

Curriculum Vitae

Dr. Emilio J. Cocinero

Physical Chemistry Department,
Universidad del País Vasco (UPV/EHU)
Instituto de Biofísica (CSIC-UPV/EHU)
Barrio Sarriena s/n, 48940, Leioa, Spain
ORCID ID: orcid.org/0000-0001-7632-3728
emiliojose.cocinero@ehu.es
<http://www.grupodeespectroscopia.es/MW/>



EDUCATION

- 2005 PhD in Chemistry, Molecular Spectroscopic Group (GEM), University of Valladolid (Spain)
Supervisors: José L. Alonso and Alberto Lesarri
Remark: Awarded *Extraordinary prize* to the best Ph. D. doctoral work conducted at the University of Valladolid.
Mark: A, Cum Laude, 10.
- 2001 Bachelor in Chemistry
University of Valladolid (Spain)

CURRENT POSITION

- 2016 – Permanent Researcher (equivalent to Tenured Professor)
University of the Basque Country (UPV/EHU), Physical Chemistry Dept., Leioa, Spain
- 2009 – now Group Leader. Spectroscopy Group
University of the Basque Country (UPV/EHU), Physical Chemistry Dept., Leioa, Spain

PREVIOUS POSITIONS

- 2006 – 2008 Postdoctoral Researcher
Oxford University, Physical and Theoretical Chemistry Laboratory, United Kingdom.
- 2001 – 2005 Ph. D. Student
University of Valladolid, Physical and Chemistry Dept., Spain.

AWARDS

- 2018 *International Dr. Barbara Mez-Starck Prize*
Barbara Mez-Starck Foundation.
For his extensive investigations of conformational behaviours and precise molecular structures of amino acids, sugars, alkaloids, anaesthetics and nicotinoids.
- 2017 *Enrique Pérez-Payá*
Spanish Biophysical Society.
For his remarkable contributions in molecular spectroscopy.
- 2015 *Flygare Award*
International Division on Molecular Spectroscopy, USA.
For outstanding contributions in molecular spectroscopy by early career independent scientist.
- 2012 *Sigma-Aldrich Award*
Spanish Royal Society of Chemistry, Spain
For the best scientific career of a Spanish young researcher in any area of Chemistry.
- 2012 *Suschem-JIQ-Postdoc*
FeiQue, JIQ and ANQUE Societies, Spain
For the best scientific publication in 2011 conducted by a Spanish young researcher in any area of Chemistry. E. J. Cocinero et al. *Nature*, 69, 76-80 (2011).
- 2008 *Extraordinary Prize*
University of Valladolid, Spain
For the best Ph. D. work conducted at the University of Valladolid, Spain.

FELLOWSHIPS

2010 – 2016	Ramón y Cajal Fellowship, Group Leader, Spanish Government, Spain.
2009 – 2010	Juan de la Cierva Fellowship, Group Leader, Spanish Government, Spain.
2008	Research Fellowship, Department Staff, Oxford University, United Kingdom.
2006 – 2008	Postdoctoral Fellowship, Spanish Government, Spain.
2003 – 2005	Ph. D Fellowship, Spanish Government, Spain.
2002	Ph. D Fellowship, University of Valladolid, Spain.
2001	Ph. D Fellowship, Ramón Areces Foundation, Spain.
2000 – 2001	Student Collaborator, University of Valladolid, Spain.

INTERNATIONAL STAYS

2013, 2019	Università di Bologna, Italy.	3 weeks
2012	University of Virginia, USA.	3 weeks
2012	Institut des sciences moléculaires d'Orsay, France.	3 weeks
2007, 2010	FELIX, FOM – Institute for Plasma Physics, Netherland.	1 month & 1 week
2006 – 2010	Oxford University, United Kingdom.	2 years & 7 months
2006, 2018	Commissariat à l'Energie Atomique (CEA), France.	3 weeks
2005, 2011	Leibniz-Universität Hannover, Germany.	3 months & 2 weeks

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2009 – 2019	6 Postdocs, 5 Ph. D. Students, 4 Master Students, 7 Undergraduate Students University of Basque Country, Physical and Chemistry Dept., Spain.
2006 – 2008	1 Postdocs, 1 Undergraduate Students Oxford University, Physical and Theoretical Chemistry Laboratory, United Kingdom.

ORGANISATION OF SCIENTIFIC MEETINGS

2018	Chairman, The 25 th International Conference on High Resolution Molecular Spectroscopy, Bilbao, Spain.
2018	Local committee, Spanish Drug Discovery Network meeting, Bilbao, Spain.
2017	Scientific committee, XIV Symposium of Young Investigators, Badajoz, Spain.
2017	International Advisory Committee, 72 nd International Symposium on Molecular Spectroscopy, Illinois, USA.
2016	Scientific committee, XIII Symposium of Young Investigators, Logroño, Spain.
2016	International Advisory Committee, 71 st International Symposium on Molecular Spectroscopy, Illinois, USA.
2015	Scientific committee, XII Symposium of Young Investigators, Barcelona, Spain.
2014	Chairman, XI Symposium of Young Investigators, Bilbao, Spain.

INSTITUTIONAL RESPONSIBILITIES

2016 – now	Member of governing board of Territorial Section of the Basque Country of Spanish Royal Society of Chemistry.
2014 – 2017	President of Young Chemical Researchers of Spanish Royal Society of Chemistry. (755 members).
2014 – 2017	Member of governing board of Spanish Royal Society of Chemistry.
2012 – 2013	Member of governing board of Young Chemical Researchers of Spanish Royal Society of Chemistry.

COMMISSIONS OF TRUST

2016, 2018	Flygare Award Committee, International Division on Molecular Spectroscopy
2014 – 2017	Evaluator, Young Chemical Researchers of Spanish Royal Society of Chemistry SusChem awards, travelling grants, fellowships for organising of scientific events.
2012	Panel Member and Evaluator, National Authority for Scientific Research
2010 – now	Panel Member and Evaluator, Spanish Evaluation National Agency National projects, Ramón y Cajal program, Postdoctoral Fellowships and Campus of international excellence of the Community of Madrid.
2009 – now	Regular Reviewer for most journals in my field, including journals of the American Chemical Society, Royal Society of Chemistry, Wiley, Elsevier.

TEACHING ACTIVITIES

- 2014 – 2018 “Chemistry II”
Physics and Geology Degree, University of Basque Country, Spain
- 2012 – 2015 “Experimentation in Physical Chemistry” and “Physical Chemistry II”
Chemistry Degree, University of Basque Country, Spain
- 2010 – 2012 “Lasers and Applications in Chemistry” and “Fundamentals of Laser Spectroscopy”
Master’s Degree, University of Basque Country, Spain
- 2004 – 2006 “Molecular Spectroscopy” and “Instrumental and laser techniques in Chemistry”
Chemistry Degree, University of Valladolid, Spain

BRIEF BIOGRAPHY

Emilio J. Cocinero (41 years-old) completed his Ph. D. in Physical Chemistry in 2005 at the University of Valladolid (Spain). In 2008, his thesis work, based on the study of the structure of amino acids by microwave spectroscopy, was recognized with a University prize to best Ph. D. doctoral work conducted at the University of Valladolid. In 2006 he moved to Oxford University and worked with Professor John P. Simons, to join the internationally leading research group studying carbohydrates in the gas phase. In January 2009 he joined the University of the Basque Country, where he leads research focused on solving various structural problems of chemistry at the molecular level, in particular, the study of biomolecules, including sugars, peptides and drugs, generated and stabilized in the gas phase. He has an excellent track record of publications (>100 papers). Several publications in the highest impact factor journals in his field including (1 *Nature*, 1 *Nat. Commun.*, 9 *J. Am. Chem. Soc.*, 10 *Angew. Chem. Int. Ed.*). His career has been recognized with several prizes. Finally, Emilio J. Cocinero was elected President of young chemical researchers (JIQ) of the Spanish Royal Society of Chemistry (RSEQ) in 2014-2017.

PRESENTATIONS

Dr. Cocinero has contributed with >150 communications in national and international conferences, including 5 plenary lectures, 10 invited talks, >50 oral presentations. In addition, he has been invited to give >20 national and international lectures in top Universities and Research Institutes.

1. *Plenary* 70th International Symposium on Molecular Spectroscopy, Champaign, Illinois, USA, 2015.
2. *Plenary* 24th Colloquium on High-Resolution Molecular Spectroscopy, Dijon, France, 2015.
3. *Plenary* Molecular Interactions from Biology to Astrochemistry, Newcastle, United Kingdom, 2019.
4. *Plenary* IX Young Investigators Meeting, RSEQ, Zaragoza, Spain, 2012.
5. *Plenary* 16th SBE Congress, Sevilla, Spain, 2017.
6. *Invited* Workshop on Mirror Images in Molecules, Bologna, Italy, 2016.
7. *Invited* XIII Iberian Meeting on Atomic and Molecular Physics, Aveiro, Portugal, 2015.
9. *Invited* XI Carbohydrate Symposium, Logroño, Spain, 2014.
9. *Invited* 2nd National conference on laboratory and molecular astrophysics, Sevilla, Spain, 2012.
10. *Invited* 26th International Carbohydrate Symposium (ICS 2012), Madrid, Spain, 2012.

FUNDED PROJECTS

Dr. Cocinero has participated in 10 international, 10 national, 13 regional, 2 infrastructure and 2 private funded projects with a total budget of ~9 Million €. As PI, despite his youth, he has also an excellent track record of peer-reviewed funding and he has managed an overall budget of ~1000 k€ with 3 international, 5 national, 4 regional and 1 private funded projects.

PUBLICATIONS

Dr. Cocinero has an excellent track record of publications: a book chapter and 108 papers, 43 in the last five years (2014-2019). Several publications in the highest impact factor journals in his field including 1 *Nature*, 1 *Nature Commun.*, 9 *J. Am. Chem. Soc.*, 10 *Angew. Chem. Int. Ed.*, among others. 63 articles (58%) have an IF > 4.4. The IF average is 6.120. His work has received >2100 citations. H index = 28, (ISI Web of Knowledge, April 2019).

FULL LIST OF PUBLICATIONS

Book Chapter

- 109 E. J. Cocinero and P. Çarçabal
Carbohydrates
Gas-Phase IR Spectroscopy and Structure of Biological Molecules.
Springer, 299-333 (2015)

2019

- 108 E. J. Juárez-Perez, L. K. Ono, I. Uriarte, E. J. Cocinero and Y. Qi
Degradation Mechanism and Relative Stability of Methylammonium Halide Based Perovskites Analyzed on the Basis of Acid–Base Theory
ACS Appl. Mater. Interfaces, 11, 12586-12593 (2019)
- 107 L. Spada, I. Uriarte, W. Li, L. Evangelisti, E. J. Cocinero and W. Caminati
Interactions between azines and alcohols: a rotational study of pyridine–tert-butyl alcohol
Phys. Chem. Chem. Phys., 21, 3545-3549 (2019)

2018

- 106 I. A. Bermejo, I. Usabiaga, I. Compañón, J. Castro-López, A. Insausti, J. A. Fernández, A. Avenoza, J. H. Busto, J. Jiménez-Barbero, J. L. Asensio, J. M. Peregrina, G. Jiménez-Osés, R. Hurtado-Guerrero, E. J. Cocinero, and Francisco Corzana
Water Sculpts the Distinctive Shapes and Dynamics of the Tumor-Associated Carbohydrate Tn Antigens: Implications for Their Molecular Recognition
J. Am. Chem. Soc., 31, 9952-9960 (2018)
Paper **Spotlight** by the Journal.
- 105 I. Uriarte, A. Insausti, A. Jabri, H. Mouhib, I. Alkorta, I. Kleiner and E. J. Cocinero
Competing Dispersive Interactions: From Small Energy Differences to Large Structural Effects in Methyl Jasmonate and Zingerone
J. Phys. Chem. Lett., 9, 5906-5914 (2018)
- 104 Z. Kisiel, L. Pszczółkowski, E. Białkowska-Jaworska, M. Jaworski, I. Uriarte, F. J. Basterretxea, E. J. Cocinero
Rotational spectroscopy update for the newly identified atmospheric ozone depleter CF₃CCl₃
J. Mol. Spectrosc., 352, 1-9 (2018)
- 103 I. Uriarte, S. Melandri, A. Maris, C. Calabrese and E. J. Cocinero
Shapes, Dynamics, and Stability of β -Ionone and Its Two Mutants Evidenced by High-Resolution Spectroscopy in the Gas Phase
J. Phys. Chem. Lett., 9, 1497-1502 (2018)
- 102 I. Uriarte, P. Écija, R. Lozada-García, P. Çarçabal, E. J. Cocinero
Investigating the Conformation of the Bridged Monosaccharide Levoglucosan
ChemPhysChem 19, 766-773 (2018)
- 101 I. Usabiaga, A. Camiruaga, A. Insausti, P. Çarçabal, E. J. Cocinero, I. León and J. A. Fernández
Phenyl- β -D-glucopyranoside and Phenyl- β -D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions
Front. Phys. 19, 766-773 (2018)

2017

- 100 M. Carini, M. P. Ruiz, I. Usabiaga, J. A. Fernández, E. J. Cocinero, M. Melle-Franco, I. Diez-Perez, and A. Mateo-Alonso
Exceptionally High Conductances in π -Folded Molecular Junctions
Nature Commun., 8, 15195-15204 (2017).

- 99 M. Vallejo-López, P. Écija, N. Vogt, J. Demaison, A. Lesarri, F. J. Basterretxea, E. J. Cocinero
N-Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine
Chem. – Eur. J., 23, 16491-16496 (2017).
Paper qualified as **Hot paper** by the Journal.
Journal cover.
- 98 A. Camiruaga, I. Usabiaga, A. Insausti, E. J. Cocinero, I. León and J. A. Fernández
Understanding the Role of Tyrosine in Glycogenin
Mol. BioSyst., 13, 1709-1712 (2017).
- 97 I. Usabiaga, J. González, I. León, P. F. Arnaiz, E. J. Cocinero and J. A. Fernández
Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose
J. Phys. Chem. Lett., 8, 1147-1151 (2017).
- 96 I. Uriarte, C. Pérez, E. Caballero-Mancebo, F. J. Basterretxea, A. Lesari, J. A. Fernández and Emilio J. Cocinero
Structural Studies of Nicotinoids: Cotinine vs. Nicotine
Chem. – Eur. J., 23, 7238-7244 (2017).
Paper qualified as **Hot paper** by the Journal.
Journal cover.
- 95 I. Uriarte, Z. Kisiel, E. Białkowska-Jaworska, L. Pszczółkowski, P. Ecija, F. J. Basterretxea and E. J. Cocinero
Comprehensive rotational spectroscopy of the newly identified atmospheric ozone depleter CF₃CH₂Cl
J. Mol. Spectrosc., 337, 37-45 (2017).
- 94 C. Calabrese, A. Maris, I. Uriarte, E. J. Cocinero, S. Melandri
Effects of Chlorination on the Tautomeric Equilibrium of 2-Hydroxypyridine: Experiment and Theory
Chem. – Eur. J., 23, 3595-3604 (2017).
Paper qualified as **Hot paper** by the Journal.
Journal cover.

2016

- 93 P. Écija, M. Vallejo-López, I. Uriarte, F. J. Basterretxea, A. Lesarri, J. A. Fernández and E. J. Cocinero
Scopine Isolated in the Gas Phase
ChemPhysChem, 15, 918-923 (2016).
Paper qualified as **VIP (Very Important paper)** by the Journal.
- 92 Q. Gou, L. Spada, M. Vallejo-López, S. Melandri, A. Lesarri, E. J. Cocinero, W. Caminati
Intermolecular Hydrogen Bonding in 2-Fluoropyridine-Water
ChemistrySelect, 6, 1273-1277 (2016).
- 91 N. Vogt, J. Demaison, E. J. Cocinero, P. Écija, A. Lesarri, H. D. Rudolph and J. Vogt
The equilibrium molecular structures of 2-deoxyribose and fructose by the semiexperimental mixed estimation method and coupled-cluster computations
Phys. Chem. Chem. Phys., 18, 15555-15563 (2016).
- 90 C. Pérez, E. Caballero-Mancebo, A. Lesarri, E. J. Cocinero, I. Alkorta, R. D. Suenram, J.-U. Grabow, B. H. Pate
The Conformational Map of Volatile Anesthetics: Enflurane Revisited
Chem - Eur. J., 22, 9804-9811 (2016).
- 89 L. B. Favero, I. Uriarte, L. Spada, P. Écija, C. Calabrese, W. Caminati and E. J. Cocinero
Solving the Tautomeric Equilibrium of Purine through Analysis of the Complex Hyperfine Structure of the Four ¹⁴N Nuclei
J. Phys. Chem. Lett., 7, 1187-1191 (2016).

- 88 P. Écija, I. Uriarte, L. Spada, B. G. Davis, W. Caminati, F. J. Basterretxea, A. Lesarri, E. J. Cocinero
Furanosic forms of sugars: Conformational equilibrium of methyl β -D-ribofuranoside
Chem. Commun., 52, 6241-6244 (2016).
- 87 I. Usabiaga, J. González, P. F. Arnáiz, I. León, E. J. Cocinero and José A. Fernández
Amino Acid-Sugar Interaction in Jets: Phenol-Glucopyranose Derivatives
Phys. Chem. Chem. Phys., 18, 12457-12465 (2016).
- 86 J. González, I. Baños, I. León, J. Contreras-García, E. J. Cocinero, A. Lesarri, J. A. Fernández and J. Millán
Unravelling Protein–DNA Interactions at Molecular Level: A DFT and NCI Study
J. Chem. Theory Comput., 12, 523-534 (2016).
- 85 I. Uriarte, P. Écija, L. Spada, E. Zabalza, A. Lesarri, F. J. Basterretxea, J. A. Fernández, W. Caminati and E. J. Cocinero
Potential energy surface of fluoroxene: experiment and theory
Phys. Chem. Chem. Phys., 18, 3966-3974 (2016).

2015

- 84 M. M. Deshmukh, S. R. Gadre and E. J. Cocinero
Stability of conformationally locked free fructose: theoretical and computational insights
New J. Chem., 39, 9006-9018 (2015).
- 83 P. Écija, I. Uriarte, F. J. Basterretxea, J. Millán, A. Lesarri, J. A. Fernández and E. J. Cocinero
*Structural distortion of the epoxy groups in norbornanes: A rotational study of *exo*-2,3-epoxynorbornane*
ChemPhysChem, 16, 2609-1614 (2015).
- 82 N. A. Seifert, C. Pérez, J. L. Neil, B. H. Pate, M. Vallejo-López, A. Lesarri, E. J. Cocinero and F. Castaño
Chiral recognition and atropisomerism in the sevoflurane dimer
Phys. Chem. Chem. Phys., 17, 18282-18287 (2015).
Journal cover.
- 81 M. K. Jahn, E. Méndez, K. P. R. Nair, P. D. Godfrey, D. McNaughton, P. Écija, F. Basterretxea, E. J. Cocinero and J.-U. Grabow
Conformational steering in dicarboxy acids: the native structure of succinic acid
Phys. Chem. Chem. Phys., 17, 19726-19734 (2015).
Journal cover.
- 80 Q. Gou, G. Feng, L. Evangelisti, M. Vallejo-López, L. Spada, A. Lesarri, E. J. Cocinero, W. Caminati
Internal Dynamics in Halogen-Bonded Adducts: A Rotational Study of Chlorotrifluoromethane-Formaldehyde
Chem - Eur. J., 21, 4148-4152 (2015).
- 79 J. Demaison, N. C. Craig, P. Groner, P. Écija, E. J. Cocinero, A. Lesarri and H. D. Rudolph
Accurate Equilibrium Structures for Piperidine and Cyclohexane
J. Phys. Chem. A, 119, 1486-1493 (2015).

2014

- 78 I. León, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández
Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures
Phys. Chem. Chem. Phys., 16, 23301-23307 (2014).

- 77 M. K. Jahn, D. A. Dewald, M. Vallejo-López, E. J. Cocinero, A. Lesarri, W. Zou, D. Cremer and J.-U. Grabow
Pseudorotational Landscape of Seven-Membered Rings: The Most Stable Chair and Twist-Boat Conformers of ϵ -Caprolactone
Chem. Eur. J., 43, 14084-14089 (2014).
- 76 I. León, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández
Water encapsulation by nanomicelles
Angew. Chem. Int. Ed., 53, 12480-12483 (2014).
- 75 I. León, I. Usabiaga, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández
Mimicking Anesthetic-Receptor Interactions in Jets: The Propofol-Isopropanol Cluster
Phys. Chem. Chem. Phys., 16, 16968-16975 (2014).
- 74 Q. Gou, L. Spada, E. J. Cocinero and W. Caminati
Halogen-halogen links and Internal dynamics in adducts of freons
J. Phys. Chem. Lett., 5, 1591-1595 (2014).
- 73 I. Algorta, C. Cancedda, E. J. Cocinero, J. Z. Dávalos, P. Écija, J. Elguero, J. González, A. Lesarri, R. Ramos, F. Reviriego, C. Roussel, I. Uriarte and N. Vanthuyne
Static and dynamic properties of Binol and its conjugated acids and bases
Chem – Eur. J., 20, 14816-14825 (2014).
- 72 P. Écija, L. Evangelisti, M. Vallejo, F. J. Basterretxea, A. Lesarri, F. Castaño, W. Caminati, E. J. Cocinero
The Conformational Flexibility of Mephesisin
J. Phys. Chem. B, 118, 5357-5364 (2014).
- 71 G. Feng, Q. Gou, L. Evangelisti, M. Vallejo-López, A. Lesarri, E. J. Cocinero, W. Caminati
Competition between weak hydrogen bonds: C-H \cdots Cl is preferred to C-H \cdots F in CH₂ClF-H₂CO, as revealed by rotational spectroscopy
Phys. Chem. Chem. Phys., 16, 12261-12265 (2014).
- 70 Q. Gou, L. Spada, M. Vallejo-López, A. Lesarri, E. J. Cocinero, W. Caminati
Interactions between alkanes and aromatic molecules: a rotational study of pyridine-methane
Phys. Chem. Chem. Phys., 16, 13041-13046 (2014).
Journal front cover.
- 69 P. Écija, M. Vallejo-López, L. Evangelisti, J. A. Fernández, A. Lesarri, W. Caminati and E. J. Cocinero
O-H \cdots N and C-H \cdots O hydrogen bonds control hydration of pivotal tropane alkaloids: Tropinone \cdots H₂O complex
ChemPhysChem., 15, 918-923 (2014).
Paper qualified as **VIP** (Very Important Paper) by the Journal.
- 68 N. A. Seifert, D. P. Zaleski, C. Pérez, J. L. Neill, B. H. Pate, M. Vallejo-López, A. Lesarri, E. J. Cocinero, F. Castaño, I. Kleiner
Probing the C-H \cdots π Weak Hydrogen Bond in Anesthetic Binding: The Gas-phase Molecular Structure of the Sevoflurane-Benzene Cluster
Angew. Chem. Int. Ed., 53, 3210-3213 (2014).
- 67 Q. Gou, G. Feng, L. Evangelisti, M. Vallejo-López, L. Spada, A. Lesarri, E. J. Cocinero, W. Caminati
How water interacts with anesthetics: the rotational spectrum of isoflurane-water
Chem – Eur. J., 20, 1980-1984 (2014).
- 66 L. Spada, Q. Gou, M. Vallejo-López, A. Lesarri, E. J. Cocinero and W. Caminati
Weak C-H \cdots N and C-H \cdots F hydrogen bonds and internal rotation in pyridine-CH₃F
Phys. Chem. Chem. Phys., 16, 2149-2153 (2014).

- 65 E. J. Cocinero and A. Lesarri
¡Disolvente fuera!: azúcares en fase gas
An. Quím., 109, 258-267 (2013).
- 64 M. Vallejo-López, L. Spada, Q. Gou, A. Lesarri, E. J. Cocinero and W. Caminati
Interactions between freons and aromatic molecules: The rotational spectrum of pyridine-difluoromethane
Chem. Phys. Lett., 591, 216-219 (2013).
- 63 E. J. Cocinero, A. Lesarri, P. Écija, A. Cimas, B. G. Davis, F. J. Basterretxea, J. A. Fernández, and F. Castaño
Naked' and Hydrated Conformers of the Conserved Core Pentasaccharide of N-linked Glycoproteins and Its Building Blocks.
J. Am. Chem. Soc., 135, 16895-16903 (2013).
- 62 E. Aguado, I León, J. Millán, E. J. Cocinero, S. Jaqx, A. Rijs, A. Lesarri and J. Fernández
Unraveling the Benzocaine-Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy
J. Phys. Chem. B, 117, 13472-13480 (2013).
- 61 M. K. Jahn, D. Dewald, M. Vallejo-López, E. J. Cocinero, A. Lesarri and J. -U. Grabow
Rotational Spectra of Bicyclic Decanes: The Trans Conformation of (-)-Lupinine
J. Phys. Chem. A, 117, 13673-13679 (2013).
- 60 I. Peña, E. J. Cocinero, C. Cabezas, A. Lesarri, S. Mata, P. Écija, A. M. Daly, Á. Cimas, C. Bermúdez, F. J. Basterretxea, S. Blanco, J. A. Fernández, J. C. López, F. Castaño and J. L. Alonso
Six Pyranoside Forms of free 2-Deoxy-D-Ribose
Angew. Chem. Int. Ed., 52, 11840-11845 (2013).
- 59 I. Haykal, L. Margulès, R. Motiyenko, T. R. Huet, P. Écija, E. J. Cocinero, F. Basterretxea, J. A. Fernández, F. Castaño, A. Lesarri, J.-C. Guillemin, B. Tercero and J. Cernicharo
The cm-, mm- and submm-wave spectrum of allyl isocyanide and radioastronomical observations in Orion KL and the PRIMOS line survey
Astrophys. J., 777, 120 (2013).
- 58 E. C. Stanka-Kaposta, P. Çarçal, E. J. Cocinero, P. Hurtado and J. P. Simons
Carbohydrate-Aromatic Interactions: Vibrational Spectroscopy and Structural Assgnment of Isolated Monosaccharide Complexes with p-Hydroxy Toluene and N-Acetyl L-Tyrosine Methylamide.
J. Phys. Chem. B, 117, 8135-8142 (2013).
- 57 I. León, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández
Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions
Angew. Chem. Int. Ed., 52, 7772-7775 (2013).
Journal inside cover.
- 56 I. León, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández
Transition from Planar to Nonplanar Hydrogen Bonds Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2-4
J. Phys. Chem. A, 117, 3396-3404 (2013).
- 55 E. J. Cocinero, A. Lesarri, P. Écija, F. J. Basterretxea, J. A. Fernández, and F. Castaño
The Distorted Tropane of Scopoline
ChemPhysChem, 14, 1830-1835 (2013)

- 54 I. León, J. Millán, E. J. Cocinero, A. Lesarri and J. A. Fernández.
Magic Numbers in the Solvation of the Propofol Dimer.
ChemPhysChem, 14, 1558-1562 (2013)
- 53 J. Demaison, M. K. Jahn, E. J. Cocinero, A. Lesarri, J.-U. Grabow, J.-C. Guillemin and H. D. Rudolph
The accurate semi-experimental structure of 1,3,4-oxadiazole by the mixed estimation method
J. Phys. Chem. A, 117, 2278-2284 (2013).
- 52 Q. Gou, G. Feng, L. Evangelisti, M. Vallejo López, A. Lesarri, E. J. Cocinero and W. Caminati
Non bonding interactions and internal dynamics in CH₂F₂...H₂CO. A rotational and model calculations study
Phys. Chem. Chem. Phys., 15, 6714-6718 (2013)
- 51 P. Écija, E. J. Cocinero, A. Lesarri, J. A. Fernández, W. Caminati and F. Castaño
Rotational Spectroscopy of Antipyretics: Conformation, Structure and Internal Dynamics of Phenazone
J. Chem. Phys., 138, 114304-114311 (2013)
- 50 P. Çarçabal, E. J. Cocinero and J. P. Simons
Binding energies of micro-hydrated carbohydrates: measurements and interpretation
Chem. Sci., 4, 1830-1836 (2013).
- 49 E. J. Cocinero, A. Lesarri, P. Écija, A. Cimas, B. G. Davis, F. J. Basterretxea, J. A. Fernández, and F. Castaño
Free Fructose is conformationally locked
J. Am. Chem. Soc., 135, 2845-1852 (2013).
- 48 I. León, E. J. Cocinero, A. M. Rijs, J. Millán, E. Alonso, A. Lesarri and J. A. Fernández
Formation of water polyhedrons in the propofol-water clusters
Phys. Chem. Chem. Phys., 15, 568-575 (2013).

2012

- 47 L. Evangelisti, P. Écija, E. J. Cocinero, F. Castaño, A. Lesarri, W. Caminati and R. Meyer
Proton tunneling in heterodimers of carboxylic acids: A rotational study of the benzoic acid-formic acid bi-molecule
J. Phys. Chem. Lett., 3, 3770-3775 (2012).
- 46 P. Écija, F. J. Basterretxea, A. Lesarri, J. Millán, F. Castaño and E. J. Cocinero.
Single hydration of the peptide bond: the case of Vince lactam
J. Phys. Chem. A, 116, 10099-10106 (2012).
- 45 I. León, E. J. Cocinero, A. Lesarri, F. Castaño and J. A. Fernández
A Spectroscopic Approach to the Solvation of Anesthetics in jets: propofol(H₂O)_n, n=4-6
J. Phys. Chem. A, 116, 8934-8941 (2012).
- 44 J. Demaison, N. Craig, E. J. Cocinero, J. -U. Grabow, A. Lesarri and H. -D. Rudolph
Semiexperimental Equilibrium Structures for the Equatorial Conformers of N-Methylpiperidone and Tropinone by the Mixed Estimation Method
J. Phys. Chem. A, 116, 8684-8692 (2012).
- 43 I. León, E. J. Cocinero, J. Millán, A. Rijs, I. Usabiaga, A. Lesarri, F. Castaño and J. A. Fernández
A Combined Spectroscopic and Theoretical Study of propofol·(H₂O)₃
J. Chem. Phys., 137, 074303 (2012).
- 42 I. León, J. Millán, E. J. Cocinero, A. Lesarri, F. Castaño and J. A. Fernández
Mimicking Anaesthetic-Receptor Interaction in Jets: a Combined Spectroscopic and Computational study of Propofol-Phenol
Phys. Chem. Chem. Phys., 14, 8956-8963 (2012).

- 41 E. J. Cocinero, A. Lesarri, P. Écija, F. J. Basterretxea, J.-U. Grabow, J. A. Fernández, and F. Castaño
Ribose Found in the Gas Phase
Angew. Chem. Int. Ed., 51, 3119-3124 (2012).
Paper qualified as **Hot paper** by the Journal.
Journal inside cover.
- 40 I. Leon, E. J. Cocinero, J. Millán, A. M. Rijs, S. Jaqx, A. Lesarri, F. Castaño and J. A. Fernández
Exploring Microsolvation of the Anesthetic Propofol
Phys. Chem. Chem. Phys., 14, 4398-4409 (2012).
Editor's choice

2011

- 39 N. Mayorkas S. Rudić, E. J. Cocinero, B. G. Davis and J. P. Simons
Carbohydrate Hydration: Heavy Water Complexes of Glucose, Galactose, Fucose and Xylose.
Phys. Chem. Chem. Phys., 13, 18671-18678 (2011).
- 38 L. Evangelisti, G. Feng, P. Écija, E. J. Cocinero, F. Castaño and W. Caminati
Halogen Bond and Internal Dynamics in CF₃Cl-H₂O.
Angew. Chem. Int. Ed., 50, 7807-7810 (2011).
- 37 P. Écija, E. J. Cocinero, A. Lesarri, J. Millán, F. Basterretxea, J. A. Fernández and F. Castaño.
Discriminating the Structure of Exo-2-Aminonorbornane Using Nuclear Quadrupole Coupling Interactions.
J. Chem. Phys., 134, 164311-164318 (2011).
- 36 E. J. Cocinero, F. J. Basterretxea, P. Écija, A. Lesarri, J. A. Fernández and F. Castaño
Conformational behaviour, hydrogen bond competition and intramolecular dynamics in vanillin derivatives: acetovanillone and 6-hydroxy-3-methoxyacetophenone
Phys. Chem. Chem. Phys., 13, 13310-13318 (2011).
- 35 L. Evangelisti, A. Lesarri, M. Jahn, E. J. Cocinero, W. Caminati and J.-U. Grabow
N-Methyl Inversion and Structure of 6-Membered Heterocyclic Rings: Rotational Spectrum 1-Methyl-4-Piperidone
J. Phys. Chem. A, 115, 9545-9551 (2011).
- 34 E. J. Cocinero, A. Lesarri, P. Écija, F. Basterretxea, J. A. Fernández and F. Castaño.
Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin
J. Mol. Spectrosc., 267, 112-117 (2011).
- 33 M. Pincu, E. J. Cocinero, N. Mayorkas, B. Brauer, B. G. Davis, R. B. Gerber and J. P. Simons.
Isotopic hydration of cellobiose: vibrational spectroscopy and dynamical simulations
J. Phys. Chem. A, 115, 9498-9509 (2011).
- 32 E. J. Cocinero, P. Çarcabal, T. D. Vaden, B. G. Davis and J. P. Simons.
Exploring carbohydrate-peptide interactions in the gas phase: Structure and selectivity in complexes of pyranosides with N-acetylphenylalanine methylamide
J. Am. Chem. Soc., 133, 4548-4557 (2011).
- 31 E. J. Cocinero, P. Çarcabal, T. D. Vaden, J. P. Simons and B. G. Davis.
Sensing the anomeric effect in a solvent-free environment
Nature, 469, 76-80 (2011).

2010

- 30 E. J. Cocinero, A. Lesarri, P. Écija, J.-U. Grabow, J. A. Fernández and F. Castaño.
Conformational equilibria in Vanillin and Ethylvanillin
Phys. Chem. Chem. Phys., 12, 12486-12493 (2010).

- 29 A. Lesarri, E. J. Cocinero, L. Evangelisti, R. D. Suenram, W. Caminati and J.-U. Grabow.
The Conformational Landscape of Nicotinoids: Solving the Conformational Disparity of Anabasine
Chem – Eur. J., 16, 10214-10219 (2010).
- 28 E. J. Cocinero, A. Lesarri, P. Écija, J.-U. Grabow, J. A. Fernández and F. Castaño.
N-Methyl Stereochemistry in Tropinone: The conformational flexibility of the tropane motif.
Phys. Chem. Chem. Phys., 12, 6076-6083 (2010).

2009

- 27 E. J. Cocinero, E. C. Stanca-Kaposta, M. Dethlefsen, B. Liu, D. P. Gamblin, B. G. Davis and J. P. Simons.
Hydration of sugars in the gas phase: regioselectivity and conformational choice in N-acetyl glucosamine and glucose
Chem – Eur. J., 15, 13427-13434 (2009).
- 26 E. Aguado, I. León, E. J. Cocinero, A. Lesarri, J. A. Fernández and F. Castaño.
Molecular Recognition in Gas Phase: Benzocaine-Phenol as a Model of Anesthetic-Receptor Interaction.
Phys. Chem. Chem. Phys., 11, 11608-11616 (2009).
- 25 E. J. Cocinero, D. P. Gamblin, B. G. Davis and J. P. Simons.
The building blocks of cellulose: the intrinsic conformational structures of cellobiose, its epimer, lactose, and their singly hydrated complexes.
J. Am. Chem. Soc., 131, 11117-11123 (2009).
- 24 Z. Su, B. Wagner, E. J. Cocinero, B. Ernst and J. P. Simons
The intrinsic conformation of a Lewis antigen: The Lewis x trisaccharide.
Chem. Phys. Lett., 477, 365-368 (2009).
- 23 J. P. Simons, B. G. Davis, E. J. Cocinero, D. P. Gamblin and E. C. Stanca-Kaposta.
Conformational change and selectivity in explicitly hydrated carbohydrates.
Tetrahedron-Asymmetr., 20, 718-722 (2009).
- 22 Z. Su, E. J. Cocinero, E. C. Stanca-Kaposta, B. G. Davis and J. P. Simons.
Carbohydrate-aromatic interactions: a computational and IR spectroscopic investigation of the complex, methyl α -L-fuco-pyranoside-toluene, isolated in the gas phase.
Chem. Phys. Lett., 471, 17-21 (2009).
- 21 E. J. Cocinero, E. C. Stanca-Kaposta, D. P. Gamblin, B. G. Davis and J. P. Simons.
Peptide secondary structures in the gas phase: the consensus motif of N-linked glycoproteins.
J. Am. Chem. Soc., 131, 1282-1287 (2009).

2008

- 20 J. P. Simons, E. C. Stanca-Kaposta, E. J. Cocinero, B. Liu, B. G. Davis, D. P. Gamblin, B. G. Davis and R. T. Kroemer.
Probing the glycosidic linkage: secondary structures in the gas phase
Phys. Scripta, 78, 058124/1-058124/7, (2008).
- 19 E. J. Cocinero, E. C. Stanca-Kaposta, E. M. Scanlan, D. P. Gamblin, B. G. Davis and J. P. Simons.
Conformational choice and selectivity in singly and multiply hydrated monosaccharides in the gas phase.
Chem – Eur. J., 14, 8947-8955 (2008).

- 18 E. C. Stanca-Kaposta, D. P. Gamblin, E. J. Cocinero, J. Frey, R. T. Kroemer, A. J. Fairbanks, B. G. Davis and J. P. Simons.
Solvent Interactions and Conformational Choice in a Core N-Glycan Segment: Gas Phase Conformation of the Central, Branching Trimannose Unit and its Singly Hydrated Complex.
J. Am. Chem. Soc., 130, 10691-10696 (2008).

2007

- 17 E. J. Cocinero, A. Lesarri, J.-U. Grabow, J. C. López and J. L. Alonso.
The shape of leucine in the gas phase.
ChemPhysChem, 8, 599-604 (2007).
- 16 E. J. Cocinero, P. Villanueva, A. Lesarri, M. E. Sanz, S. Blanco, S. Mata, J. C. López and J. L. Alonso.
The shape of neutral sarcosine in gas phase.
Chem. Phys. Lett., 435, 336-341 (2007).

2006

- 15 J. L. Alonso, E. J. Cocinero, A. Lesarri, M. E. Sanz and J. C. López.
The glycine-water complex.
Angew. Chem. Int. Ed., 45, 3471-3474 (2006).
Paper qualified as **VIP** (Very Important Paper) by the Journal.
Journal cover.
- 14 E. J. Cocinero, A. Lesarri, M. E. Sanz, J. C. López and J. L. Alonso.
Conformations of α -aminobutyric acid in gas-phase.
ChemPhysChem, 7, 1481-1487 (2006).
- 13 D. Banser, M. Schnell, J.-U. Grabow, E. J. Cocinero, A. Lesarri and J. L. Alonso.
The pure rotational spectrum of TeSe: rotational parameters, Born-Oppenheimer break down corrections and hyperfine constants.
J. Mol. Struct., 795, 163-172 (2006).

2005

- 12 D. Banser, M. Schnell, J.-U. Grabow, E. J. Cocinero, A. Lesarri and J. L. Alonso.
The internuclear potential, electronic structure, and chemical bond of tellurium selenide.
Angew. Chem. Int. Ed., 44, 6311-6315 (2005).
Paper qualified as **VIP** (Very Important Paper) by the Journal
- 11 A. Lesarri, R. Sánchez, E. J. Cocinero, J. C. López and J. L. Alonso.
Coded amino acids in the gas phase: the shape of isoleucine.
J. Am. Chem. Soc., 127, 12952-12956 (2005).
- 10 A. Lesarri, E. J. Cocinero, J. C. López and J. L. Alonso.
Gas-phase structure of N,N-dimethylglycine.
ChemPhysChem, 5, 1559-1566 (2005).
- 9 E. J. Cocinero, R. Sánchez, A. Lesarri, J. C. López and J. L. Alonso.
Weak hydrogen bonds C-H \cdots S and C-H \cdots F-C in the thirane-trifluoromethane dimer.
Chem. Phys. Lett., 402, 4-10 (2005).
- 8 A. Lesarri, E. J. Cocinero, J. C. López and J. L. Alonso.
The shape of 4(S)- and 4(R)-hydroxyproline in gas phase.
J. Am. Chem. Soc., 127, 2572-2577 (2005).

2004

- 7 A. Lesarri, E. J. Cocinero, J. C. López and J. L. Alonso.
The shape of neutral valine.
Angew. Chem. Int. Ed., 43, 605-610 (2004).

2002

- 6 A. Lesarri, S. Mata, E. J. Cocinero, S. Blanco, J. C. López and J. L. Alonso.
The structure of neutral proline
Angew. Chem. Int. Ed., 41, 4673-4676 (2002).

Non-Peer Reviewed

- 5 J. P. Simons, N. Mayorkas, B. G Davis, E. J Cocinero, M. Pincu, R. B. Gerber and B. Brauer.
Isotopic hydration of cellobiose: vibrational spectroscopy and dynamical simulations
Annual Report, Central Laser Facility, Rutherford Appleton Laboratory, 60 (2010-2011).
- 4 J. P. Simons, Z. Su, E. J. Cocinero, B. Ernst and B. Wagner.
Antigens laid bare: The intrinsic conformation of Lewisx
Annual Report, Central Laser Facility, Rutherford Appleton Laboratory, 204-205 (2009-2010).
- 3 Z. Su, E. J. Cocinero, J. P Simons, E C. Stanca-Kaposta and B. G Davis.
Carbohydrate molecular recognition: probing CH- π interactions
Annual Report, Central Laser Facility, Rutherford Appleton Laboratory, 206-207 (2009-2010).
- 2 E. J. Cocinero, J. P Simons, E C. Stanca-Kaposta, B. G Davis and D. P. Gamblin.
Hydrophilic and Hydrophobic Carbohydrate Interactions
Annual Report, Central Laser Facility, Rutherford Appleton Laboratory, 187-189 (2008-2009).
- 1 E. C. Stanca-Kaposta, B. Liu, E. J. Cocinero, T. D. Vaden, J. Frey, J. P. Simons and L. C. Snoek.
Towards the elucidation of the 3D structure of N-linked glycoproteins: does rigidity play an important role?
Annual Report, Central Laser Facility, Rutherford Appleton Laboratory, 143-146 (2006-2007).