

Angeles Peñ̃a-Gallego

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	A Tetracyanobutadiene Spirobifluorene: Synthesis, Enantiomeric Resolution and Chiroptical Properties. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	2.4	6
2	ON/OFF Spiroconjugation through Peripheral Functionalization: Impact on the Reactivity and Chiroptical Properties of Spirobifluorenes. <i>ChemPlusChem</i> , 2022, 87, e202100554.	2.8	3
3	Chemoselectivity on the synthesis of iridacycles: A theoretical and experimental study. <i>Inorganica Chimica Acta</i> , 2021, 517, 120189.	2.4	5
4	Key factors in the synthesis of polycyclic iridaaromatics <i>via</i> the methoxyalkenylcarbene pathway. <i>Dalton Transactions</i> , 2021, 50, 11216-11220.	3.3	8
5	The effect of spin polarization on the electron transport of molecular wires with diradical character. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4777-4783.	2.8	7
6	Tracking the Transition from Pericyclic to Pseudopericyclic Reaction Mechanisms Using Multicenter Electron Delocalization Analysis: The [1,3] Sigmatropic Rearrangement. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8337-8344.	2.5	0
7	Detecting Molecular Plasmons by Means of Electron Density Descriptors. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1585-1593.	3.1	6
8	Distinct Helical Molecular Orbitals through Conformational Lock**. <i>Chemistry - A European Journal</i> , 2020, 26, 17342-17349.	3.3	17
9	Unimolecular Electrical Rectification Understood Through Electron Deformation Orbitals. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17924-17931.	3.1	1
10	Clar Goblet and Aromaticity Driven Multiradical Nanographenes. <i>Chemistry - A European Journal</i> , 2020, 26, 16138-16143.	3.3	9
11	Design and synthesis of chiral spirobifluorenes. <i>Chirality</i> , 2020, 32, 464-473.	2.6	6
12	Spirobifluorene Metallaaromatics. <i>Chemistry - A European Journal</i> , 2019, 25, 13496-13499.	3.3	17
13	Chiroptical Symmetry Analysis of Trianglimines: A Case Study. <i>Symmetry</i> , 2019, 11, 1245.	2.2	3
14	Assessing the Reversed Exponential Decay of the Electrical Conductance in Molecular Wires: The Undeniable Effect of Static Electron Correlation. <i>Nano Letters</i> , 2019, 19, 7394-7399.	9.1	13
15	Chiroptical Symmetry Analysis: Exciton Chirality-Based Formulae to Understand the Chiroptical Responses of C _n and D _n Symmetric Systems. <i>Molecules</i> , 2019, 24, 141.	3.8	5
16	NMR spectroscopy for assessing cocaine-functional monomer interactions when preparing molecularly imprinted polymers. <i>Microchemical Journal</i> , 2019, 147, 813-817.	4.5	21
17	Metallaaromatic biaryl atropisomers. <i>Chemical Communications</i> , 2018, 54, 10974-10976.	4.1	21
18	Kinetic study of the formation of <i>N</i> -chloro compounds using <i>N</i> -chlorosuccinimide. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 407-418.	1.9	12

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19	Theoretical study of the decomposition of ethyl and ethyl 3-phenyl glycidate. Journal of Molecular Modeling, 2013, 19, 315-320.	1.8	0
20	A MP2 and DFT study of the influence of complexation on the aromatic character of phosphole. Journal of Molecular Modeling, 2012, 18, 765-770.	1.8	2
21	Molecular recognition-based catalysis in nucleophilic aromatic substitution: a mechanistic study. New Journal of Chemistry, 2012, 36, 1519.	2.8	6
22	Effect of microhydration on the guanidinium ⁺ benzene interaction. Journal of Chemical Physics, 2011, 135, 214301.	3.0	17
23	A computational study of the mechanism of the unimolecular elimination of α,β -unsaturated aldehydes in the gas phase. Journal of Molecular Modeling, 2011, 17, 21-26.	1.8	11
24	A MP2 and DFT study of the aromatic character of polyphosphaphospholes. Is the pyramidal character the only factor to take into consideration?. Journal of Molecular Modeling, 2011, 17, 1267-1272.	1.8	14
25	Study of the interaction between aniline and CH ₃ CN, CH ₃ Cl and CH ₃ F. Theoretical Chemistry Accounts, 2011, 128, 531-539.	1.4	8
26	Computational study of the interaction of indole-like molecules with water and hydrogen sulfide. Journal of Chemical Physics, 2011, 135, 134310.	3.0	10
27	Study of the ferrocene-lithium cation interaction by DFT calculations: an in-depth analysis of the existence of a planetary system. Tetrahedron, 2009, 65, 2368-2371.	1.9	17
28	Cation- π and anion- π interactions: Changes in aromaticity upon complexation. Chemical Physics Letters, 2008, 452, 49-53.	2.6	25
29	Computational Study on the Characteristics of the Interaction in Naphthalene- π - π -(H ₂ X) _n (X = O, S) Clusters. Journal of Physical Chemistry A, 2008, 112, 6344-6350.	2.5	54
30	Comment on "A Theoretical Investigation of the Interactions between Water Molecules and Ionic Liquids". Journal of Physical Chemistry B, 2008, 112, 13465-13466.	2.6	3
31	Study of the interaction in clusters formed by phenol and CH ₃ X (X=CN,F,Cl) molecules. Journal of Chemical Physics, 2008, 128, 194311.	3.0	11
32	Characteristics of the interaction of azulene with water and hydrogen sulfide: A computational study. Journal of Chemical Physics, 2008, 129, 084305.	3.0	20
33	A Comparative Theoretical Study of the Pericyclic-pseudopericyclic Character in a Group of Cyclizations of Dienylketenes to Cyclohexadienones. Journal of Physical Chemistry A, 2007, 111, 2935-2940.	2.5	12
34	Theoretical study of the walk rearrangement in perfluorotetramethyl (Dewar thiophene) exo-S-oxide. Tetrahedron, 2007, 63, 2191-2198.	1.9	10
35	A DFT study of the [4+2] cycloadditions of conjugated ketenes (vinylketene, imidoalkylketene and) properties. Tetrahedron, 2007, 63, 4937-4943.	1.9	13
36	A theoretical study of the influence of BF ₃ on the reaction path of the [4+2] cycloaddition of vinylketene with formaldimine. Tetrahedron, 2007, 63, 11617-11621.	1.9	4

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37	A computational study of the electrocyclization of o-divinylbenzene and derivatives. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 141-151.	1.5	6
38	A DFT Study of the Concerted Cyclisation of 3-Azidopropenal to Isoxazole: Is it a Pseudopericyclic Reaction According to Its Magnetic Properties?. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3228-3232.	2.4	17
39	A Density Functional Theory Study on the Electrocyclization of 1,2,4,6-Heptatetraene Analogues: Converting a Pericyclic to a Pseudopericyclic Reaction. <i>Chemistry - A European Journal</i> , 2005, 11, 5966-5974.	3.3	24
40	A DFT Study of the Pericyclic/Pseudopericyclic Character of Cycloaddition Reactions of Ethylene and Formaldehyde to Buta-1,3-dien-1-one and Derivatives. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5636-5644.	2.5	17
41	Are Electrocyclization Reactions of (3Z)-1,3,5-Hexatrienone and Nitrogen Derivatives Pseudopericyclic? A DFT Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 3921-3928.	3.2	34
42	A DFT Study of the Boulton-Katritzky Rearrangement of (5R)-4-Nitrosobenz[c]isoxazole and Its Anion: Pseudopericyclic Reactions with Aromatic Transition States. <i>Journal of Organic Chemistry</i> , 2004, 69, 7013-7017.	3.2	41
43	Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. <i>Chemical Physics Letters</i> , 2003, 369, 1-7.	2.6	4
44	DFT Study of Pericyclic and Pseudopericyclic Thermal Cheletropic Decarbonylations. Evaluation of Magnetic Properties. <i>Journal of Organic Chemistry</i> , 2003, 68, 8823-8830.	3.2	39
45	The Role of Aromaticity in the Planarity of Lumiflavin. <i>Journal of Organic Chemistry</i> , 2002, 67, 6347-6352.	3.2	34
46	Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. <i>Chemical Physics Letters</i> , 2002, 353, 418-425.	2.6	17
47	The unimolecular dissociation of the propionyl radical: A classical dynamics study. <i>Journal of Chemical Physics</i> , 2001, 114, 3546-3553.	3.0	5
48	Direct dynamics simulation of the methanethiol cation decomposition. <i>Chemical Physics Letters</i> , 2000, 324, 88-94.	2.6	11
49	A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. <i>Computational and Theoretical Chemistry</i> , 2000, 497, 105-113.	1.5	9
50	Intermolecular interactions and cooperative effects in acetonitrile clusters. An ab initio molecular orbital study. <i>Computational and Theoretical Chemistry</i> , 2000, 498, 21-28.	1.5	45
51	DFT conformational study of cysteine in gas phase and aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2000, 498, 191-200.	1.5	64
52	Dynamics of the cis-trans isomerization and Cl-O dissociation of chlorine nitrite. Classical trajectory and statistical calculations. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5393-5399.	2.8	8
53	MRCI Calculation, Scaling of the External Correlation, and Modeling of Potential Energy Curves for HCl and OCl. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6241-6246.	2.5	9
54	An ab initio study of a model compound of penicillins. <i>Computational and Theoretical Chemistry</i> , 1999, 491, 177-185.	1.5	10

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55	A DFT study of a model compound of vitamin D. Computational and Theoretical Chemistry, 1999, 492, 143-150.	1.5	2
56	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. Journal of Chemical Physics, 1999, 110, 11323-11334.	3.0	17
57	Classical Trajectory Study of the Cis \rightleftharpoons Trans Isomerization and F \rightleftharpoons O Dissociation of FONO. Journal of Physical Chemistry A, 1998, 102, 8708-8715.	2.5	7