

JOSE ANTONIO DOBADO JIMENEZ

Grupo de Investigación: **MODELIZACION Y DISEÑO MOLECULAR** (Cod.: FQM174)

Departamento: Universidad de Granada. Química Orgánica

Citas en Google Scholar: <https://scholar.google.es/citations?user=7XFo1xwAAAAJ&hl=es>

Código ORCID: <http://orcid.org/0000-0001-7714-1715>

RG: https://www.researchgate.net/profile/Jose_Dobado

Correo electrónico: dobado@ugr.es

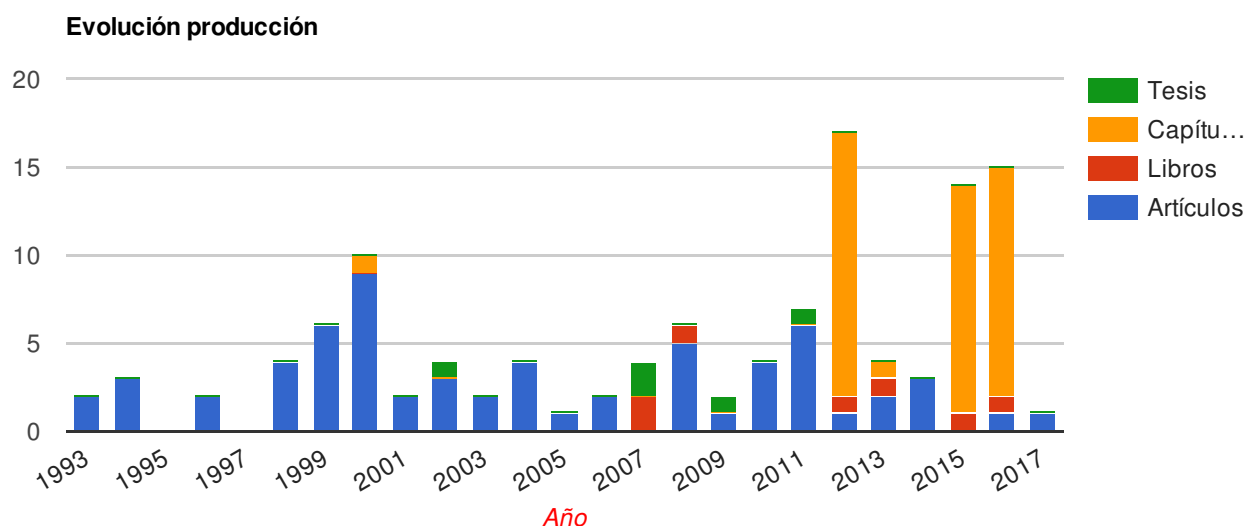
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Ficha del Directorio

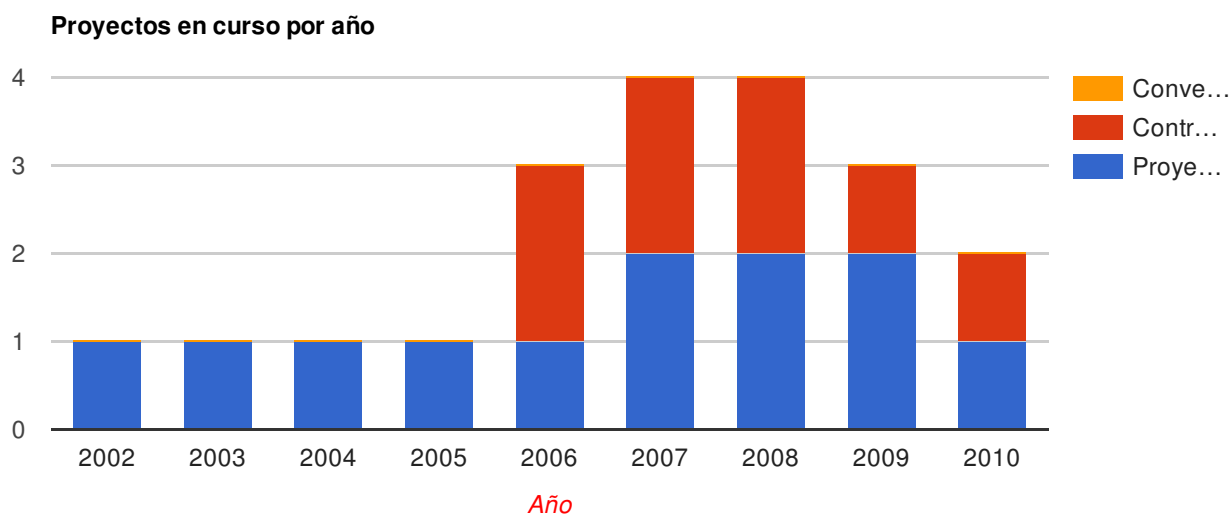
Producción 119

Artículos (64) Libros (7) Capítulos de Libros (43) Tesis dirigidas (5)



Proyectos dirigidos 5

Proyectos (3) Contratos (2) Convenios (0)



Actividades 0

Título publicación	Fuente	Tipo	Fecha
The role of weak interactions in lignin polymerization	Journal of molecular modeling	Artículo	2017
A computational study of bulk porous two-dimensional polymers related to graphyne	Physical chemistry chemical physics	Artículo	2016
Advanced organic synthesis experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Basic laboratory operations	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Basic operation experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Basic operation experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Determining physical and spectroscopic properties	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Experimental organic chemistry: laboratory manual	Academic press - elsevier	Libros	2016
Functional-group analysis	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Green chemistry	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Green chemistry experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Laboratory equipment	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Laboratory safety	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Microscale	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Microscale experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Organic synthesis experiments	Experimental organic chemistry: laboratory manual	Capítulo de libro	2016
Applications of modified and unmodified lignins	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Background and overview	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Biological properties of lignans	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Biosynthesis of lignin	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Chemical characterization and modifications of lignins	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Chemical characterization and modifications of lignins	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Detection and determination	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Functional and spectroscopic characterization of lignins	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
High-value chemical products	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Isolation of lignins	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Lignin and lignans as renewable raw materials	John wiley & sons	Libros	2015

Structure and chemical properties of lignans	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Structure and physicochemical properties	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Summary, conclusions, and prespectives on lignin chemistry	Lignin and lignans as renewable raw materials	Capítulo de libro	2015
Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage	International journal of hydrogen energy	Articulo	2014
Insight into the informational-structure behavior of the diels-alder reaction of cyclopentadiene and maleic anhydride	Journal of molecular modeling	Articulo	2014
Study by fluorescence of calix[4]arenes bearing heterocycles with anions: highly selective detection of iodide	Journal of inclusion phenomena and macrocyclic chemistry	Articulo	2014
Decoding the building blocks of life from the perspective of quantum information	Advances in quantum mechanics	Capítulo de libro	2013
From 7-azaindole to adenine: molecular recognition aspects on mixed-ligand cu(ii) complexes with deaza-adenine ligands	Dalton transactions	Articulo	2013
Structural consequences of the n7 and c8 translocation on the metal binding behavior of adenine	Inorganic chemistry	Articulo	2013
Tratado de quimica organica experimental	Editorial garceta	Libros	2013
Acidos carboxílicos y derivados	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Alcanos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Alcoholes, éteres y oxiranos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Aldehídos y cetonas	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Alquenos y dienos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Alquinos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Aminas	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Compuestos aromaticos sustituidos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Enolatos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Estructura y representación de las moléculas orgánicas	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Haloalcanos	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Insights on the binding ability of a new adenine analog: 7-amine-1,2,4-triazole[1,5-a]pyrimidine. synthesis and magnetic study of the first copper(ii) complexes	Dalton transactions	Articulo	2012
Introducción a la síntesis orgánica	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Isomería en las moléculas orgánicas	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012
Quimica orgánica: ejercicios comentados	Garceta grupo editorial	Libros	2012
Reacciones orgánica	Quimica orgánica: ejercicios comentados	Capítulo de libro	2012

Sustitución aromática en benceno y derivados	Química orgánica: ejercicios comentados	Capítulo de libro	2012
Contub v2.0 - algorithms for constructing c3-symmetric models of three-nanotube junctions	Journal of chemical information and modeling	Artículo	2011
Dinuclear silver(i) complexes for the design of metal-ligand networks based on triazolopyrimidines	Dalton transactions	Artículo	2011
Edge effects, electronic arrangement, and aromaticity patterns on finite-length carbon nanotubes	Physical chemistry chemical physics	Artículo	2011
Modelización molecular de nanotubos de carbono	Universidad de granada. química orgánica	Tesis doctoral	2011
N, p and as ylides and aza- and arsa-wittig reactions from topological analyses of electron density	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Artículo	2011
Nmr assignment in regioisomeric hydroquinones	Magnetic resonance in chemistry	Artículo	2011
Protecting-group-free synthesis of chokols	Journal of organic chemistry	Artículo	2011
Causes of energy destabilization in carbon nanotubes with topological defects	Theoretical chemistry accounts	Artículo	2010
Porous nanotube network: a novel 3-d nanostructured material with enhanced hydrogen storage capacity	Chemical communications	Artículo	2010
Reversible attachment of platinum alloy nanoparticles to nonfunctionalized carbon nanotubes	Acs nano	Artículo	2010
Weakening c-o bonds: ti(iii), a new reagent for alcohol deoxygenation and carbonyl coupling olefination	Journal of the american chemical society	Artículo	2010
Carbon···carbon weak interactions	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Artículo	2009
Estudio mecanocuántico, docking y dinámica molecular de tioazúcares como inhibidores de la proteína fucosidasa: algoritmos para el análisis conformacional y programa para el cálculo de constantes de acoplamiento vecinales (cal3jhh)	Universidad de granada. química orgánica	Tesis doctoral	2009
Cal3jhh: a java program to calculate the vicinal coupling constants (3jh,h) of organic molecules	Journal of computer - aided molecular design	Artículo	2008
Clar-kekule structuring in armchair carbon nanotubes	Organic letters	Artículo	2008
Electrochemically and photochemically active palladium(ii) heterotopic metallacalix[3]arenes	Chemical communications	Artículo	2008
Estudio computacional sobre la naturaleza del enlace carbono-metal: análisis topológico, qtaim y elf	Ugr	Libros	2008
Evidence of an unexpectedly long c-c bond (> 2.7 angstrom) in 1,3-metalladiyne complexes [cp2mccr](2) (m = ti, zr): qtaim and elf analyses	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Artículo	2008
Química sostenible: una alternativa creíble	Anales de química	Artículo	2008
Caracterización del enlace químico en compuestos de boro, iluros y reacciones de aza- y arsa-wittig	Ugr	Libros	2007
Caracterización del enlace químico en compuestos de boro, iluros y reacciones de aza- y arsa-wittig: qtaim y análisis elf de la densidad electrónica.	Universidad de granada. química orgánica	Tesis doctoral	2007
Estudio computacional sobre la naturaleza del enlace carbono-	Universidad de granada.	Tesis	2007

metal	química orgánica	doctoral	2007
Problemas resueltos de química orgánica	Thomson-paraninfo	Libros	2007
Conformational analysis of thiosugars: theoretical nmr chemical shifts and (3j)(h),(h) coupling constants of 5-thio-pyranose monosaccharides	Journal of carbohydrate chemistry	Articulo	2006
On the existence of alpha-agostic bonds: bonding analyses of titanium alkyl complexes	Organometallics	Articulo	2006
On the nature of metal-carbon bonding: aim and elf analyses of mchn (n=1-3) compounds containing early transition metals	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2005
Chemical bonding to n, p and as in ylides and their boron analogs	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2004
Contub: an algorithm for connecting two arbitrary carbon nanotubes	Journal of chemical information and computer sciences	Articulo	2004
On the 1,3-dipolar cycloaddition reactions of indenone with n-n-c dipoles: density functional theory calculations	Spectrochimica acta, part a: molecular and biomolecular spectroscopy	Articulo	2004
Structure and theoretical nmr chemical shifts of modified cyclodextrins	Journal of molecular structure. theochem	Articulo	2004
Bonding of atomic phosphorus to polycyclic hydrocarbons and curved graphitic surfaces	Journal of physics and chemistry of solids	Articulo	2003
Epoxides, cyclic sulfites, and sulfate from natural pentacyclic triterpenoids: theoretical calculations and chemical transformations	Journal of organic chemistry	Articulo	2003
Nanotubos grafiticos con disclinaciones: estructura electrónica, conductividad y topología	Universidad de granada. química orgánica	Tesis doctoral	2002
Structural and electronic effects of the interaction of metal cations with benzene	Journal of molecular structure. theochem	Articulo	2002
Structurally different dinuclear copper(ii) complexes with the same triazolopyrimidine bridging ligand	European journal of inorganic chemistry	Articulo	2002
Structure and bonding of weak hydrogen peroxide complexes	Journal of molecular structure. theochem	Articulo	2002
Recognizing a triple bond between main group atoms	Theoretical chemistry accounts	Articulo	2001
The three-center-four-electron (3c-4e) bond nature revisited. an atoms-in-molecules theory (aim) and elf study	Theoretical chemistry accounts	Articulo	2001
Chemical bonding in hypervalent molecules revised. 3. application of the atoms in molecules theory to y3x-ch2 (x = n, p, or as ; y = h or f) and h2x-gh(2) (x = o, s, or se) ylides	Journal of physics and chemistry of solids	Articulo	2000
Multiple bonding in four-coordinated titanium(iv) compounds	Inorganic chemistry	Articulo	2000
N-o and p-o bond nature in hypervalent compounds: is bader analysis basis-set and geometry independent?	Quantum systems in chemistry and physics, vol. 2:	Capítulo de libro	2000
On the aromaticity and meisenheimer rearrangement of strained heterocyclic amine, phosphine, and arsine oxides	Journal of organic chemistry	Articulo	2000
Regioselective enzymatic acylations of polyhydroxylated eudesmanes: semisynthesis, theoretical calculations, and biotransformation of cyclic sulfites	Journal of organic chemistry	Articulo	2000
Semi-synthesis of triterpene a-ring derivatives from cleanolic and			

Semi-synthesis of triterpene a-ring derivatives from oleanolic and maslinic acids. part ii. theoretical and experimental c-13 chemical shifts	Journal of chemical research	Articulo	2000
Semi-synthesis of triterpene a-ring derivatives from oleanolic and maslinic acids. theoretical and experimental c-13 chemical shifts	Journal of chemical research	Articulo	2000
Stabilization in neutral bicyclic sulfoxide compounds	Journal of computational chemistry	Articulo	2000
Structure and bonding of h ₂ o ₂ center dot center dot center dot x complexes with (x = no+, cn-, hcn, hnc, co)	Physical chemistry chemical physics	Articulo	2000
Theoretical characterization of 5-oxo, 7-oxo and 5-oxo-7-amino[1,2,4]triazolo[1,5-a]pyrimidines	Journal of the chemical society. perkin transactions. ii	Articulo	2000
Adenine-hydrogen peroxide system: dft and mp2 investigation	Journal of physical chemistry (1952)	Articulo	1999
Basis set superposition error-counterpoise corrected potential energy surfaces. application to hydrogen peroxide center dot center dot center dot x (x=f-, cl-, br-, li+, na+) complexes	Journal of chemical physics	Articulo	1999
Chemical bonding in hypervalent molecules revised. 2. application of the atoms in molecules theory to y(2)xz and y(2)xz(2) (y = h, f, ch ₃ ; x = o, s, se; z = o, s) compounds	Journal of physics and chemistry of solids	Articulo	1999
Metal-metal closed-shell interaction in m ₂ x ₂ (m = ag, cu; x = cl, br, i) and related compounds [ag ₂ br ₂](ph ₃)(3) and [cu ₂ cl ₂](ph ₃)(2): an rhf, mp2 and dft study	Journal of molecular structure. theochem	Articulo	1999
On the bonding isomerism in three-co-ordinated copper(i) thiocyanates	Journal of the chemical society. faraday transactions	Articulo	1999
Theoretical bonding description of alkylidene chalcogen (o, s, se) difluorides (h ₂ c=x ₂): planar versus bent conformations	Inorganic chemistry	Articulo	1999
Ab initio molecular study of hydrogen peroxide.: application of density functional methods	Journal of molecular structure. theochem	Articulo	1998
Chemical bonding in hypervalent molecules revised. application of the atoms in molecules theory to y-3 x and y-3 xz (y = h or ch ₃ ; x = n, p or as; z = o or s) compounds	Journal of physics and chemistry of solids	Articulo	1998
Para-fluor benzyl substituted bis indenyl metallocenes as catalyst precursors in ethylene polimerization	Journal of organometallic chemistry	Articulo	1998
Theoretical study on the urea¿hydrogen peroxide 1:1 complexes	Journal of physical chemistry (1952)	Articulo	1998
A theoretical investigation on the reactivity of 6-amino-3-methylpyrimidin-4(3h)-ones towards dmad. tandem diels-alder retro diels-alder (da/rda) reaction.	Tetrahedron	Articulo	1996
Mrci calculations of the ground and excited state potential energy surfaces of the 2,4-pentadien-1-iminium cation	Journal of physical chemistry (1952)	Articulo	1996
A comparative molecular mechanics, semiempirical and ab-initio study of saturated 5-membered rings	Journal of molecular structure. theochem	Articulo	1994
Ab-initio calculations of the hydrogen-peroxide hydrogen halide-complexes (hooh...xh, x=f, cl)	Journal of physical chemistry (1952)	Articulo	1994
Ab-initio molecular-orbital study of the hydrogen peroxide-water complex (hooh ... h ₂ o)	Journal of physical chemistry (1952)	Articulo	1994
Ab initio molecular orbital calculation of the hydrogen peroxide dimer: study of basis set superposition error	Journal of physical chemistry (1952)	Articulo	1993
The structure and molecular mechanics calculations of the cyclic (1-¿)-beta-d-glucan secreted by rhizobium-tropicci ciat 899	Journal of molecular structure	Articulo	1993

	Título proyecto	Tipo	Inicio	Fin
1	Modelización y diseño molecular de uniones de tres nanotubos grafíticos para su aplicación como transistores	Proyecto	10/1/07	9/30/10
2	Fenómenos de transporte electrónico en uniones de múltiples nanotubos grafíticos	Contrato	4/1/06	4/1/10
3	Fenómenos de transporte electrónico en uniones de múltiples nanotubos grafíticos	Proyecto	2/1/06	2/28/09
4	Fenómenos de transporte electrónico en uniones de múltiples nanotubos grafíticos	Contrato	4/1/06	4/1/08
5	Estudios teóricos sobre la naturaleza del enlace químico	Proyecto	11/1/02	10/31/05

Actividades 0

Título actividad	Fuente	Tipo	Fecha
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Colaboradores

- FRANCISCO GARCIA CALVO-FLORES (47)
- JOAQUIN ISAC GARCIA (42)
- SANTIAGO MELCHOR FERRER (20)
- ISAAC VIDAL DAZA (8)
- ANDRES PARRA SANCHEZ (3)
- JUAN MANUEL SALAS PEREGRÍN (3)
- ALEJANDRO FERNANDEZ BARRERO (2)
- ALICIA DOMINGUEZ MARTIN (2)
- ANDRES GARCIA-GRANADOS LOPEZ DE HIERRO (2)
- DUANE CHOQUESILLO LAZARTE (2)
- JESÚS SÁNCHEZ-DEHESA MORENO-CID (2)
- JOSE FRANCISCO QUILEZ DEL MORAL (2)
- JOSEFA MARIA GONZALEZ PEREZ (2)
- JUAN NICLOS GUTIERREZ (2)
- MARIA DEL MAR HERRADOR DEL PINO (2)
- RODOLFO OCTAVIO ESQUIVEL OLEA (2)
- ANA BELÉN CABALLERO HERNÁNDEZ (1)
- ANTONIO RODRÍGUEZ DIÉGUEZ (1)
- FRANCISCO SANTOYO GONZALEZ (1)
- FÁTIMA LINARES ORDOÑEZ (1)
- JORGE ANDRÉS RODRÍGUEZ NAVARRO (1)
- JOSE MARIA ARIAS PEÑALVER (1)
- JOSÉ HORACIO RODRÍGUEZ DIÉGUEZ (1)
- JUAN CARLOS ANGULO IBÁÑEZ (1)
- JULIETA VERÓNICA CATALÁN (1)
- MIGUEL ANGEL GALINDO CUESTA (1)
- MIGUEL QUIRÓS OLOZÁBAL (1)
- M^a CARMEN PÉREZ MORALES (1)
- PILAR LOPEZ RODRIGUEZ (1)