



Part A. PERSONAL INFORMATION		CV date	31/03/2023
First and Family name	Alkorta Osoro, Ibon		
ID number	15365423C	Age	58
Researcher numbers	Researcher ID	I-7828-2014	
	Orcid code	0000-0001-6876-6211	

A.1. Current position

Name of Institution	Consejo Superior Investigaciones Científicas		
Department	Instituto de Química Médica		
Address	Juan de la Cierva, 3. 28006-Madrid		
Phone number	915622900	E-mail	ibon@iqm.csic.es
Current position	Prof. Investigación	From	2008
UNESCO codes	2390, 2306, 2307		
Keywords	Hydrogen bonds, weak interactions.		

A.2. Education

Degree/PhD	University	Year
Degree in Chemistry	Universidad Autónoma de Madrid	1986
PhD in Chemistry	Universidad Autónoma de Madrid	1990

A.3. JCR articles, h Index, thesis supervised

Number of sexennia	5
Date of last sexennium	2017
PhDs supervised in the last 10 years	2
Total number of citations (Web of Science)	26839
Average number of citations/year	1500
Number of publications in the first quartile (Q1) in the last 5 years	50
h index	71

Part B. CV SUMMARY (max. 3500 characters, including spaces)

Prof. Alkorta has more than 30 years research experience. His main areas of interest are the theoretical study of weak interactions (hydrogen, halogen and pnicoen bonds as well as beryllium interactions) and the prediction of physicochemical properties of heterocycles. Prof Alkorta has published a total of 849 articles in international journals. Of these, 8 have been published in 2023. The number of articles has grown steadily, culminating in an h-index of 71 and a total number of ~26000 citations. 39 of his articles have been cited more than 100 times.

Prof. Alkorta started his scientific carrier as synthetic organic chemist under the direction of Dr. Vicente Aran. During his PhD under the direction of Prof. Pilar Goya, he became familiarized with the molecular modeling techniques while carrying out the synthesis of heterocyclic compounds. In his post-doctoral stage at the MRI (Palo Alto, California, USA) under the direction of Dr. Hugo Villar he extended his knowledge in molecular modeling and started to use quantum-mechanism programs to characterize molecular interactions. Since then, he has specialized in the study of weak interactions. He has spent variable periods of time (between 6 and 12 weeks) during 10 summers (from 2009-2018) as invited researcher in the group of Prof. Paul Popelier (Manchester University, UK).

Prof. Alkorta has formed and maintains ongoing collaborations with several groups of researchers worldwide:

- Prof. José Elguero (IQM-CSIC, Madrid) and Prof Rosa Claramunt (UNED, Madrid): physicochemical properties of heterocycles.



- Prof. Janet Del Bene (Youngstown University, USA): study of coupling constants in weak interactions.
- Prof. Manuel Yáñez and Prof. Otilia Mó (Univ. Autónoma, Madrid): hydrogen bonds and beryllium bonds.
- Prof. Elies Molins (CSIC, Barcelona) and Prof Enrique Espinosa (CNRS, Nancy, France): electron density in hydrogen bonds.
- Prof. Paul Popelier (Univ. Manchester, Britain): pK_a prediction and conformational analysis of carbohydrates.

Academic and Professional achievements

- B. Chemistry (1987; Autónoma University Madrid, Spain)
- PhD Chemistry (1990; Autónoma University Madrid, Spain).
- Post-doctoral researcher (1991-1993, Molecular Research Institute, Palo Alto, California, USA)
- Post-doctoral researcher (1993-1996, Institute of Medicinal Chemistry, Spain)
- Tenured Scientist (1996-2004, Institute of Medicinal Chemistry, Spain)
- Scientist (2004-2008, Institute of Medicinal Chemistry, Spain)
- Full professor (2008-now, Institute of Medicinal Chemistry, Spain)

Mentoring of early-stage researchers.

Prof. Alkorta has been the PhD thesis supervisor of Marina Sánchez (Title: Theoretical calculation of physical properties in complexes of chemical interest) presented in 2011 and PhD thesis supervisor of Luis Miguel Azofra (Title: Theoretical study of reactivity in carbohydrates), presented in 2014. At present time he is supervising the PhD thesis of Maxime Ferrer. In addition, Prof. Alkorta has guided in the last 5 years three young researchers in their Master work (Iñigo Irribarren, I-Ting and Ruben López), two predoctoral researcher (Carlos Martín Fernández and Maxime Ferrer) and two researchers from Iran (Saber Mohammadi Chalanchi and Esmail Vessally).

Several post-doctoral researchers have worked with Prof. Alkorta:

- Dr. M. Merced Montero-Campillo (2017-2018): sequestration of CO₂
- Dr. Marta Marín-Luna (2014-2015): beryllium bonds
- Dr. Goar Sánchez Sanz (2011-2012): theoretical study of chalcogen interactions.
- Dr. Cristina Trujillo (2010): new photoactive materials.
- Dr. Fernando Blanco (2007-2009): chiral discrimination in hydrogen-bonded clusters.
- Dr. Krzysztof Zborowski (2005-2006): chiral discrimination in reactive processes.
- Dr. Markku Sundberg (2005): chiral discrimination in metallic complexes.

Part C. RELEVANT MERITS

C.1. Publicacions

Articles (A selection of the most representatives published in the last 4 years)

- M. Ferrer, I. Alkorta, J. Elguero, J. M. Oliva-Enrich "Reactivity of a model of B3P3 -doped nanographene with up to three CO₂ molecules" *Sci. Rep.* **13**, 2407 (2023).
- D. Homma, S. Taketani, T. Shirai, E. Caytan, C. Roussel, J. Elguero, I. Alkorta, O. Kitagawa "Rotational Behavior of N-(5-Substituted-pyrimidin-2-yl)anilines: Relayed Electronic Effect in Two N–Ar Bond Rotations" *J. Org. Chem.* **87**, 8118–8125 (2022)
- A. Bauzá, I. Alkorta, J. Elguero, T. J. Mooibroek, A. Frontera, "Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements" *Angew. Chem. Int. Ed.*, **59**, 17482–17487 (2020)



- J.E. Del Bene, I. Alkorta, J. Elguero "Hydrogen bonds and halogen bonds in complexes of carbon L->C<-L as electron donors to HF and ClF, for L = CO, N₂, HNC, PH₃, and SH₂", *Phys. Chem. Chem. Phys.* **22**, 15966-15975 (2020)
- O. Mó, M. M. Montero-Campillo, I. Alkorta, J. Elguero, M. Yáñez "Ternary Complexes Stabilized by Chalcogen and Alkaline-Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions" *Chem. Eur. J.* **25**, 11688-11695 (2019). DOI: 10.1002/chem.201901641
- I. Uriarte, F. Reviriego, C. Calabrese, J. Elguero, Z. Kisiel, I. Alkorta, E. J. Cocinero "Bond Length Alternation Observed Experimentally: The Case of 1H-Indazole" *Chem. Eur. J.* **25**, 10172–10178 (2019). DOI: 10.1002/chem.201901666

Chapters in scientific books

- O. Brea, I. Alkorta, I. Corral, O. Mó, M. Yáñez, J. Elguero "Intramolecular Beryllium Bonds. Further Insights into Resonance Assistance Phenomena" in *Intermolecular Interactions in Crystals: Fundamentals of Crystal Engineering*, Edited by Juan J. Novoa, The Royal Society of Chemistry, 2017
- J. E. Del Bene, I. Alkorta, J. Elguero "The Pnicogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnicogen Bonds" en el libro "Noncovalent forces" S. Scheiner ed., Springer, 2015.
- I. Alkorta, J. Elguero "¿Interacciones débiles? No tanto" in the book "A través del cristal. Cómo la cristalografía ha cambiado la visión del mundo", M. Martínez-Ripoll; J. A. Hermoso; A. Albert Ed., Editorial CSIC, 2014.
- I. Alkorta and J. Elguero "How Aromaticity Affects the Chemical and Physicochemical Properties of Heterocycles: A Computational Approach" *Aromaticity in Heterocyclic Compounds*, Ed. T.M Krygowski and M. Cyrański, Vol. 19 Topics Heterocyclic Chemistry, Springer-Verlag, Berlin 2009.
- I. Alkorta, J. Elguero "Chirality and Chiral Recognition" in *Practical Aspects of Computational Chemistry*, Ed. J. Leszczynski and M. K. Shukla, Springer, 2009. DOI: 10.1007/978-90-481-2687-3_3
- Mata, I. Alkorta, E. Espinosa, E. Molins, J. Elguero "Topological properties of the electron distribution in hydrogen-bonded systems" *The Quantum Theory of Atoms in Molecules* Ed. C.F. Matta and R.J. Boyd, Wiley-VCH, 2007.

C.2. Research projects

Period September 2022- August 2025
IP Dr. Ibon Alkorta (subproject-IP)
Title Frustrated Lewis Pairs and New Materials based on boron and beryllium.
Code PID2021-125207NB-C32
Financier Ciencia, e Innovación.

Period January 2019- December 2021
IP Dr. Ibon Alkorta (subproject-IP)
Title Design and characterization of new molecular materials and improved drugs:
 synergy between experiment and theory
Code PGC2018-094644-B-C22
Financier Ciencia, Innovación y Universidades

Period January 2016-December 2018
IP Dr. Ibon Alkorta (subproject-IP)
Title Modificación de la reactividad y diseño de nuevos materiales mediante
 enlaces berilio y otras interacciones no-covalentes.

Code CTQ2015-63997-C2-2-P
Financier Ministerio de Economía y Competitividad

Period October 2014-September 2017
IP Dr. Nazario Martín
Title Materiales avanzados de carbono para fotovoltaica molecular
Code FOTOCARBON, S2013/MIT-2841
Financier Comunidad de Madrid.

Period January 2013-December 2015
IP Dr. Ibon Alkorta (subproject-IP)
Title Interacciones no-covalentes y quiralidad en nuevos materiales
Code CTQ2012-35513-C02-02
Financier Ministerio de Economía y Competitividad

Period January 2010-December 2013
IP Dr. Nazario Martín
Title Materiales foto- y electroactivos para células solares orgánicas e híbridas
Code MADRISOLAR2, S2009/PPQ-1533
Financier Comunidad de Madrid

Period January 2010- December 2012
IP Dr. Ibon Alkorta (subproject-IP)
Title Reactividad en fase gas: nuevos materiales moleculares y discriminación quiral
Code CTQ2009-13129-C02-02
Financier Ministerio de Ciencia e Innovación

Period January 2006-December 2009
IP Dr. Nazario Martín
Title Materiales foto- y electroactivos para células solares orgánicas e híbridas
Code MADRISOLAR, S2505/PPQ/0225
Financier Comunidad de Madrid.

Period December 2006-November 2007
IP Dr. Ibon Alkorta
Title Estudio de organocatálisis quiral por interacciones débiles
Code CTQ2006-14487-C02-01
Financier Ministerio de Educación y Ciencia

Period December 2007-November 2008
IP Dr. Ibon Alkorta
Title Racionalización y optimización de la discriminación quiral a través de enlaces de hidrógeno
Code CTQ2007-61901/BQU
Financier Ministerio de Educación y Ciencia

C3. Other

Prof. Alkorta has been part of the IUPAC task group that redefined the Hydrogen Bond term (2004-2011). The results were published in *Pure Appl. Chem.*, 83, 1619-1636 and 1637-1641 (2011), these articles have been cited more than 500 times each.