Iker LeÃ³n

List of Publications by Year
in descending order

83 papers	1,191 citations	430874 18 h-index	477307 29 g-index
89 all docs	89 docs citations	89 times ranked	880 citing authors

#	Article	IF	Citations
1	Millimetre-wave laboratory study of glycinamide and a search for it with ALMA towards Sagittarius B2(N). Astronomy and Astrophysics, 2022, 657, A99.	5.1	7
2	Unleashing the shape of l-DOPA at last. Physical Chemistry Chemical Physics, 2022, 24, 3546-3554.	2.8	2
3	Rotational Spectrum and Conformational Analysis of Perillartine: Insights into the Structureâ€“Sweetness Relationship. Molecules, 2022, 27, 1924.	3.8	1
4	Shapeâ€Shifting Molecules: Unveiling the Valence Tautomerism Phenomena in Bare Barbaralones. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
5	Computational study on the affinity of potential drugs to SARS-CoV-2 main protease. Journal of Physics Condensed Matter, 2022, 34, 294005.	1.8	2
6	Noncovalent interactions in isolated molecular aggregates: From single molecules to nanostructures. , 2021, , 143-188.		0
7	The role of the intramolecular interactions in the structural behavior of biomolecules: Insights from rotational spectroscopy. , 2021, , 93-141.		15
8	Revisiting the Spectroscopy of Water Dimer in Jets. Journal of Physical Chemistry Letters, 2021, 12, 1316-1320.	4.6	7
9	Attosecond state-resolved carrier motion in quantum materials probed by soft x-ray XANES. Applied Physics Reviews, 2021, 8, .	11.3	30
10	Exploring the Maze of Cycloserine Conformers in the Gas Phase Guided by Microwave Spectroscopy and Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 2121-2129.	2.5	19
11	Rotational spectroscopic study and astronomical search for propiolamide in Sgr B2(N). Astronomy and Astrophysics, 2021, 647, A55.	5.1	5
12	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie, 2021, 133, 17550-17554.	2.0	0
13	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. ChemPlusChem, 2021, 86, 1374-1386.	2.8	14
14	Laboratory Detection of Cyanoacetic Acid: A Jet-cooled Rotational Study. Astrophysical Journal, 2021, 915, 76.	4.5	4
15	Shape of Testosterone. Journal of Physical Chemistry Letters, 2021, 12, 6983-6987.	4.6	12
16	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie - International Edition, 2021, 60, 17410-17414.	13.8	10
17	An innovative approach for the generation of species of the interstellar medium. Angewandte Chemie - International Edition, 2021, 60, 24461-24466.	13.8	9
18	Intrinsic folding of the cysteine residue: competition between folded and extended forms mediated by the â€“SH group. Physical Chemistry Chemical Physics, 2020, 22, 20284-20294.	2.8	9

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19	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie - International Edition, 2020, 59, 14081-14085.	13.8	14
20	A rotational study of the AlaAla dipeptide. Physical Chemistry Chemical Physics, 2020, 22, 13867-13871.	2.8	10
21	Formation of interstellar cyanoacetamide: a rotational and computational study. Astronomy and Astrophysics, 2020, 644, A3.	5.1	4
22	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie, 2020, 132, 14185-14189.	2.0	0
23	Gasâ€Phase Conformational Map of the Amino Acid Isovaline. ChemPhysChem, 2020, 21, 525-530.	2.1	1
24	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	2.8	0
25	The Shape of the Archetypical Oxocarbon Squaric Acid and Its Water Clusters. Chemistry - A European Journal, 2019, 25, 10748-10755.	3.3	7
26	Frontispiece: Unveiling the Neutral Forms of Glutamine. Angewandte Chemie - International Edition, 2019, 58, .	13.8	0
27	The Laboratory Millimeter and Submillimeter Rotational Spectrum of Lactaldehyde and an Astronomical Search in Sgr B2(N), Orion-KL, and NGC 6334I. Astrophysical Journal, 2019, 883, 18.	4.5	8
28	Unveiling the Neutral Forms of Glutamine. Angewandte Chemie, 2019, 131, 16148-16153.	2.0	8
29	Unveiling the Neutral Forms of Glutamine. Angewandte Chemie - International Edition, 2019, 58, 16002-16007.	13.8	27
30	Elucidating the multiple structures of pipecolic acid by rotational spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 4155-4161.	2.8	8
31	Excited state dynamics of aniline homoclusters. Physical Chemistry Chemical Physics, 2019, 21, 3098-3105.	2.8	5
32	Influence of the solvent in the electronic excitation of aromatic alcohols: Excited state IR-UV of propofol(H2O)8. Journal of Chemical Physics, 2019, 150, 214306.	3.0	2
33	Rotational Spectrum of Saccharin: Structure and Sweetness. Journal of Physical Chemistry A, 2019, 123, 2756-2761.	2.5	5
34	Laser Ablation Assists Cyclization Reactions of Hydantoic Acid: A Proof for the Near-Attack Conformation Theory?. Journal of Physical Chemistry Letters, 2019, 10, 1325-1330.	4.6	15
35	Frontispiz: Unveiling the Neutral Forms of Glutamine. Angewandte Chemie, 2019, 131, .	2.0	0
36	Unveiling the nâ†'Ï€* interactions in dipeptides. Communications Chemistry, 2019, 2, .	4.5	30

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37	The effect of N-methylation on the conformational landscape of alanine: the case of N-methyl-l-alanine. Physical Chemistry Chemical Physics, 2018, 20, 29159-29165.	2.8	2
38	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
39	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19
40	Probing the structures and bonding of auropolyynes, Auâ€"(Câ‰¡C)nâ€"Auâ¯ (n = 1â€“3), using high-resolution photoelectron imaging. Journal of Chemical Physics, 2018, 149, 144307.	3.0	13
41	The Structural Signs of Sweetness in Artificial Sweeteners: A Rotational Study of Sorbitol and Dulcitol. ChemPhysChem, 2018, 19, 3334-3340.	2.1	16
42	Glycinamide, a Glycine Precursor, Caught in the Gas Phase: A Laser-ablation Jet-cooled Rotational Study. Astrophysical Journal, 2018, 861, 70.	4.5	10
43	The last link of the x-aminobutyric acid series: the five conformers of Î²-aminobutyric acid. Physical Chemistry Chemical Physics, 2018, 20, 15574-15580.	2.8	4
44	Dispersive soft x-ray absorption fine-structure spectroscopy in graphite with an attosecond pulse. Optica, 2018, 5, 502.	9.3	47
45	Phenyl-Î²-D-glucopyranoside and Phenyl-Î²-D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions. Frontiers in Physics, 2018, 6, .	2.1	8
46	Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, 10291-10295.	3.3	12
47	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	4.6	14
48	Sugarâ€"peptidic bond interactions: spectroscopic characterization of a model system. Physical Chemistry Chemical Physics, 2017, 19, 12013-12021.	2.8	7
49	Competition between stacked and hydrogen bonded structures of cytosine aggregates. Physical Chemistry Chemical Physics, 2017, 19, 8826-8834.	2.8	9
50	Axialâ€"equatorial isomerism and semiexperimental equilibrium structures of fluorocyclohexane. Physical Chemistry Chemical Physics, 2017, 19, 29162-29169.	2.8	18
51	The role of amino acid side chains in stabilizing dipeptides: the laser ablation Fourier transform microwave spectrum of Ac-Val-NH₂. Physical Chemistry Chemical Physics, 2017, 19, 24985-24990.	2.8	28
52	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
53	Femtosecond Excited State Dynamics of Size Selected Neutral Molecular Clusters. Journal of Physical Chemistry Letters, 2016, 7, 2797-2802.	4.6	10
54	Probing the electronic structure and Auâ€"C chemical bonding in AuCnâ¯ and AuCnHâ¯ (n = 2, 4, and 6) using high-resolution photoelectron spectroscopy. Journal of Chemical Physics, 2016, 145, 064304.	3.0	18

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55	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	2.8	23
56	Mass resolved IR spectroscopy of anilineâ€“water aggregates. Physical Chemistry Chemical Physics, 2016, 18, 27336-27341.	2.8	15
57	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
58	Influence of dispersive forces on the final shape of a reverse micelle. Physical Chemistry Chemical Physics, 2015, 17, 2241-2245.	2.8	13
59	The design and construction of a high-resolution velocity-map imaging apparatus for photoelectron spectroscopy studies of size-selected clusters. Review of Scientific Instruments, 2014, 85, 083106.	1.3	131
60	Probing the electronic structure and Auâ€“C chemical bonding in AuC2â^' and AuC2 using high-resolution photoelectron spectroscopy. Journal of Chemical Physics, 2014, 140, 084303.	3.0	26
61	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	2.8	9
62	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	2.8	4
63	Behind the Reactivity of Lactones: A Computational and Spectroscopic Study of PhenolÂ·Î³-Butyrolactone. Journal of Physical Chemistry A, 2014, 118, 2568-2575.	2.5	3
64	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	13.8	14
65	IR mass-resolved spectroscopy of complexes without chromophore: CyclohexanolÂ·(H2O)n, n = 1â€“3 and cyclohexanol dimer. Journal of Chemical Physics, 2013, 139, 174312.	3.0	15
66	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	2.6	11
67	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	2.8	16
68	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	2.1	8
69	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	13.8	31
70	Transition from Planar to Nonplanar Hydrogen Bond Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2â€“4. Journal of Physical Chemistry A, 2013, 117, 3396-3404.	2.5	3
71	High resolution photoelectron imaging of Au2â^'. Journal of Chemical Physics, 2013, 138, 184304.	3.0	46
72	Resonant photoelectron spectroscopy of Au2â^' via a Feshbach state using high-resolution photoelectron imaging. Journal of Chemical Physics, 2013, 139, 194306.	3.0	11

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73	Communication: Vibrational spectroscopy of Au4 from high resolution photoelectron imaging. Journal of Chemical Physics, 2013, 139, 021106.	3.0	38
74	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	3.0	18
75	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	2.8	25
76	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	2.8	40
77	Mass-Resolved Infrared Spectroscopy of Complexes without Chromophore by Nonresonant Femtosecond Ionization Detection. Journal of Physical Chemistry A, 2012, 116, 6798-6803.	2.5	19
78	A Spectroscopic Approach to the Solvation of Anesthetics in Jets: Propofol(H2O)n, n = 4â€“6. Journal of Physical Chemistry A, 2012, 116, 8934-8941.	2.5	18
79	A Spectroscopic and Computational Study of Propofol Dimers and Their Hydrated Clusters. ChemPhysChem, 2012, 13, 3819-3826.	2.1	23
80	Combined Experimental and Theoretical Study of the Benzocaine/Ar van der Waals System in Supersonic Expansions. Journal of Physical Chemistry A, 2009, 113, 982-988.	2.5	11
81	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	2.8	21
82	An innovative approach for the generation of species of the interstellar medium. Angewandte Chemie, 0, , .	2.0	3
83	Shapeâ€Shifting Molecules: Unveiling the Valence Tautomerism Phenomena in Bare Barbaralones. Angewandte Chemie, 0, , .	2.0	0