ESPINOSA FERAO, Arturo

PERSONAL DETAILS & CAREER

Nationality: Spanish.

E-mail: artuesp@um.es Website: http://www.um.es/funcmolecmat/artuesp/

Current Position

Professor in Organic Chemistry, University of Murcia, since December 2017 ("*Acreditation*" to Full Professor on February 2014).

Department of Organic Chemistry (Faculty of Chemistry, Univ. Murcia, Spain).

Previous positions held

* Predoctoral grant ("*F.P.U.*" from the Spanish ministry of education) with associated academic duties (Univ. Murcia): January 1987 to October 1990.

* Postdoctoral grant ("*Reincorporación de doctores y tecnólogos*" from the Spanish ministry of education) with associated academic duties (Univ. Murcia): October 1991 to December 1993.

* Lecturer in Organic Chemistry, University of Murcia, since January 1st 1994. Associate Professor in Organic Chemistry, University of Murcia, since April 8th 1995.

* Head of the Department of Organic Chemistry along ca. 2.5 years (December 2002 to May 2005).

Degrees held

* Degree in Science (section of Chemistry) in 1986 by the University of Murcia, with average mark of 9.83 [from 0.00 (lowest) to 10.00 (highest)]. *"Extraordinary Prize"* from the University of Murcia and *"National Extraordinary Prize"*.

* PhD in "Chemical Sciences" in 1990 by the University of Murcia, with Honors (with the highest "Sobresaliente *Cum Laude*" mark). *"Extraordinary Prize of PhD"* from the University of Murcia.

Other positions

- Postdoctoral research fellow at the École Polytechnique (Palaiseau, France), October 1990 to October 1991.
- Visiting professor (*Erasmus/Erasmus+ program*) at the Rheinische Friedrich-Wilhelms-Universität Bonn (Germany), summer semesters of 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019 and 2021.

- Visiting professor at the Institute for Chemical Research, Kyoto University ("*Funding Program for Next Generation Researchers from Kyoto University Research Coordination Alliance*"), in March 2016.

PARTICIPATION IN FUNDED PROJECTS

Participation in 18 funded projects including:

* 15 from the national or regional funding agencies (one of them as external collaborator)

* 3 as co-leader in German-Spanish collaborative research projects financed by the Deutsche Forschungsgemeinschaft (DFG):

- "*Open-shell three-membered phosphorus heterocycles: ring opening and ring expansion reactions – a combined experimental and theoretical study" (STR 411/28-1)*. Period July 2009 to December 2010.

- "*Open-shell three-membered phosphorus heterocycles: ring opening and ring expansion reactions – a combined experimental and theoretical study*" (*STR 411/31-1*). Period July to December 2011

- "*Chemistry of thiaphosphiranes and isomers: An experimental and theoretical study" (STR 411/36-1)*. Period July to December 2014.

RESEARCH INTERESTS

- intramolecular electron-transfer,

- multisignalling (redox, optical and/or fluorescent) molecular recognition,

- platinum, iridium, rhodium and ruthenium-based antitumor agents

- ring strain

- highly reactive phosphorus intermediates

- quantum chemical calculations

PUBLICATIONS

Original Papers & Communications published:	156
Further Original Papers & Communications accepted:	0
Further Original Papers & Communications submitted:	3
Total publications	**159**

H-Index: **38** [source: Web of Science, 13.10.2021, on 155 publications found]

Total number of times cited:	4126 (3389 excluding self-citations)
Total number of citing articles:	2599 (2472 excluding self-citations)

SELECTED RECENT (2012-2021) PUBLICATIONS

► A. Espinosa, C. Gómez, R. Streubel, "Single electron transfer-mediated selective endo- and exocyclic bond cleavage processes in azaphosphiridine chromium(0) complexes: a computational study*" Inorg. Chem.*, **2012**, *51*, 7250-7256. DOI: 10.1021/ic300522g.

► A. Espinosa, R. Streubel, "Exocyclic bond cleavage in oxaphosphirane complexes?" *Chem. Eur. J.*, **2012**, *18*, 13405-13411. DOI: 10.1002/chem.201201057.

► L. Abdrakhmanova, G. Schnakenburg, A. Espinosa, R. Streubel, "Reaction of Li/Cl phosphinidenoid complexes with a phosphite substituted ketone: access to complexes with a novel mixed-valence polycyclic P,C-ligand system" *Dalton Trans.*, **2013**, *42*, 10510-10514. DOI: 10.1039/C3DT50902H.

► J. M. Villalba Franco, A. Espinosa Ferao, G. Schnakenburg, R. Streubel, "The azaphosphiridine to terminal phosphinidene complex rearrangement – looking for non-covalent interactions of a highly reactive species" *Chem. Commun.*, **2013**, *49*, 9648-9650. DOI: 10.1039/C3CC45477K.

► G. von Frantzius, A. Espinosa Ferao, R. Streubel, "Coordination of CO to low-valent phosphorus centres and other related P-C bonding situations. A theoretical case study" *Chem. Sci.*, **2013**, *4*, 4309-4322. DOI: 10.1039/C3SC52027G.

► G. Sánchez, A. Espinosa, D. Curiel, A. Tárraga, P. Molina, "Bis(carbazolyl)ureas as Selective Receptors for the Recognition of Hydrogenpyrophosphate in Aqueous Media" *J. Org. Chem.*, **2013**, *78*, 9725-9737. DOI: 10.1021/jo401430d.

► V. Nesterov, A. Espinosa, G. Schnakenburg, R. Streubel, "Novel N,P,C-cage complex via rearrangement of a tricyclic phosphirane complex. On the importance of non-covalent interactions" *Chem. Eur. J.*, **2014**, *20*, 7010-7016. DOI: 10.1002/chem.201305061.

► A. Espinosa, É. de las Heras, R. Streubel, "Oxaphosphirane-borane complexes: Ring strain and migratory insertion reactions" *Inorg. Chem.*, **2014**, *53*, 6132-6140. DOI: 10.1021/ic500536h.

► J. M. Villalba Franco, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Unprecedented ring/ring interconversion of N,P,C-cage ligands" *Chem. Eur. J.*, **2015**, *21*, 3727-3735. DOI: 10.1002/chem.201405754.

► J. M. Villalba Franco, T. Sasamori, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Going for strain: synthesis of the first 3-imino-azaphosphiridine complexes and their surprising conversion into oxaphosphirane complex valence isomers" *Chem. Commun.*, **2015**, *51*, 3878-3881. DOI: 10.1039/C4CC10266E.

► J. M. Villalba Franco, G. Schnakenburg, T. Sasamori, A. Espinosa Ferao, R. Streubel, "Stimuli-Responsive Frustrated Lewis-Pair-Type Reactivity of a Tungsten Iminoazaphosphiridine Complex" *Chem. Eur. J.*, **2015**, *21*, 9650-9655. DOI: 10.1002/chem.201501628.

► M. Klein, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Rearrangement and deoxygenation of 3,3-bis(2-pyridyl)oxaphosphirane complexes" *Dalton Trans.*, **2016**, *45*, 2085-2094. DOI: 10.1039/C5DT03404C.

► C. Murcia García, A. Espinosa Ferao, G. Schnakenburg, R. Streubel, "CPh_3 as a functional group in P-heterocyclic chemistry: elimination of $HCPh_3$ in the reaction of P-CPh_3 substituted Li/Cl phosphinidenoid complexes with $Ph_2C{=}O$" *Dalton Trans.*, **2016**, *45*, 2378-2385. DOI: 10.1039/c5dt04595a.

► J. M. Villalba Franco, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Coordination chemistry of a low-coordinate non-metal element: the case of

electrophilic terminal phosphinidene complexes" *Dalton Trans.*, **2016**, *45*, 13951-13956. DOI: 10.1039/C6DT02909D.

► P. Malik, A. Espinosa Ferao, G. Schnakenburg, R. Streubel, "Cycloaddition of P-C single bonds. Stereoselective formation of novel benzo-1,3,6,2-trioxaphosphepine complexes via a ditopic van der Waals complex", *Angew. Chem. Int. Ed.*, **2016**, *55*, 12693-12697. DOI: 10.1002/anie.201606264.

► A. Espinosa Ferao, R. Streubel, "Thiaphosphiranes and their complexes: systematic study on ring strain and ring cleavage reactions", *Inorg. Chem.*, **2016**, *55*, 9611-9619. DOI: 10.1021/acs.inorgchem.6b01322.

► T. Sugahara, J.-D. Guo, T. Sasamori, Y. Karatsu, Y. Furukawa, A. Espinosa Ferao, S. Nagase, N. Tokitoh, "Reaction of a Diaryldigermyne with Acetylenes: Synthesis of a 1,2-Digermabenzene and a 1,4-Digermabarrelene", *Bull. Chem. Soc. Jpn.*, **2016**, *89*, 1375-1384. DOI: 10.1246/bcsj.20160269.

► A. Espinosa Ferao, "Kinetic energy density per electron as quick insight into ring strain energies", *Tetrahedron Lett.*, **2016**, *57*, 5616-5619. DOI: 10.1016/j.tetlet.2016.10.115.

► A. Espinosa Ferao, R. García, "Fulvenization as characteristic geometric distortion in electron deficient ferrocenes", *Tetrahedron*, **2017**, *73*, 952-956. DOI: 10.1016/j.tet.2017.01.019.

► A. Espinosa Ferao, R. Streubel, "Coordination of N_2 and other small molecules to the phosphorus center of RPW$(CO)_5$ - A theoretical study on the Janus facets of the stabilization/activation problem", *Chem. Eur. J.*, **2017**, *23*, 8632-8643. DOI: 10.1002/chem.201700524. ***(Hot paper)***

► A. Espinosa Ferao, "Comparative computational study on the reaction of chloroacetone with trimethylphosphite: Perkow versus Michaelis-Arbuzov reaction paths", *J. Phys. Chem. A*, **2017**, *121*, 6517-6522. DOI: 10.1021/acs.jpca.7b06262.

► J. Faßbender, N. Künemund, A. Espinosa Ferao, G. Schnakenburg, R. Streubel, "Epoxide-like chemistry: 1,2-bifunctional P-ligands via stereo- and regioselective ring opening of an oxaphosphirane complex", *Organometallics*, **2018**, *37(8)*, 1331-1336. DOI: 10.1021/acs.organomet.8b00116.

► A. W. Kyri, F. Gleim, A. García Alcaraz, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Low-coordinate" 1,2-oxaphosphetanes – a new opportunity in coordination and main group chemistry", *Chem Commun.*, **2018**, *54(52)*, 7123-7126. DOI: 10.1039/C8CC02963F.

► A. Espinosa Ferao, "On the mechanism of trimethylphosphine-mediated reductive dimerization of ketones", *Inorg. Chem.*, **2018**, *57(14)*, 8058-8064. DOI: 10.1021/acs.inorgchem.7b02816.

► J. Faßbender, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Effects of diminished steric protection at phosphorus on stability and reactivity of oxaphosphirane complexes", *Dalton Trans.*, **2018**, *47(28)*, 9347-9354. DOI: 10.1039/C8DT01979G.

► J. Faßbender, G. Schnakenburg, D. P. Gates, A. Espinosa Ferao, R. Streubel, "Unconventional ionic ring-deconstruction pathways of a three-membered heterocycle", *Chem. Commun.*, **2018**, *54(99)*, 14013-14016. DOI: 10.1039/c8cc08713j.

► A. W. Kyri, F. Gleim, D. Becker, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Synthesis of free and ligated 1,2-thiaphosphetanes – expanding the pool of strained P-ligands", *Chem. Commun.*, **2019**, *55(11)*, 1615-1618. DOI: 10.1039/C8CC09892A.

► A. Khan, P. Junker, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "Competitive or sequential reaction of an electrophilic terminal phosphinidene metal(0) complex with allyl halides? [2+1]-Cycloaddition vs C-X bond insertion", *Chem Commun.*, **2019**, *55*, 9987-9990. DOI: 10.1039/C9CC05328J.

► V. Nesterov, R. Baierl, F. Hanusch, A. Espinosa Ferao, S. Inoue, "NHC-Stabilized Germanium and Tin Analogues of Heavier Nitriles: Synthesis, Reactivity, and Catalytic Application", *J. Am. Chem. Soc.*, **2019**, *141(37)*, 14576-14580, DOI: 10.1021/jacs.9b08741.

► A. Espinosa Ferao, R. Streubel, "1,2-Thiaphosphetanes: The quest for Wittig-type ring cleavage, rearrangement and sulfur atom transfer", *Inorg. Chem.*, **2020**, *59(5)*, 3110-3117, DOI: 10.1021/acs.inorgchem.9b03471.

► R. Kunzmann, Y. Omatsu, G. Schnakenburg, A. Espinosa Ferao, T. Yanagisawa, N. Tokitoh, R. Streubel, "A synthetic equivalent for unknown 1,3-zwitterions? – A K/OR phosphinidenoid complex with an additional Si-Cl function", *Chem. Commun.*, **2020**, *56,* 3899-3902, DOI: 10.1039/D0CC00024H.

► M. Más-Montoya, M. F. Montenegro, A. Espinosa Ferao, A. Tárraga, J. N. Rodriguez-Lopez, D. Curiel, "Rigid π-Extended Boron Difluoride Complex with Mega-Stokes Shift for Bioimaging", *Org. Lett.*, **2020**, *22(9)*, 3356-3360, DOI: 10.1021/acs.orglett.0c00782.

► T. Sugahara, A. Espinosa Ferao, A. Rey Planells, J.-D. Guo, S. Aoyama, K. Igawa, K. Tomooka, T. Sasamori, D. Hashizume, S. Nagase, N. Tokitoh, "1,2-Insertion Reactions of Alkynes into Ge–C Bonds of Arylbromogermylene", *Dalton Trans.*, **2020**, *49*, 7189-7196, DOI: 10.1039/D0DT01223H.

► A. Rey Planells, A. Espinosa Ferao, "Accurate ring strain energy calculations on saturated three-membered heterocycles with one group 13-16 element", *Inorg. Chem*, **2020**, *59*, 11503-11513, DOI: 10.1021/acs.inorgchem.0c01316.

► A. Espinosa Ferao, A. García Alcaraz, S. Zaragoza Noguera, R. Streubel "Terminal phosphinidene complex adducts with neutral and anionic O-donors and halides, and the search for a differentiating bonding descriptor", *Inorg. Chem*, **2020**, *59*, 12829-12841, DOI: 10.1021/acs.inorgchem.0c01874.

► P. Junker, Z.-W. Qu, T. Kalisch, G. Schnakenburg, A. Espinosa Ferao, R. Streubel, "A case study on the conversion of Li/Cl phosphinidenoid into phosphinidene complexes", *Dalton Trans.*, **2021**, *50*, 739-745, DOI: 10.1039/D0DT03884A.

► N. Volk, P. Malik, A. García Alcaraz, A. Espinosa Ferao, R. Streubel, "Chemistry of Oxaphosphirane Complexes", *Coord. Chem. Rev.*, accepted (ref: CCR_213818).

OTHERS

83 Participations (attendance and/or communication) in conferences either national (24) or international (59).

27 Scientific lectures upon invitation.

Substitute Management Committee (MC) and "Work Group 5" member of the European COST action CM0802 (*PhoSciNet*) since August 2009 (extinguished). Member of the COST action CM1302 (*SIPs*), "Work Group 1", since May 2014.

Member of the Editorial Board of *Journal of Chemistry*, Hindawi Publishing Corporation.

Member of the Editorial Board of *Journal of Inorganic Chemistry*, Hindawi Publishing Corporation (extinguished).

Projects evaluator for the National Science Agency of Argentina.

External collaborator in the German SFB-813 (Chemistry of Spin Centers) priority research cluster (project B4).

Member of the Spanish Royal Society of Chemistry (R.S.E.Q.)

Tetrahedron *"Top 25 cited author for 2010-11"* award for publication: *Tetrahedron*, **2010**, *66*, 3662-3667.

Bull. Chem. Soc. Jpn. award article for publication: *Bull. Chem. Soc. Jpn.*, **2016**, *89*, 1375-1384.

"Hot paper" for publication: *Chem. Eur. J.*, **2017**, *23*, 8632-8643.

Member of the Organizing Committee and editor of the Book of Abstracts (ISBN 978-84-693-2615-2) for the *XXIIIth Biennial Meeting of the Organic Chemistry Group of the Spanish Royal Chemical Society (R.S.E.Q.)*, June 2010.

Organizer and responsible for the workshop "*Computation of Ring Strain Energies*" at the Institute of Inorganic Chemistry - University of Bonn on December 4th - 8th, 2017, sponsored by the "IPID4all funding program" of the german DAAD agency.

Referee for various international journals, such as: J. Org. Chem., Chem. Phys. Letters, Synthetic Metals, J. Mol. Struct., Arkivoc, Bioorg. Med. Chem. Lett., Cen. Eur. J. Chem., PhysChemChemPhys, Eur. J. Inorg. Chem., Inorg. Chem., WIREs Comp. Mol. Sci., J. Lumin., Organometallics, Appl. Organometal. Chem., New J. Chem., Angew. Chem. Int. Ed., Open Chem., Appl. Catal., Organometallics, Comput. Chem., Polyhedron, J. Mol. Model., Arab. J. Chem., Lett. Org. Chem., J. Theor. Comput. Chem., Appl. Cat., Chem. Select, Synthesis