scientific paper

Format: Journal

- 111** C SARASOLA; X LOPEZ; A ARRIETA; C BARRIENTOS; A LARGO; JM UGALDE. ABINITIO CHARACTERIZATION OF NOVEL GASEOUS (PO)₂⁺ SPECIES. JOURNAL OF PHYSICAL CHEMISTRY. 97 - 22, pp. 5860 - 5863. 06/1993. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 112** X LOPEZ; C SARASOLA; B LECEA; A LARGO; C BARRIENTOS; JM UGALDE. ABINITIO CHARACTERIZATION OF GASEOUS P₂O₂. JOURNAL OF PHYSICAL CHEMISTRY. 97 - 16, pp. 4078 - 4079. 04/1993. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 113** X LOPEZ; JM UGALDE; C BARRIENTOS; A LARGO; P REDONDO. THEORETICAL-STUDY OF POSSIBLE PROCESSES FOR THE INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - REACTION OF P⁺ WITH SH₂. JOURNAL OF PHYSICAL CHEMISTRY. 97 - 8, pp. 1521 - 1525. 02/1993. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 114** C BARRIENTOS; A LARGO; P REDONDO; F PAUZAT; Y ELLINGER. THEORETICAL-STUDY OF A BASIC PROCESS IN INTERSTELLAR CHLORINE CHEMISTRY - REACTION OF C⁺ WITH HCL. JOURNAL OF PHYSICAL CHEMISTRY. 97 - 1, pp. 173 - 176. 01/1993. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 115** C BARRIENTOS; I MARTIN. QUANTUM-DEFECT STUDIES OF SYSTEMATIC TRENDS OF F-VALUES - TRANSITIONS IN SUBORDINATE SPECTRAL SERIES. JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER. 48 - 3, pp. 287 - 293. 09/1992. ISSN 0022-4073

Type of production: Scientific paper

Format: Journal

- 116** C BARRIENTOS; A LARGO. A THEORETICAL-STUDY OF THE STRUCTURES AND STABILITIES OF SC₂H₂⁺ SPECIES - THE REACTION OF S⁺ WITH ACETYLENE. JOURNAL OF PHYSICAL CHEMISTRY. 96 - 14, pp. 5808 - 5814. 07/1992. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 117** C LAVIN; C BARRIENTOS; I MARTIN. QUANTUM-DEFECT STUDIES OF TRANSITIONS IN THE DIFFUSE SPECTRAL SERIES OF THE POTASSIUM ISOELECTRONIC SEQUENCE. JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER. 47 - 5, pp. 411 - 419. 05/1992. ISSN 0022-4073

Type of production: Scientific paper

Format: Journal

- 118** I MARTIN; C LAVIN; C BARRIENTOS. FINE-STRUCTURE OSCILLATOR-STRENGTHS FOR EXCITED-STATE TRANSITIONS IN CU-LIKE IONS. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 26, pp. 465 - 474. 1992. ISSN 0020-7608

Type of production: Scientific paper

Format: Journal

- 119** A LARGO; C BARRIENTOS. THEORETICAL-STUDIES OF POSSIBLE PROCESSES FOR THE INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - REACTION OF P⁺ WITH HCN AND PROTONATION OF CNP COMPOUNDS. JOURNAL OF PHYSICAL CHEMISTRY. 95 - 24, pp. 9864 - 9868. 11/1991. ISSN 0022-3654

Type of production: Scientific paper

Format: Journal

- 120** I MARTIN; C LAVIN; C BARRIENTOS. SYSTEMATIC TRENDS ALONG THE POTASSIUM SEQUENCE - STUDY OF NS₂S-MP₂P₀ TRANSITIONS. CANADIAN JOURNAL OF PHYSICS. 69 - 10, pp. 1273 - 1283. 10/1991. ISSN 0008-4204

Type of production: Scientific paper

Format: Journal

- 121** C BARRIENTOS; A LARGO. AN ABINITIO STUDY OF C₂S PROTONATION. CHEMICAL PHYSICS LETTERS. 184 - 1-3, pp. 168 - 174. 09/1991. ISSN 0009-2614
Type of production: Scientific paper **Format:** Journal
- 122** A LARGO; JR FLORES; C BARRIENTOS; JM UGALDE. THEORETICAL-STUDIES OF POSSIBLE PROCESSES FOR INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - REACTION OF P⁺ WITH METHANE. JOURNAL OF PHYSICAL CHEMISTRY. 95 - 17, pp. 6553 - 6557. 08/1991. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 123** A LARGO; P REDONDO; C BARRIENTOS; JM UGALDE. THEORETICAL-STUDIES OF POSSIBLE PROCESSES FOR THE INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - REACTION OF P⁺ WITH WATER. JOURNAL OF PHYSICAL CHEMISTRY. 95 - 14, pp. 5443 - 5445. 07/1991. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 124** P REDONDO; A LARGO; C BARRIENTOS; JM UGALDE. A THEORETICAL-STUDY OF THE STRUCTURES AND STABILITIES OF (H₂PO)⁺ SPECIES AND THE PROTON AFFINITIES OF HPO AND POH. JOURNAL OF PHYSICAL CHEMISTRY. 95 - 11, pp. 4318 - 4323. 05/1991. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 125** I MARTIN; C BARRIENTOS. ANALYTICAL WAVE-FUNCTIONS FOR ATOMIC QUANTUM-DEFECT THEORY - COMMENT. PHYSICAL REVIEW A. 43 - 7, pp. 4061 - 4062. 04/1991. ISSN 1050-2947
Type of production: Scientific paper **Format:** Journal
- 126** A LARGO; JR FLORES; C BARRIENTOS; JM UGALDE. THEORETICAL-STUDIES OF POSSIBLE PROCESSES FOR THE INTERSTELLAR PRODUCTION OF PHOSPHORUS-COMPOUNDS - REACTION OF P⁺ WITH AMMONIA. JOURNAL OF PHYSICAL CHEMISTRY. 95 - 1, pp. 170 - 175. 01/1991. ISSN 0022-3654
Type of production: Scientific paper **Format:** Journal
- 127** C BARRIENTOS; I MARTIN. QUANTUM-DEFECT STUDIES OF SYSTEMATIC TRENDS OF F VALUES. PHYSICAL REVIEW A. 42 - 1, pp. 432 - 439. 07/1990. ISSN 1050-2947
Type of production: Scientific paper **Format:** Journal
- 128** I MARTIN; C BARRIENTOS; I GUTIEZ. THEORETICAL-STUDY OF TRANSITIONS INVOLVING 3 RYDBERG SERIES IN 2-VALENCE ELECTRON-SYSTEMS - MGI AND ITS ELECTRONIC SEQUENCE. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 37 - 3, pp. 221 - 240. 03/1990. ISSN 0020-7608
Type of production: Scientific paper **Format:** Journal
- 129** A LARGO; C BARRIENTOS. A THEORETICAL-STUDY OF THE C₂H, C₂F AND C₂CL RADICALS AND THEIR POSITIVE-IONS. CHEMICAL PHYSICS. 138 - 2-3, pp. 291 - 301. 11/1989. ISSN 0301-0104
Type of production: Scientific paper **Format:** Journal
- 130** C BARRIENTOS; I MARTIN. CORE-POLARIZATION EFFECTS IN SUBORDINATE SERIES OF THE ALKALI ATOMS. CANADIAN JOURNAL OF PHYSICS. 67 - 10, pp. 996 - 1001. 10/1989. ISSN 0008-4204
Type of production: Scientific paper **Format:** Journal
- 131** A LARGOCABRERIZO; C BARRIENTOS. THEORETICAL-STUDIES OF POTENTIAL ASTROPHYSICAL MOLECULES - THE CLCC AND SC₂H RADICALS. CHEMICAL PHYSICS LETTERS. 155 - 6, pp. 550 - 556. 03/1989. ISSN 0009-2614
Type of production: Scientific paper **Format:** Journal
- 132** A LARGOCABRERIZO; C BARRIENTOS. AN ABINITIO STUDY OF THE HBS⁺, FBS⁺, CLBS⁺ CATIONS. THEOCHEM-JOURNAL OF MOLECULAR STRUCTURE. 52, pp. 183 - 189. 01/1989. ISSN 0166-1280
Type of production: Scientific paper **Format:** Journal



- 133** A LARGOCABRERIZO; C BARRIENTOS. A COMPARATIVE THEORETICAL-STUDY OF THE C₂N⁺ AND SiCN⁺ IONS AND THEIR FORMATION PROCESSES. CHEMICAL PHYSICS LETTERS. 148 - 1, pp. 79 - 85. 07/1988. ISSN 0009-2614
Type of production: Scientific paper **Format:** Journal
- 134** C BARRIENTOS; I MARTIN. OSCILLATOR STRENGTH DISTRIBUTION IN THE ALKALINE-EARTH ELEMENTS. CANADIAN JOURNAL OF PHYSICS. 66 - 1, pp. 29 - 33. 01/1988. ISSN 0008-4204
Type of production: Scientific paper **Format:** Journal
- 135** C BARRIENTOS; I MARTIN; J MAZON. CORE POLARIZATION EFFECTS IN ELECTRON TRANSITIONS - OSCILLATOR-STRENGTHS FOR THE NA ISOELECTRONIC SEQUENCE. JOURNAL DE CHIMIE PHYSIQUE ET DE PHYSICO-CHIMIE BIOLOGIQUE. 84 - 5, pp. 715 - 718. 05/1987. ISSN 0021-7689
Type of production: Scientific paper **Format:** Journal
- 136** C BARRIENTOS; I MARTIN. INTERACTION BETWEEN 2 RYDBERG SERIES IN THE ABSORPTION-SPECTRA OF CA, SR AND BA. JOURNAL DE CHIMIE PHYSIQUE ET DE PHYSICO-CHIMIE BIOLOGIQUE. 84 - 5, pp. 719 - 724. 05/1987. ISSN 0021-7689
Type of production: Scientific paper **Format:** Journal
- 137** C BARRIENTOS; I MARTIN. OSCILLATOR-STRENGTH DISTRIBUTION IN THE DISCRETE AND CONTINUOUS SPECTRA OF THE ALKALI ELEMENTS. CANADIAN JOURNAL OF PHYSICS. 65 - 4, pp. 435 - 437. 04/1987. ISSN 0008-4204
Type of production: Scientific paper **Format:** Journal
- 138** Carmen Barrientos; Inmaculada Martín. Photoionisation cross sections of one-valence electron atomic species through the Quantum defect Orbital Method. Anales de Química. 83, pp. 514 - 521. 1987.
Type of production: Scientific paper **Format:** Journal
- 139** I MARTIN; C BARRIENTOS. CORE-POLARIZATION EFFECTS IN THE ALKALI ATOMS - OSCILLATOR-STRENGTH CALCULATIONS. CANADIAN JOURNAL OF PHYSICS. 64 - 8, pp. 867 - 871. 08/1986. ISSN 0008-4204
Type of production: Scientific paper **Format:** Journal
- 140** C BARRIENTOS; I MARTIN. QUANTUM DEFECT ORBITAL CALCULATIONS ON THE ALKALINE-EARTH ELEMENTS - OSCILLATOR-STRENGTHS AND PHOTOIONIZATION CROSS-SECTIONS. CANADIAN JOURNAL OF PHYSICS. 63 - 11, pp. 1441 - 1445. 1985. ISSN 0008-4204
Type of production: Scientific paper **Format:** Journal
- 141** J.J. Novoa; A. Largo; C. Barrientos; E. Besalú. Computational Techniques: Computer Programming and Numerical Calculus. LIBRO: Theoretical and Computational Chemistry: Foundations, Methods and techniques, p. 279-384; (eds.: J. Andrés, J. Bertrán), Universidad Jaume I, Castellón, 2007 (. ISBN 978-84-8021-615-9)
- 142** A. Largo; E. Del Río; C. Barrientos. Interstellar Chemistry of Binary Phosphorus-Carbon Compounds. LIBRO: Electronic Structure: Predictions and Applications, p.111-150; (eds. A. Irigoras, J.M. Ugalde), Donostia ,1996 (. ISBN 84-8021-312-4)
- 143** J.J. Novoa y A. Largo. Técnicas Computacionales. LIBRO: Química Teórica y Computacional, p. 143-215; (eds.: J. Andrés, J. Bertrán), Universidad Jaume I, Castellón, 2000 (. ISBN 84-8021-312-4)

Works submitted to national or international conferences

- 1** **Title of the work:** Computer Simulations in Astrochemistry: Structure and Reactivity of Interstellar Molecules
Name of the conference: XXII CAFQI
Type of event: Conference
Type of participation: Participatory - Plenary session
Geographical area: Non EU International
Reasons for participation: Upon invitation
Corresponding author: Yes
City of event: La Plata, Argentina
Date of event: 19/04/2021
End date: 29/04/2021
Carmen Barrientos.
- 2** **Title of the work:** Structure and spectroscopic properties of imine and amine acetaldehyde: possible interstellar molecules
Name of the conference: The Physics and Chemistry of the Interstellar Medium. Celebrating the first 40 years of Alexander Tielens' contribution to Science. International
Type of event: Conference
Type of participation: 'Participatory - poster
Geographical area: Non EU International
Corresponding author: No
City of event: Avignon, France
Date of event: 02/09/2019
End date: 06/09/2019
Pilar Redondo; Miguel Sanz-Novo; Carmen Barrientos; Antonio Largo.
- 3** **Title of the work:** Hydrogenation of Isocyanic acid on Water Ice Surfaces: a Computational Approach
Name of the conference: Our Astro-Chemical History Past, Present, and Future. International
Type of event: Conference
Type of participation: 'Participatory - poster
Geographical area: Non EU International
Corresponding author: No
City of event: Assen, Holland
Date of event: 10/09/2018
End date: 14/09/2018
Pilar Redondo; Carmen Barrientos; Antonio Largo.
- 4** **Title of the work:** Complex Organic Molecules Formation through the Gas-Phase Reaction
Name of the conference: 11th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Type of event: Conference
Type of participation: 'Participatory - poster
Geographical area: Non EU International
Corresponding author: No
City of event: Toledo, Spain
Date of event: 17/07/2018
End date: 19/07/2014
Pilar Redondo; Henar Martínez; Antonio Largo; Carmen Barrientos.



- 5** **Title of the work:** Structural Trends in Monoboronyl Compounds
Name of the conference: 11th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Toledo, Spain
Date of event: 17/07/2018
End date: 19/07/2014
Carmen Barrientos; Pilar Redondo; Víctor M. Rayón; Antonio Largo.
- 6** **Title of the work:** Formation of Peptide Bond in Space through Gas-phase Reactions: Formamide and Acetamide
Name of the conference: WATOC-2014. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Santiago de Chile, Chile
Date of event: 05/10/2014
End date: 10/10/2014
P. Redondo; C. Barrientos; A. Largo.
- 7** **Title of the work:** Possible Ion-Molecule Reactions Leading to Interstellar Glycine
Name of the conference: WATOC-2014. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Santiago de Chile, Chile
Date of event: 05/10/2014
End date: 10/10/2014
A. Largo; Henar Martínez; P. Redondo; C. Barrientos.
- 8** **Title of the work:** Reactivity of Alkaline-Earth Monocations with Halomethane Molecules: A Computational Kinetic Study
Name of the conference: WATOC-2014. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Santiago de Chile, Chile
Date of event: 05/10/2014
End date: 10/10/2014
C. Barrientos; P. Redondo; A. Largo; Víctor M. Rayón; Germán Molpeceres; José A. Sordo.
- 9** **Title of the work:** Gas-Phase Reactions of Metal Monocations with CH₃X (X= Cl, Br): Mechanism for the C-X Bond Activation
Name of the conference: 9th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Badajoz, Spain
Date of event: 01/07/2014
End date: 04/07/2014

C. Barrientos; P. Redondo; A. Largo; Víctor M. Rayón; Germán Molpeceres; José A. Sordo.

- 10 Title of the work:** Molecular Structure of Plutonium Tricarbide: a Computational Study
Name of the conference: 9th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Badajoz, Spain
Date of event: 01/07/2014
End date: 04/07/2014
A. Largo; Germán Molpeceres; C. Barrientos; Víctor M. Rayón; P. Redondo.
- 11 Title of the work:** Structure and Spectroscopic Properties of Neutral and Cationic Tetratomic [C,H,N,Zn] Isomers: A Theoretical Study
Name of the conference: 9th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Badajoz, Spain
Date of event: 01/07/2014
End date: 04/07/2014
P. Redondo; C. Barrientos; A. Largo.
- 12 Title of the work:** Study of ion-molecule reactions leading to interstellar glycine
Name of the conference: 9th Congress on Electronic Structure: Principles and Applications. ESPA 2014. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Badajoz, Spain
Date of event: 01/07/2014
End date: 04/07/2014
Henar Martínez; A. Largo; P. Redondo; C. Barrientos.
- 13 Title of the work:** Reactivity of first-row transition metal monocations with methyl fluoride: a computational kinetic study
Name of the conference: The VIIIth Congress of the International Society of Theoretical Chemical Physics (ISTCP-VIII). Internacional
Geographical area: Non EU International
Type of participation: Participatory - poster
City of event: Budapest, Hungary
Date of event: 29/08/2013
End date: 31/08/2013
C. Barrientos; P. Redondo; V. M. Rayón; A. Largo; J. A. Sordo.
- 14 Title of the work:** Theoretical studies of possible routes for synthesis of amino acids in space
Name of the conference: The VIIIth Congress of the International Society of Theoretical Chemical Physics (ISTCP-VIII). Internacional
Geographical area: Non EU International
Type of participation: Participatory - poster
City of event: Budapest, Hungary
Date of event: 29/08/2013
End date: 31/08/2013



A. Largo; C. Barrientos; P. Redondo; H. Martínez.

- 15 Title of the work:** C-F Bond Activation by Main-Fourth-Period Mono-Cations(Ga⁺, Ge⁺, As⁺, and Se⁺)
Name of the conference: XXXIXth Congress of theoretical Chemists of Latin Expression QUITEL 2012. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Granada, Spain
Date of event: 01/07/2013
End date: 05/07/2013
P. Redondo; C. Barrientos; V. M. Rayón; A. Largo; J. A. Sordo.
- 16 Title of the work:** Peptide bond formation in the gas phase: on the mechanism of the reaction of protonated glycine with neutral glycine
Name of the conference: XXXIXth Congress of theoretical Chemists of Latin Expression QUITEL 2012. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Granada, Spain
Date of event: 01/07/2013
End date: 05/07/2013
H. Martínez; P. Redondo; A. Cimas; C. Barrientos; A. Largo.
- 17 Title of the work:** Small carbides of third-row main group elements: Structure and bonding
Name of the conference: Theoretical Chemistry in Spain told by women A symposium in Honour of Rosa Caballol. Internacional
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Tarragona, Spain
Date of event: 30/01/2013
End date: 31/01/2013
P. Redondo; E.F. Villanueva; V.M. Rayón; A. Largo; C.Barrientos.
- 18 Title of the work:** Exploration of Different Routes for the Formation of Formamide in Space
Name of the conference: XXVIIIth Congress of theoretical Chemists of Latin Expression QUITEL 2012. Internacional
Type of participation: 'Participatory - poster
City of event: Natal-RN,
Date of event: 02/12/2012
End date: 07/12/2012
P. Redondo; C. Barrientos; A. Largo. 02/2007.
- 19 Title of the work:** Peptide bond formation through gas-phase ion-molecule reactions: A Computational study
Name of the conference: XXVIIIth Congress of theoretical Chemists of Latin Expression QUITEL 2012. Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Natal-RN,
Date of event: 02/12/2012
End date: 07/12/2012
A. Largo; H. Martínez; A. Cimas; P. Redondo; C. Barrientos. 12/2012.



- 20** **Title of the work:** Structure and bonding in small carbides
Name of the conference: XXVIIIth Congress of theoretical Chemists of Latin Expression QUITEL 2012. Internacional
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Natal-RN,
Date of event: 02/12/2012
End date: 07/12/2012
C. Barrientos; P. Redondo; V.M. Rayón; E. Fernández; A. Largo.
- 21** **Title of the work:** Applications of Computational Chemistry in Astrochemistry: possible ion-molecule routes toward interstellar glycine
Name of the conference: Theory and Applications of Computational Chemistry TACC 2012. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Pavia, Italy
Date of event: 02/09/2012
End date: 07/09/2012
C. Barrientos; P. Redondo; A. Largo.
- 22** **Title of the work:** Searching for the Origin of Biomolecules in Space
Name of the conference: VIIIth Congress on Electronic Structure: Principles and Applications ESPA 2012. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Barcelona, Spain
Date of event: 26/06/2012
End date: 29/06/2012
P. Redondo; A. Largo; C. Barrientos.
- 23** **Title of the work:** Structure and bonding in third-row main group tricarbides
Name of the conference: VIIIth Congress on Electronic Structure: Principles and Applications ESPA 2012. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - poster
City of event: Barcelona, Spain
Date of event: 26/06/2012
End date: 29/06/2012
P. Redondo; E. Fernández; V.M. Rayón; A. Largo; C. Barrientos.
- 24** **Title of the work:** Gas phase reactions between fluoremethane and third-row monocations
Name of the conference: QUITEL 2011. Internacional.
Geographical area: Non EU International
Type of participation: Participatory - poster
City of event: Riviera Maya, Mexico
Date of event: 04/12/2011
End date: 09/12/2011
P. Redondo; C. Barrientos; V.M. Rayón; A. Largo; J.A. Sordo.



- 25** **Title of the work:** On the search for synthetic routes leading to interstellar glycine.
Name of the conference: QUITEL 2011. Internacional.
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Riviera Maya, Mexico
Date of event: 04/12/2011
End date: 09/11/2012
C. Barrientos; P. Redondo; L. Largo; V.M. Rayón; A. Largo.
- 26** **Title of the work:** Competitive kinetical study of the C-F bond activation in methyl fluoride by third-row cations in gas phase
Name of the conference: WATOC-2011. Internacional. The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Santiago de Compostela, Spain
Date of event: 17/07/2011
End date: 22/07/2011
P. Redondo; J.A. Sordo; C. Barrientos; V.M. Rayón; A. Largo.
- 27** **Title of the work:** Computational Astrochemistry: Ion-molecule processes in the synthesis of interstellar glycine.
Name of the conference: WATOC-2011. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Santiago de Compostela, Spain
Date of event: 17/07/2011
End date: 22/07/2011
A. Largo; P. Redondo; C. Barrientos; L. Largo; V.M. Rayón. 07/2011.
- 28** **Title of the work:** Neutral polycyanides of Transition metals
Name of the conference: WATOC-2011. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Santiago de Compostela, Spain
Date of event: 17/07/2011
End date: 22/07/2011
C. Barrientos; P. Redondo; V.M. Rayón; A. Largo.
- 29** **Title of the work:** Reactions of $\text{NH}_2\text{OH}^+/\text{NH}_3\text{OH}^+$ with acetic acid.
Name of the conference: WATOC-2011. Internacional The World Association of Theoretical and Computational Chemists (WATOC)
City of event: Santiago de Compostela, Spain
Date of event: 17/07/2011
End date: 22/07/2011
L. Largo; P. Redondo; V.M. Rayón; C. Barrientos; A. Largo. 07/2011.
- 30** **Title of the work:** Could the reactions of acetic acid with hydroxylamine-derived ions produce glycine precursors?
Name of the conference: The Molecular Universe (IAU SYMPOSIUM "280



Type of participation: 'Participatory - poster

City of event: Toledo, Spain

Date of event: 30/05/2011

P. Redondo; L. Largo; C. Barrientos; V.M. Rayón; A. Largo. 30/05/2003.

- 31 Title of the work:** C-F bond activation in methyl fluoride by alkaline-earth metal cations: analysis of the potential energy hypersurface and kinetics calculations

Name of the conference: 36ème CHITEL. Internacional.

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Anglet, France

Date of event: 29/07/2010

End date: 04/10/2010

P. Redondo; A. Varela; J. A. Sordo; C. Barrientos; V. M. Rayón; A. Largo. 2004.

- 32 Title of the work:** C-F bond activation by bare metal cations: kinetics and mechanism

Name of the conference: 7th Congress on Electronic Structure: Principles and Applications ESPA2010. Internacional.

Geographical area: Non EU International

Type of participation: Participatory - invited/keynote talk

City of event: Oviedo, Spain

Date of event: 29/06/2010

End date: 02/07/2010

V. M. Rayón; A. Largo; A. Varela. C. Barrientos; P. Redondo; J. A. Sordo.

- 33 Title of the work:** Reactions of formic acid with $\text{CH}_3\text{NH}_2^+/\text{CH}_3\text{NH}_3^+$: astrochemical implications

Name of the conference: 7th Congress on Electronic Structure: Principles and Applications ESPA2010. Internacional.

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Oviedo, Spain

Date of event: 29/06/2010

End date: 02/07/2010

P. Redondo; L. Largo; C. Barrientos; V. M. Rayón; A. Largo.

- 34 Title of the work:** Structure and bonding in third-row main group dicarbides C_2X ($\text{X}=\text{K}-\text{Br}$)

Name of the conference: 7th Congress on Electronic Structure: Principles and Applications ESPA2010. Internacional.

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Oviedo, Spain

Date of event: 29/06/2010

End date: 02/07/2010

C. Barrientos; V. M. Rayón; P. Redondo; A. Largo.

- 35 Title of the work:** Structure and stability of neutral cyanide complexes of iron

Name of the conference: 7th Congress on Electronic Structure: Principles and Applications ESPA2010. Internacional.

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Oviedo, Spain

Date of event: 29/06/2010

End date: 02/07/2010

A. Largo; V. M. Rayón; P. Redondo; C. Barrientos.

- 36 Title of the work:** Complejos de Ti(IV) con Ligandos CN-: Un Estudio Teórico
Name of the conference: XXXV Congreso Internacional de Químicos Teóricos de Expresión Latina-QUITEL09. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: San Andrés, Colombia
Date of event: 18/09/2009
End date: 22/09/2009
P. Redondo; V.M. Rayón; C. Barrientos; A. Largo.

- 37 Title of the work:** Estructura y propiedades de FeCn, FeCn⁺ y FeCn⁻ (n = 1-8)
Name of the conference: XXXV Congreso Internacional de Químicos Teóricos de Expresión Latina-QUITEL09. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: San Andrés, Colombia
Date of event: 18/09/2009
End date: 22/09/2009
L. Largo; C. Barrientos; P. Redondo.

- 38 Title of the work:** Estudio Teórico de Reacciones Ion-Molécula de Posible Relevancia en la Síntesis Interestelar de Glicina
Name of the conference: XXXV Congreso Internacional de Químicos Teóricos de Expresión Latina-QUITEL09. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: San Andrés, Colombia
Date of event: 18/09/2009
End date: 22/09/2009
A. Largo; P. Redondo; L. Largo; V.M. Rayón; C. Barrientos.

- 39 Title of the work:** Estudio termodinámico y cinético de la reacción entre fluorometano y el monocatión calcio
Name of the conference: XXXV Congreso Internacional de Químicos Teóricos de Expresión Latina-QUITEL09. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: San Andrés, Colombia
Date of event: 18/09/2009
End date: 22/09/2009
A. Varela-Álvarez; V.M. Rayón; P. Redondo; C. Barrientos; J.A. Sordo.

- 40 Title of the work:** Some Ion-Molecule Reactions Related to the Interstellar Formation of Glycine
Name of the conference: "13th ICQC". Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Helsinki, Finland



Date of event: 22/06/2009

End date: 26/06/2009

P. Redondo; L. Largo; V.M. Rayón; C. Barrientos; A. Largo. 06/2009.

41 Title of the work: Theoretical study of Neutral $Ti[CN]_n$ complexes

Name of the conference: "13th ICQC". Internacional

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Helsinki, Finland

Date of event: 22/06/2009

End date: 26/06/2009

C. Barrientos; V.M. Rayón; P. Redondo; H. Valdés; A. Largo. 06/2009.

42 Title of the work: Computational study of the reactivity of metal cations with methyl fluoride

Name of the conference: WATOC 2008. Eighth triennial Congress of the World Association of Theoretical and Computational Chemists. Internacional

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Sydney, Australia

Date of event: 14/09/2008

End date: 19/09/2008

C. Barrientos; A. Varela; V.M. Rayón; P. Redondo; L. Largo; A. Cimas; J.A. Sordo. 09/2008.

43 Title of the work: Cyanide vs. isocyanide competition in transition metal complexes

Name of the conference: WATOC 2008. Eighth triennial Congress of the World Association of Theoretical and Computational Chemists. Internacional

Geographical area: Non EU International

Type of participation: Participatory - oral communication

City of event: Sydney,

Date of event: 14/09/2008

End date: 19/09/2008

A. Largo; V.M. Rayón; H. Valdés; P. Redondo; C. Barrientos. 09/2008.

44 Title of the work: Small carbon clusters doped with first-row transition metals: structures and stabilities

Name of the conference: WATOC 2008. Eighth triennial Congress of the World Association of Theoretical and Computational Chemists. Internacional

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Sydney, Australia

Date of event: 14/09/2008

End date: 19/09/2008

P. Redondo; C. Barrientos; L. Largo; A. Largo. 09/2008.

45 Title of the work: A possible ion-molecule reaction leading to precursor of glycine in the interstellar medium

Name of the conference: 6th Congress on Electronic Structure: Principles and Applications: ESPA2008. Internacional

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Palma de Mallorca, Spain

Date of event: 02/09/2008

End date: 05/09/2008



L. Largo; P. Redondo; V.M. Rayón; C. Barrientos; A. Largo. 09/2008.

- 46 Title of the work:** Gas-phase reactivity of bare metal cations with CH₃F: the importance of formation of intermediates in chemical reactivity
Name of the conference: 6th Congress on Electronic Structure: Principles and Applications: ESPA2008. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Palma de Mallorca, Spain
Date of event: 02/09/2008
End date: 05/09/2008
C. Barrientos; A. Varela; V.M. Rayón; P. Redondo; L. Largo; A. Cimas; J.A. Sordo. 09/2008.

- 47 Title of the work:** Stability trends on small first-row transition metal carbides TMC_n (n = 1-8)
Name of the conference: 6th Congress on Electronic Structure: Principles and Applications: ESPA2008. Internacional
City of event: Palma de Mallorca, Spain
Date of event: 02/09/2008
End date: 05/09/2008
P. Redondo; C. Barrientos; L. Largo; A. Largo. 09/2008.

- 48 Title of the work:** Transition metal cyanide complexes: an ab initio study on the cyanide-isocyanide competition
Name of the conference: 6th Congress on Electronic Structure: Principles and Applications: ESPA2008. Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Palma de Mallorca, Spain
Date of event: 02/09/2008
End date: 05/09/2008
V.M. Rayón; P. Redondo; H. Valdés; C. Barrientos; A. Largo. 09/2008.

- 49 Title of the work:** Complejos de metales de transición con el ion cianuro: un análisis de la competencia cianuro isocianuro
Name of the conference: "CHITEL 08". Internacional
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Cetraro, Italy
Date of event: 03/07/2008
End date: 08/07/2008
A. Largo; V.M. Rayón; H. Valdés; P. Redondo; C. Barrientos. 07/2008.

- 50 Title of the work:** A systematic study of cyanides and isocyanides of first-row transition metals
Name of the conference: "ICCMSE 2007". Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Corfu, Greece
Date of event: 25/09/2007
End date: 30/09/2007
P. Redondo; V.M. Rayón; H. Valdés; C. Barrientos; A. Largo. 09/2007.



- 51 Title of the work:** Complexes of Fe+2 with CN- ligands: A theoretical Study of cyanide vs. isocyanide competition
Name of the conference: "ICCMSE 2007". Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Corfu, Greece
Date of event: 25/09/2007
End date: 30/09/2007
V.M. Rayón; H. Valdés; P. Redondo; C. Barrientos; A. Largo. 09/2007.
- 52 Title of the work:** Theoretical study of the reaction between NH₂⁺ and CH₃COOH
Name of the conference: "ICCMSE 2007". Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Corfu, Greece
Date of event: 25/09/2007
End date: 30/09/2007
L. Largo; P. Redondo; C. Barrientos; V. M. Rayón; A. Largo. 09/2007.
- 53 Title of the work:** Complejos de Fe+2 con ligandos CN-: Estudio teórico de la competencia entre la formación de cianuros e isocianuros
Name of the conference: "XXXIII QUITEL". Internacional
City of event: La Habana, Cuba
Date of event: 09/2007
V.M. Rayón; H. Valdés; P. Redondo; C. Barrientos; A. Largo. 09/2007.
- 54 Title of the work:** Estructura molecular, enlace y barreras de isomerización de cianuros e isocianuros de metales de transición
Name of the conference: "XXXIII QUITEL". Internacional
City of event: La Habana, Cuba
Date of event: 09/2007
A. Largo; P. Redondo; V.M. Rayón; H. Valdés; C. Barrientos. 09/2007.
- 55 Title of the work:** Estudio comparativo de la estructura y estabilidad en pequeños clusters de carbono monosustituidos por V y Co
Name of the conference: "XXXIII QUITEL". Internacional
City of event: La Habana, Cuba
Date of event: 09/2007
P. Redondo; C. Barrientos; A. Largo. 09/2007.
- 56 Title of the work:** Estudio teórico de la reacción entre el catión NH₂⁺ y el ácido acético
Name of the conference: "XXXIII QUITEL". Internacional
City of event: La Habana, Cuba
Date of event: 09/2007
L. Largo; P. Redondo; C. Barrientos; V.M. Rayón; A. Largo. 09/2007.
- 57 Title of the work:** Cyanides and isocyanides of first-row transition metals: molecular structure, bonding and isomerization barriers
Name of the conference: "Molecular Quantum Mechanics Conference - Analytic Gradients and Beyond". Internacional



City of event: Budapest, Hungary

Date of event: 06/2007

V.M. Rayón; P. Redondo; H. Valdés; C. Barrientos; A. Largo. 06/2007.

58 Title of the work: Molecular structure and stability of the first-row transition metal cyanides and isocyanides

Name of the conference: "Molecules in Space & Laboratory". Internacional

City of event: París, France

Date of event: 05/2007

P. Redondo; V.M. Rayón; H. Valdés; C. Barrientos; A. Largo. 05/2007.

59 Title of the work: Molecular structure and reactivity of small carbon radicals

Name of the conference: Electronic Structure: Principles and Applications (ESPA 2006)

Type of participation: Participatory - invited/keynote talk

City of event: Santiago de Compostela,

Date of event: 07/2006

A. Largo; C. Barrientos. 2021.

60 Title of the work: Structure and bonding in first-row transition metal dicarbide cations

Name of the conference: Electronic Structure: Principles and Applications (ESPA 2006)

City of event: Santiago de Compostela, Spain

Date of event: 07/2006

C. Barrientos; V.M. Rayón; P. Redondo; A. Largo. 07/2006.

61 Title of the work: Structure and stabilities of XC_2^+ and $X_2C_4^+$ ($X=Ti, V$) ions: A theoretical study

Name of the conference: Electronic Structure: Principles and Applications (ESPA 2006)

City of event: Santiago de Compostela, Spain

Date of event: 07/2006

P. Redondo; V.M. Rayón; C. Barrientos; A. Largo. 07/2006.

62 Title of the work: Structure and stability of TiC_n ($n=2-8$) clusters

Name of the conference: Electronic Structure: Principles and Applications (ESPA 2006)

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Santiago de Compostela, Spain

Date of event: 07/2006

L. Largo; A. Cimas; P. Redondo; V.M. Rayón; C. Barrientos; A. Largo. 07/2006.

63 Title of the work: The reaction of ground-state nitrogen atoms with bromomethyl radicals

Name of the conference: Electronic Structure: Principles and Applications (ESPA 2006)

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: Santiago de Compostela, Spain

Date of event: 07/2006

A. Cimas; M. Aschii; C. Barrientos; V.M. Rayón; J. A. Sordo; A. Largo. 07/2006.

64 Title of the work: Estudio teórico de la estructura y propiedades electrónicas de clusters lineales VC_n ($n=1-8$)

Name of the conference: "XXXI QUITEL". Internacional

City of event: Isla Margarita, Venezuela

Date of event: 10/2005

P. Redondo; C. Barrientos; A. Largo. 10/2005.



- 65** **Title of the work:** Molecular structure and bonding in first-row transition metal dicarbides
Name of the conference: "28th International Symposium on Free Radicals". Internacional
City of event: Leysin, Switzerland
Date of event: 09/2005
V.M. Rayón; P. Redondo; C. Barrientos; A. Largo. 09/2005.
- 66** **Title of the work:** Radical-radical reactions involving very high internal energies: a computational study of $N(2D)+CH_2F$
Name of the conference: "28th International Symposium on Free Radicals". Internacional
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Leysin, Switzerland
Date of event: 09/2005
A. Cimas; V.M. Rayón; M. Aschii; J. A. Sordo; C. Barrientos; A. Largo. 09/2005.
- 67** **Title of the work:** Estudio teórico de la competencia entre isómeros cíclicos y lineales en compuestos XC_2 ($X=Na-Cl$)
Name of the conference: "XXX QUITEL". Internacional
City of event: Oporto, Portugal
Date of event: 09/2004
P. Redondo; C. Barrientos; A. Largo. 09/2004.
- 68** **Title of the work:** On the competition between cyclic and linear isomers in second-row dicarbides
Name of the conference: "ESPA-2004". Internacional
City of event: Valladolid, Spain
Date of event: 09/2004
A. Largo; P. Redondo; C. Barrientos. 09/2004.
- 69** **Title of the work:** Small carbon clusters doped with early transition metals: a theoretical study of ScC_n ($n=1-8$) compounds
Name of the conference: "ESPA-2004". Internacional
City of event: Valladolid, Spain
Date of event: 09/2004
P. Redondo; C. Barrientos; A. Largo. 09/2004.
- 70** **Title of the work:** Structure and properties of open-chain and monocyclic calcium-doped carbon clusters CaC_n , CaC_n^+ , and CaC_n^- ($n=1-8$)
Name of the conference: "ESPA-2004". Internacional
City of event: Valladolid, Spain
Date of event: 09/2004
C. Barrientos; P. Redondo; A. Largo. 09/2004.
- 71** **Title of the work:** Theoretical investigation of the $N(4S, 2D) + CH_2X$ ($X=Cl, Br$) reactions: a comparative ab initio and DFT study
Name of the conference: "ESPA-2004". Internacional
City of event: Valladolid, Spain
Date of event: 09/2004
A. Cimas; V. M. Rayón; J. A. Sordo; C. Barrientos; A. Largo. 09/2004.



- 72** **Title of the work:** Theoretical study on the kinetics of the $N(4S)+CH_2F$ reaction
Name of the conference: "ESPA-2004". Internacional
City of event: Valladolid, Spain
Date of event: 09/2004
A. Cimas; M. Aschii; C. Barrientos; V. M. Rayón; J. A. Sordo; A. Largo. 09/2004.
- 73** **Title of the work:** "Compuestos binarios policarbonados de Calcio: un estudio teórico"
Name of the conference: "29ème Congrès International des Chimistes Théoriciens d'Expression Latine ". Internacional
City of event: Marrakech, Morocco
Date of event: 09/2003
P. Redondo; C. Barrientos; A. Largo. 09/2003.
- 74** **Title of the work:** "Theoretical studies of small carbon clusters doped with alkaline and alkaline-earth elements"
Name of the conference: "XIth International Congress of Quantum Chemistry 2003". Internacional
City of event: Bonn, Germany
Date of event: 07/2003
P. Redondo; C. Barrientos; A. Largo. 07/2003.
- 75** **Title of the work:** Estudio teórico de moléculas de interés en Astrofísica: Compuestos binarios policarbonados
Name of the conference: Primer Congreso Nacional de Astrofísica Molecular
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Ciudad Real,
Date of event: 07/2003
A. Largo; C. Barrientos; P. Redondo; A. Cimas. 07/2003.
- 76** **Title of the work:** Structure and synthesis of small heteroatom-doped carbon clusters. A theoretical study
Name of the conference: XIX Reunió de la Xarxa de Química Teórica.
Type of participation: Participatory - invited/keynote talk
City of event: Gerona,
Date of event: 07/2003
A. Largo; C. Barrientos; P. Redondo; A. Cimas. 07/2003.
- 77** **Title of the work:** "DFT study of small Magnesium-doped carbon clusters"
Name of the conference: "ESPA2002. Electronic Structure: Principles and Applications". Internacional
City of event: Sevilla, Spain
Date of event: 09/2002
P. Redondo; C. Barrientos; A. Largo. 09/2002.
- 78** **Title of the work:** "Theoretical study of AlC_n , AlC_n^+ and AlC_n^- ($n=1-7$) clusters. Open-chain and monocyclic structures"
Name of the conference: "Fourth European Conference on Computational Chemistry (EUCC-4)". Internacional
City of event: Assisi, Italy
Date of event: 09/2002
P. Redondo; C. Barrientos; A. Largo. 09/2002.



- 79** **Title of the work:** "Theoretical study of the reaction of HCl with C₃H₂⁺: A possible source of carbon-chlorine compounds in space"
Name of the conference: "ESPA2002. Electronic Structure: Principles and Applications". Internacional
City of event: Sevilla, Spain
Date of event: 09/2002
P. Redondo; J.R. Redondo; A. Largo. 09/2002.
- 80** **Title of the work:** "Ionization and protonation of NaC₃: a theoretical study"
Name of the conference: "6th World Congress of Theoretically Oriented Chemists (WATOC02)". Internacional
City of event: Lugano, Switzerland
Date of event: 08/2002
P. Redondo; C. Barrientos; A. Largo. 08/2002.
- 81** **Title of the work:** "Etapas prohibidas por el espín en procesos globalmente permitidos por el espín. Aplicaciones en Química Interestelar"
Name of the conference: "27ème Congrès des Chimistes Théoriciens d'Expression Latine". Internacional
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Toulouse, France
Date of event: 09/2001
A. Largo; M. Aschi; C. Barrientos; P. Redondo. 09/2001.
- 82** **Title of the work:** "Procesos ion-molécula para la formación de compuestos cloro-carbonados"
Name of the conference: "27ème Congrès des Chimistes Théoriciens d'Expression Latine". Internacional
City of event: Toulouse, France
Date of event: 09/2001
J.R. Redondo; P. Redondo; C. Barrientos; A. Largo. 09/2001.
- 83** **Title of the work:** "The role of spin-forbidden steps in globally spin-allowed processes. The S⁺ + C₂H₂ reaction as a test case"
Name of the conference: "Electronic Structure and Chemical Reactivity. An International Symposium in Honor of Prof. Juan Bertran". Internacional
City of event: Bellaterra, Spain
Date of event: 09/2001
A. Largo; M. Aschi; C. Barrientos; P. Redondo. 09/2001.
- 84** **Title of the work:** Estudio comparativo ab initio y DFT de la reacción N(4S) + CH₂F"
Name of the conference: "27ème Congrès des Chimistes Théoriciens d'Expression Latine". Internacional
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Toulouse, France
Date of event: 09/2001
A. Cimas; C. Barrientos; A. Largo; B. Menéndez; J. A. Sordo. 09/2001.
- 85** **Title of the work:** "Theoretical study of C_nCl, C_nCl⁺, C_nCl⁻ (n=1-7) Clusters"
Name of the conference: "Electronic Structure: Prediction and Applications"
City of event: San Sebastián, Spain
Date of event: 10/2000



A. Cimas; P. Redondo; C. Barrientos; A. Largo. 10/2000.

- 86 Title of the work:** "Theoretical study of MgC3 and its cationic and protonated derivatives"
Name of the conference: "Electronic Structure: Prediction and Applications". Internacional
City of event: San Sebastián, Spain
Date of event: 10/2000
P. Redondo; C. Barrientos; A. Largo. 10/2000.
- 87 Title of the work:** "Theoretical study of CnCl, CnCl+, CnCl- (n=1-7) Clusters"
Name of the conference: "Third European Conference on Computational Chemistry, EUCCO-CC3". Internacional
City of event: Budapest, Hungary
Date of event: 09/2000
A. Cimas; P. Redondo; C. Barrientos; A. Largo. 09/2000.
- 88 Title of the work:** "Experiencias del laboratorio de Química con apoyo audiovisual e informático"
Name of the conference: "III Congreso Internacional de Formación y Medios Audiovisuales". Internacional
City of event: Valladolid, Spain
Date of event: 07/2000
M.J. Insausti; P. Redondo; E. Charro. 07/2000.
- 89 Title of the work:** "Theoretical study of Aluminum-Carbon compounds: structure and synthesis of AlC3"
Name of the conference: "Xth International Congress of Quantum Chemistry". Internacional
City of event: Menton, France
Date of event: 06/2000
F. García; P. Redondo; C. Barrientos; A. Largo. 06/2000.
- 90 Title of the work:** "Estudio teórico de la reacción S+ + C3H2"
Name of the conference: "XXV Congreso Internazionale dei Chimici Teorici di Espressione Latina"
City of event: Nápoles, Italy
Date of event: 09/1999
P. Redondo; E. Calleja; C. Barrientos; A. Largo. 09/1999.
- 91 Title of the work:** "Procesos ion-molécula en la formación de cianopoliacetilenos: estudio teórico de la reacción C2H2+ + CN"
Name of the conference: "XXV Congreso Internazionale dei Chimici Teorici di Espressione Latina". Internacional
City of event: Napoles, Italy
Date of event: 09/1999
P. Redondo; R. Boronat; C. Barrientos; A. Largo. 1999.
- 92 Title of the work:** "Theoretical studies of interstellar molecules: structure and synthesis"
Name of the conference: "Workshop on Computational Chemistry". Internacional
City of event: Miraflores de la Sierra, Spain
Date of event: 06/1998
C. Barrientos; P. Redondo; A. Largo. 06/1998.
- 93 Title of the work:** "Theoretical studies of possible processes for the interstellar production of silicon-carbon compounds"
Name of the conference: "Second European Conference on Computational Chemistry". Internacional
City of event: Lisboa, Portugal



Date of event: 1997

P. Redondo; A. Sagüillo; C. Barrientos; A. Largo. 1997.

- 94** **Title of the work:** Síntesis de compuestos clorocarbonados en el medio interestelar"
Name of the conference: "XXIII Congreso de Químicos Teóricos de Expresión Latina". Internacional
Geographical area: Non EU International
Type of participation: Participatory - oral communication
City of event: Cáceres, Spain
Date of event: 09/1996
V. M. Rayón; C. Barrientos; A. Largo. 1999.

- 95** **Title of the work:** Theoretical study of the C2P radical
Name of the conference: 22nd International Symposium on Free Radicals. Internacional
Type of participation: Participatory - oral communication
City of event: Doorwerth, Holland
Date of event: 09/1993
A. Largo; C. Barrientos; X. López; J.M. Ugalde. 09/1993.

- 96** **Title of the work:** "Reactions of CH₃⁺ with free second-row atoms: an ab initio study
Name of the conference: IAU Colloquium146: Molecular Opacities in the Stellar Environment
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Copenhagen, Denmark
Date of event: 1993
J. R. Flores; A. Largo; C. Barrientos.

- 97** **Title of the work:** "Theoretical study of the C2P radical"
Name of the conference: 22nd International Symposium on Free Radicals
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Doorwerth, Holland
Date of event: 1993
A. Largo; C. Barrientos; X. López; J. M. Ugalde.

- 98** **Title of the work:** "Relativistic Quantum Defect Orbital study of electron transitions in highly ionized atomic systems
Name of the conference: Sanibel Symposia
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Gainesville, Florida, United States of America
Date of event: 1992
I. Martín; C. Lavín; C. Barrientos.

- 99** **Title of the work:** Relativistic Quantum defect calculations of transition probabilities from excited levels"
Name of the conference: 7th International Congress of Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Menton, France
Date of event: 1991
C. Lavín; C. Barrientos; I. Martín.



- 100** **Title of the work:** "A basic process of interstellar chemistry: $C^+ + HCl \rightarrow CCl^+ + H$
Name of the conference: 7th International Congress of Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Menton, France
Date of event: 1991
A. Largo; C. Barrientos; F. Pauzat; Ellinger.
- 101** **Title of the work:** "Systematic trends of oscillator strengths for $n=0$ transitions in the Cu isoelectronic sequence
Name of the conference: 7th International Congress of Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Menton, France
Date of event: 1991
C. Barrientos; C. Lavín; I. Martín.
- 102** **Title of the work:** "Theoretical studies of the interstellar chemistry of sulfur compounds. The C_2S radical.
Name of the conference: 7th International Congress of Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Menton, France
Date of event: 1991
A. Largo; C. Barrientos.
- 103** **Title of the work:** " Estudio teórico de transiciones electrónicas en átomos con dos electrones de valencia"
Name of the conference: XII Reunión Bienal de la Real Sociedad Española de Física
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Palma de Mallorca, Spain
Date of event: 1989
I. Martín; C. Barrientos.
- 104** **Title of the work:** "Regularities in transitions involving levels of the principal spectral series of Potassium-like systems"
Name of the conference: Third European Conference on Atomic and Molecular Physics
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Burdeos, France
Date of event: 1989
C. Lavín; C. Barrientos; I. Martín.
- 105** **Title of the work:** Influencia de la polarización del core atómico por el electrón activo en las transiciones electrónicas"
Name of the conference: XII Reunión Bienal de la Real Sociedad Española de Física
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Palma de Mallorca, Spain
Date of event: 1989
C. Lavín; I. Martín; C. Barrientos.



- 106 Title of the work:** Systematic trends of oscillator strengths involving subordinate series"
Name of the conference: Third European Conference on Atomic and Molecular Physics
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Burdeos, France
Date of event: 1989
C. Barrientos; I. Martín.
- 107 Title of the work:** An ab initio study of the formation processes of C₂N⁺ and SiCN⁺"
Name of the conference: NATO Advanced Study Institute on New Theoretical Concepts for Understanding Organic Reactions
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: San Feliú de Guixols, Spain
Date of event: 1988
C. Barrientos; A. Largo.
- 108 Title of the work:** Regularities in transition probabilities from excited states: sharp series in the Potassium isoelectronic sequence"
Name of the conference: Workshop on Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Girona, Spain
Date of event: 1988
C. Lavín; I. Martín; C. Barrientos.
- 109 Title of the work:** Trends of oscillator strengths in the lithium isoelectronic sequence"
Name of the conference: Sixth International Congress on Quantum Chemistry
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Jerusalem, Israel
Date of event: 1988
C. Barrientos; I. Martín; I. Charro.
- 110 Title of the work:** "Fractal Orbitals"
Name of the conference: 20th Quantum Theory Conference
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Edimburgo, United Kingdom
Date of event: 1987
C. Barrientos; L. L. Boyle.
- 111 Title of the work:** Fuerzas de oscilador para Mg y su serie isoelectrónica"
Name of the conference: XVII Congreso de Químicos Teóricos de Expresión Latina
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Peñíscola, Spain
Date of event: 1987
I. Martín; I. Gútiez; C. Barrientos.



- 112** **Title of the work:** Tendencias sistemáticas en series isoelectrónicas. Cálculos relativos a la serie del potasio"
Name of the conference: XVII Congreso de Químicos Teóricos de Expresión Latina
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Peñíscola, Spain
Date of event: 1987
C. Lavín; I. Martín; C. Barrientos.
- 113** **Title of the work:** Transiciones electrónicas desde estados excitados. Regularidades en átomos análogos"
Name of the conference: XVII Congreso de Químicos Teóricos de Expresión Latina
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Peñíscola, Spain
Date of event: 1987
C. Barrientos; I. Martín.
- 114** **Title of the work:** "Aplicación de los orbitales de Defecto Cuántico al estudio teórico del espectro de absorción de los elementos alcalinotérreos"
Name of the conference: XVIe Congrès des Chimistes theoriciciens d'expression Latine
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Lyon, France
Date of event: 1986
C. Barrientos; I. Martín.
- 115** **Title of the work:** "Efectos de la polarización del core atómico en las transiciones electrónicas: fuerzas de oscilador de la serie isoelectrónica del sodio
Name of the conference: XVIe Congrès des Chimistes theoriciciens d'expression Latine
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Lyon, France
Date of event: 1986
C. Barrientos; I. Martín; J. Mazón.

Other dissemination activities

Title of the work: Colaboración en Revista de divulgación científica
Name of the event: ALKAID
Reasons for participation: Upon invitation
Date of event: 2008
"Química Interestelar". 1, pp. 16 - 21. (Spain): Alkaid Ediciones, ISSN 1888-8860

R&D management and participation in scientific committees

Scientific, technical and/or assessment committees

Committee title: Nobel Committee for Chemistry (Royal Swedish Academy of Sciences)
Primary (UNESCO code): 230000 - Chemistry
City affiliation entity: Sweden

Organization of R&D activities

Title of the activity: International Conference on Electronic Structure : Principles and Applications (ESPA-2004)
Type of activity: Organización de Congreso
Geographical area: Non EU International
City convening entity: Valladolid, Spain
Type of participation: Organiser
Start-End date: 15/09/2004 - 17/09/2004

R&D management

- 1** **Name of the activity:** IP del Proyecto: Simulaciones Computacionales en Astroquímica: Propiedades Espectroscópicas y Reactividad de Moléculas Interestelares - PID2020-117742GB-I00
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal y Gestión del Proyecto
Entity: Universidad de Valladolid
Type of entity: University
Start date: 01/09/2021
Duration: 4 years
Average annual budget: 10
Nº of people: 7
Geographical area: Regional
- 2** **Name of the activity:** IP del Proyecto: Laser Abaltion Spectroscopic Techniques: from buiding blocks and sweeteners to interstellar molecules VA244P20
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal y Gestión del Proyecto
Entity: Universidad de Valladolid
Type of entity: University
Start date: 01/09/2020
Duration: 4 years
Average annual budget: 10
Nº of people: 7
Geographical area: Regional
- 3** **Name of the activity:** Investigadora del Proyecto: Astroquímica computacional: formación de moléculas prebióticas - AYA2017-87515-P
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora
Entity: Universidad de Valladolid
Type of entity: University
Start date: 01/09/2018
Duration: 3 years
Average annual budget: 10
Nº of people: 7
Geographical area: Regional



- 4** **Name of the activity:** IP del Proyecto: Astroquímica computacional: formación de moléculas prebióticas y predicción de parámetros espectroscópicos - VA010G18
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal y Gestión del Proyecto
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 01/09/2018 **Duration:** 3 years
Average annual budget: 10 **Nº of people:** 7
Geographical area: Regional
- 5** **Name of the activity:** IP del Proyecto: Procesos ion-molécula en fase gas: síntesis interestelar de biomoléculas y reactividad de derivados halocarbonados
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto total
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 03/09/2013 **Duration:** 3 years
Average annual budget: 10 **Nº of people:** 7
Geographical area: Regional
- 6** **Name of the activity:** IP del Proyecto: Estudio mecano-cuántico y cinético de sistemas y procesos ion-molécula de
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto total
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 01/01/2011 **Duration:** 3 years - 6 months
Average annual budget: 25
- 7** **Name of the activity:** IP del Proyecto: Reacciones ion-molécula en fase gas. Implicaciones en Química sintética y
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto total
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 01/01/2009 **Duration:** 3 years
Average annual budget: 15
- 8** **Name of the activity:** IP del Proyecto: Reactividad en fase gas de cationes metálicos con CH₃X (X=H,F,Cl). La
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 13/12/2007 **Duration:** 3 years
Average annual budget: 25
- 9** **Name of the activity:** IP del Proyecto: Estudio de la estructura y síntesis de compuestos de interés en química
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto total
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 01/01/2006 **Duration:** 3 years
Average annual budget: 5



- 10** **Name of the activity:** IP del Proyecto: Estructura y procesos de síntesis de compuestos policarbonados: estudio teórico (VA085/03)
Type of management: Management of R&D&I actions and projects
Performed tasks: Investigadora Principal, Gestora y Coordinadora del Proyecto total
Entity: Universidad de Valladolid **Type of entity:** University
Start date: 01/01/2003 **Duration:** 3 years
Average annual budget: 15

Evaluation and revision of R&D projects and articles

- 1** **Performed tasks:** Evaluador de Proyectos de Investigación
Entity where activity was carried out: Barcelona Supercomputing Center- Red Española de Supercomputación
City of entity: Spain
Start date: 01/05/2021
- 2** **Performed tasks:** Evaluador de Proyectos de Investigación
Entity where activity was carried out: Ministerio de Educación y Ciencia (Ministerio de Ciencia y Tecnología, etc.)
City of entity: Spain
Start date: 2010
- 3** **Performed tasks:** Evaluador de Proyectos de Investigación
Entity where activity was carried out: Ministerio de Educación y Ciencia (Ministerio de Ciencia y Tecnología, etc.)
City of entity: Spain
Start date: 2009
- 4** **Performed tasks:** Evaluador de Proyectos de Investigación
Entity where activity was carried out: Ministerio de Educación y Ciencia (Ministerio de Ciencia y Tecnología, etc.)
City of entity: Spain
Start date: 2008
- 5** **Performed tasks:** Evaluador de Proyectos de Investigación
Entity where activity was carried out: Ministerio de Educación y Ciencia (Ministerio de Ciencia y Tecnología, etc.)
City of entity: Spain
Start date: 1997



Other achievements

Stays in public or private R&D centres

- 1** **Entity:** Università di L'Aquila **Type of entity:** University
Faculty, institute or centre: Dipartimento di Chimica e Materiali
City of entity: L'Aquila, Italy
Start-End date: 26/03/2005 - 31/03/2005 **Duration:** 6 days
Goals of the stay: Guest
Provable tasks: Acción Integrada Hispano-Italiana HI2002-0025
- 2** **Entity:** Ecole Normale Supérieure **Type of entity:** University
Faculty, institute or centre: Laboratorio de Radioastronomía
City of entity: París, France
Start-End date: 11/07/1992 - 24/07/1992 **Duration:** 14 days
Goals of the stay: Guest
Provable tasks: Acción Integrada Hispano-Francesa HF-304
- 3** **Entity:** Ecole Normale Supérieure **Type of entity:** University
Faculty, institute or centre: Laboratorio de Radioastronomía
City of entity: París, France
Start-End date: 10/12/1990 - 20/12/1990 **Duration:** 13 days
Goals of the stay: Guest
Provable tasks: Acción Integrada Hispano-Francesa HF-316
- 4** **Entity:** Ecole Normale Supérieure **Type of entity:** University
Faculty, institute or centre: Laboratorio de Radioastronomía
City of entity: París, France
Start-End date: 15/07/1990 - 30/07/1990 **Duration:** 15 days
Goals of the stay: Guest
Provable tasks: Acción Integrada Hispano-Francesa HF-236
- 5** **Entity:** University of Kent **Type of entity:** University
City of entity: Canterbury, United Kingdom
Start-End date: 01/01/1987 - 31/12/1987 **Duration:** 1 year
Goals of the stay: Post-doctoral

Obtained grants and scholarships

Name of the grant: Beca Postdoctoral del CSIC
Aims: Post-doctoral
Awarding entity: Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
Conferral date: 01/01/1987 **Duration:** 1 year
End date: 31/12/1987
Entity where activity was carried out: University of Kent, Canterbury (UK)

Prizes, mentions and distinctions

Description: Premio Extraordinario de Doctorado

Awarding entity: Universidad de Valladolid

Type of entity: University

City awarding entity: Valladolid, Castile and León, Spain

Conferral date: 01/09/1986

Periods of research activity

1 Nº of recognized periods: 6

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora (CNEAI) **Type of entity:** State agency

Date of recognition: 31/12/2020

2 Nº of recognized periods: 5

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora **Type of entity:** State agency

Date of recognition: 31/12/2014

3 Nº of recognized periods: 4

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora **Type of entity:** State agency

Date of recognition: 31/12/2008

4 Nº of recognized periods: 3

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora **Type of entity:** State agency

Date of recognition: 31/12/2002

5 Nº of recognized periods: 2

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora **Type of entity:** State agency

Date of recognition: 31/12/1996

6 Nº of recognized periods: 1

Certifying entity: Comisión Nacional Evaluadora de la Actividad Investigadora **Type of entity:** State agency

Date of recognition: 31/12/1990

Obtained accreditations/recognitions

1 **Description:** Evaluación excelente Programa Docencia

Accrediting entity: Universidad de Valladolid

Date of recognition: 04/02/2013

2 **Description:** Evaluación positiva de seis tramos docentes (quinquennios)

Accrediting entity: Universidad de Valladolid

Type of entity: University

Date of recognition: 2013



Summary of other achievements

- 1** **Description of the achievement:** Miembro del Claustro de la Universidad de Valladolid. Elegida en representación del colectivo de Catedráticos de Universidad.
Accrediting entity: Universidad de Valladolid **Type of entity:** University
Conferral date: 01/05/2018
- 2** **Description of the achievement:** Miembro de la Comisión de Reclamaciones de la Universidad de Valladolid
Accrediting entity: Universidad de Valladolid **Type of entity:** University
Conferral date: 01/06/2016
- 3** **Description of the achievement:** Miembro del Claustro de la Universidad de Valladolid. Elegida en representación del colectivo de Profesores Titulares de Universidad.
Accrediting entity: Universidad de Valladolid **Type of entity:** University
Conferral date: 01/10/2010
- 4** **Description of the achievement:** Secretaria del Departamento de Química Física. Universidad de Valladolid.
Accrediting entity: Universidad de Valladolid **Type of entity:** University
Conferral date: 03/03/1997