CURRICULUM VITAE ABREVIADO (CVA)

***IMPORTANT** – The Curriculum Vitae **cannot exceed 4 pages**. Instructions to fill this document are available in the website.*

Part A. PERSONAL INFORMATION

First name	Antonio			
Family name	Fernandez Ramos			
Gender	Male	Birth date		-----
Social Security, Passport, ID number		----		
e-mail:	----	URL:https://www.usc.es/ciqus/es/grupos/fernandez-ramos		
ORCID	0000-0002-6468-1592			
Scopus	A-5690-2008			
Google Scholar	https://scholar.google.es/citations?user=zXPf7uUAAAAJ&hl=es			

A.1. Current position

Position	Full profesor		
Initial date	April 2023		
Institution	Universidade de Santiago de Compostela		
Department/Center	Physical Chemistry	Centro singular de investigación en química biológica y materiales moleculares (CIQUS)	
Country	Spain	Teleph. number	
Keywords	Chemical reaction dynamics, instanton theory, variational transition state theory, tunneling effect, proton transfer reactions, combustion reactions, automated computational methods, astrochemistry		

A.2. Previous positions (research activity interuptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
Dec. 2007- Mar 2023	Associate profesor/Univ. de Santiago de Compostela
Oct. 2006 - Dec. 2007	Assistant profesor/Univ. de Santiago de Compostela
Nov. 2001 – Sep. 2006	Ramón y Cajal/ Univ. de Santiago de Compostela
Jan. 2001 – Oct. 2001	Posdoctoral fellow FCT/ Univ. Coimbra/Portugal
Sep. 1998 – Dec. 2000	Posdoctoral fellow National Research Council/ Steacie Institute for Molecular Sciences/Ottawa/Canada

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
PhD	U. de Santiago de Compostela	1998
Licensed	U. de Santiago de Compostela	1993

Part B. CV SUMMARY *(max. 5000 characters, including spaces)*

Antonio Fernández Ramos (AFR) earned his PhD in Chemistry from the University of Santiago de Compostela (USC) in 1998, under the supervision of Miguel A. Ríos and Jesús Rodríguez Otero. From 1998 until the end of 2000, he served as a Visiting Fellow at the National Research Council of Canada (NRCC) in Ottawa, collaborating with Zorka Smedarchina, Willem Siebrand, and Marek Zgierki. During this time, he contributed to the development of an approximate method for simulating multidimensional proton transfer reactions at low temperatures. This semiclassical method, known as the Approximated Instanton Method (AIM), enables accurate calculations of tunneling splittings and thermal rate constants in low-temperature environments. The AIM methodology has since been integrated into the DOIT (Dynamics of Instanton Tunneling) program (JCC2001). In addition to these studies, AFR pioneered the incorporation of explicit and implicit solvation to accurately explain the zwitterion-to-neutral conversion in glycine (JCP2000).

In 2001, he received a scholarship from the Fundação para a Ciência e a Tecnologia of the Portuguese government to work at the Universidade de Coimbra under the supervision of Antonio Varandas. Later that year, he was awarded a Ramón y Cajal contract and joined the Group of Theoretical and Computational Chemistry at USC. By 2006, he became an Assistant Professor at USC and successfully passed the National Habilitation in Physical Chemistry. From December 2007 until April 2023, he served as an Associate Professor. In 2003, he received the Prize from the Royal Spanish Society of Chemistry for Young Researchers. AFR has supervised two PhD theses: Rubén Meana-Pañeda in 2011 [staff scientist at the National Institutes of Health (USA)] and Luis Simon-Carballido in 2017 (high-school teacher)

Currently, AFR holds the position of Full Professor at USC. Since 2014, he has been the Principal Investigator for two Central Government projects and is the author of 105 scientific articles, five book chapters, and two review articles on bimolecular reactions and variational transition state theory (VTST), respectively. He has been cited more than 5600 times and his current h-index is 39 (source: Google Scholar).

Throughout his research career, AFR has focused on chemical reaction dynamics, particularly proton transfer reactions, and is an expert in the VTST and instanton methodologies. From 2001 to 2018, he collaborated closely with researchers at the NRCC, where they developed a new method for hydrogen transfer reactions called the 'Rainbow' Instanton Model (JCP2012) and a innovative multidimensional Hamiltonian with mass dependence on the coordinate (PRE2014).

In collaboration with Donald Truhlar at the University of Minnesota, AFR has explored various approaches that incorporate quantum effects within the VTST framework, creating the large curvature tunneling method (JCP2001) and the least-action path (JCTC2010) for polyatomics, implemented in different versions of the POLYRATE program (CPC2024). This collaboration also led to the release of a new software program on VTST called Pilgrim in 2020 (CPC2020). AFR also contributed to the developed of a novel application of VTST that spans from ultra-low (interstellar) to very high (combustion) temperatures (JACS2018) and investigates the accuracy of complete basis set extrapolation (JPCA2024).

More recently, he has spent the last seven years developing methods and designing software to simulate complex reactions. Recent contributions include: (i) extending VTST to systems with high conformational flexibility (JACS2012, JPCA2018), (ii) applying VTST to simulate reactions at ultra-low temperatures (PCCP2020) and in combustion (PCCP2022), (iii) developing a new method that incorporates anharmonic effects due to internal rotations (JCP2013, JCTC2017), and implementing VTST for heterogeneous catalysis (JPCC2024) and large systems using QM/MM (JCIM2024). Additionally, he has employed computational automated methods to discover new reaction pathways in the interstellar medium (SciAdv2024). A notable collaboration with Elena Jimenez from the University of Castilla-La Mancha has successfully combined theory and experiment to study bimolecular reactions involving the OH radical (PCCP2022, PCCP2024).

In relation to conformational analysis in combustion reactions involving biofuels, two new software programs from his research group, Q2DTor (CPC2018) and Torsiflex (JCheminfor2021), focus on evaluating accurate thermochemical functions and searching for all torsional conformers in flexible molecules, respectively. These tools are part of a long-term project called the Cathedral Package aimed at integrating various computational programs to simulate complex reaction networks without relying on external software. His current scientific interests center on the development of methods and software for chemical reaction dynamics, with applications in astrochemistry and combustion.

Part C. RELEVANT MERITS *(sorted by typology)*

C.1. Publications (10 contributions related to the proposal)

1. M. Castiñeira-Reis(*), E. Martínez-Núñez, **A. Fernández-Ramos(*)**. Comprehensive computational automated search of barrierless reactions leading to the formation of benzene and other C_6-membered rings. Science Advances, 10, eadq4077 (2024).

Brief overview: computational study that employs automated methods to discover possible reaction pathways for the formation of benzene and benzyne in the interstellar medium.

2. A. M. Parameswaran, A**. Fernández-Ramos**, D. G. Truhlar(*). Evaluating cost and accuracy in two-point complete basis set extrapolation schemes using diffuse basis sets. The Journal of Physical Chemistry A, 128, 10673 (2024).
Brief overview: A method to perform a complete basis set extrapolation to obtain very accurate energies at a reasonable computational cost.
3. D. González, A. Canosa, E. Martínez-Núñez, **A. Fernández-Ramos(*)**, B. Ballesteros, M. Agúndez, J. Cernicharo, E. Jiménez(*). Effect of temperature on the gas-phase reaction of CH_3CN with OH radicals: experimental (T=11.7-177.5 K) and computational (T=10-400 K) kinetic study. Physical Chemistry Chemical Physics, 26, 3632 (2024).
Brief overview: a combined experimental/computational study for a bimolecular reaction at ultra-low temperatures.
4. L. Guerrero-Méndez, A. Lema-Saavedra, E. Jiménez, **A. Fernández-Ramos(*)**, E. Martínez-Núñez(*). Gas-phase formation of glycolonitrile in the interstellar medium. Physical Chemistry Chemical Physics, 25, 20988 (2023).
Brief overview: Computational simulation about the formation of glycolonitrile in the interstellar medium.
5. D. Ferro-Costas(*), I. Mosquera-Lois, **A. Fernández-Ramos(*)**. Torsiflex: and automatic generator of torsional conformers. Application to the twenty proteogenic amino acids. Journal of Cheminformatics, 13:100 (2021).
Brief overview: This program based on a novel algorithm allows obtaining all torsional conformers of a flexible molecule.
6. D. Ferro-Costas, D. G. Truhlar, **A. Fernández-Ramos(*)**. Pilgrim: A thermal rate constant calculator and a chemical kinetics generator. Computer Physics Communications, 256, 107457 (2020).
Brief overview: Program that employs variational transition state theory to evaluate elementary thermal rate constants and kinetic Monte Carlo dynamics to simulate reaction mechanisms.
7. I. Mosquera-Lois, D. Ferro-Costas, **A. Fernández-Ramos(*)**. Chemical reactivity from the vibrational ground-state level. The role of the tunneling path in the tautomerization of urea and derivatives. Physical Chemistry Chemical Physics, 22, 24951 (2020).
Brief overview: theoretical study of a chemical reaction at ultra-low temperatures.
8. L. G. Gao, J. Zheng, **A. Fernández-Ramos**, D. G. Truhlar(*), X. Xu(*). Kinetics of the methanol reaction with the OH at interstellar, atmospheric and combustion temperatures. Journal of the American Chemical Society, 140, 2906 (2018).
Brief overview: In this application we have used a modification of variational transition state theory called competitive canonical unified statistical theory that allows to calculate thermal rate constants in a wide range of temperatures and in the limit of low and high pressures.
9. L. Simón-Carballido, J. L. Bao, T. V. Alves, R. Meana-Pañeda, D. G. Truhlar(*), A. **Fernández-Ramos(*)**. Anharmonicity of coupled torsions: the extended two-dimensional torsion method and its use to assess more approximate methods. Journal of Chemical Theory and Computation, 13, 3478 (2017).
Brief overview: We have developed a new method called Extended Two-Dimensional Torsions (E2DT) that allows an accurate treatment of partition functions and thermodynamical properties in systems presenting two hindered rotors. This method has been implemented in the Q2DTor program.
10. Z. Smedarchina, W. Siebrand, E. Martínez-Núñez(*), **A. Fernández-Ramos(*)**. Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature. Phys. Chem. Chem. Phys. 18, 22712 (2016).
Brief overview: In this applicaion we explain the pressure dependence of the OH + methanol reaction and the implications for this process to occur in the interstellar medium.

C.2. Congress (10 contributions)
1. Title: Two relevant issues in variational transition state theory: tunneling and multiple structures. Conference: Summer modeling. Venue: Castiglione della Pescaia, Italy. Date: September 2024. Participation: Plenary lecture.
2. Tittle: Approaching fifty years of variational transition state theory: a personal perspective. Conference: ACS Fall meeting 2024. Venue: Denver (USA), Date: August 2024. Participation: Invited conference.

3. Title: The role of hydrogen-bonded complexes in bimolecular reactions involving OH at ultra-low temperatures. Conference: 25th International Conference on Horizons in Hydrogen Bond Research. Venue: Bologna (Italy). Date: September 2023. Participation: Contributed talk.
4. Title: Algorithms for tackling the conformers of flexible molecules. Conference: The 26th International Conference on High Resolution Molecular Spectroscopy. Venue: Prague (Czech Republic). Date: August 2022. Participation: Contributed talk.
5. Title: Advances in the development and implementation of automated methods to study complex reaction mechanisms using variational transition state theory. Conference: Configurating Interactions: Computational Chemistry in São Paulo (CI-CCSP), Venue: São Paulo (Brasil); Date: July 2019. Participation: Plenary lecture.
6. Tittle: The OH + methanol reaction at ultracold temperatures: A tough nut to crack for theory. Conference: The XIXth Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases (QAMTS). Venue: The Borovets (Bulgaria). Date: May 2019. Participation: Invited conference.
7. Title: Proton transfer tunneling splittings and the imaginary mode Hamiltonian: the beginning of a beautiful friendship. Conference: The 25th International Conference on High Resolution Molecular Spectroscopy; Venue: Bilbao. Date: September 2018. Participation: Contributed talk.
8. Title: The methanol + OH reaction and its role in astrophysics: a theorist's point of view. Conference: Joint Iberian Meeting in Atomic and Molecular Physics (IBER); Venue: Barcelona. Date: September 2017. Participation: Invited conference.
9. Title: The mechanism of double-proton transfer at very low temperatures. Conference: XVIIIth Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases (QAMTS); Venue: Madison (EEUU). Date: May 2017. Participation: Invited conference.
10. Title: Why is hydrogen abstraction reaction from methanol by OH drastically enhanced at low temperatures? Conference: Electronic structure, Principles and applications, ESPA 2016. Venue: Castellón; Date: June 2016. Participation: Invited conference.

C.3. Research projects, indicating your personal contribution. In the case of young researchers, indicate lines of research for which they have been responsible.

Projects for the last 10 years as principal investigator:
1. Simulación de biocombustibles y aditivos de gasolina. Funding entity: MICINN (Retos); Period: from 1/6/2020 to 31/5/2024: Amount: 60500 euros.
Principal researcher: Antonio Fernández Ramos

2. Simulación de procesos de combustión de bioalcoholes. Funding entity: MINECO (Retos); Period: from 01/01/2015 to 12/31/2018; Amount: 87120 euros.
Principal researcher: Antonio Fernández Ramos

C.4. Contracts, technological or transfer merits.
The main technological transfer is the software licensed by the research group:

Torsiflex (2021): A program that allows obtaining the all torsional conformers of a flexible molecule. Citations: 41 citations (Scholar).
Pilgrim (2020): This program calculated thermal rate constants using variational transition state theory and multi-path variational transition state theory calculations. Citations: 50 (Scholar).
Q2DTor: a program that calculates hindered rotor tunneling splittings and rovibrational partition functions in systems with two coupled hindered rotors. Citations: 26 (Scholar)

Contributions to software from other research groups:
POLYRATE (several versions): a computer program from the University of Minnesota that contains most of the advances in variational transition state theory. Version 9.7: 340 citations; version 2008: 278 citations; version 2017-C: 174 citations (Scholar).