Lucas C. Ducati

List of Publications by Year
in descending order

60	826	516710 16	552781 26
papers	citations	h-index	g-index

61	61	61	946
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecules with All Triple Bonds: OCBBCO, N₂BBN₂, and [OBBBBO]^{2â^'}. Journal of Physical Chemistry A, 2009, 113, 11693-11698.	2.5	69
2	Transuranic Hybrid Materials: Crystallographic and Computational Metrics of Supramolecular Assembly. Journal of the American Chemical Society, 2017, 139, 10843-10855.	13.7	58
3	Engaging the Terminal: Promoting Halogen Bonding Interactions with Uranyl Oxo Atoms. Chemistry - A European Journal, 2017, 23, 15355-15369.	3.3	46
4	The unexpected roles of Ïƒ and Ï€ orbitals in electron donor and acceptor group effects on the ¹³C NMR chemical shifts in substituted benzenes. Chemical Science, 2017, 8, 6570-6576.	7.4	39
5	The halogen effect on the ¹³C NMR chemical shift in substituted benzenes. Physical Chemistry Chemical Physics, 2018, 20, 11247-11259.	2.8	34
6	Heavy Halogen Atom Effect on ¹³C NMR Chemical Shifts in Monohalo Derivatives of Cyclohexane and Pyran. Experimental and Theoretical Study. Journal of Chemical Theory and Computation, 2009, 5, 2222-2228.	5.3	32
7	Experimental, SOPPA(CCSD), and DFT Analysis of Substitutent Effects on NMR1JCFCoupling Constants in Fluorobenzene Derivatives. Journal of Physical Chemistry A, 2011, 115, 1272-1279.	2.5	32
8	Conformational preferences for some 5-substituted 2-acetylthiophenes through infrared spectroscopy and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1071-1076.	3.9	28
9	Proposal for crystallization of 3-amino-4-halo-5-methylisoxazoles: an energetic and topological approach. CrystEngComm, 2015, 17, 7381-7391.	2.6	27
10	Analysis of Canonical Molecular Orbitals to Identify Fermi Contact Coupling Pathways. 1. Through-Space Transmission by Overlap of 31P Lone Pairs. Journal of Physical Chemistry A, 2010, 114, 1044-1051.	2.5	23
11	Are hydrogen bonds responsible for glycine conformational preferences?. Chemical Physics, 2011, 387, 85-91.	1.9	23
12	Thermochromic Uranyl Isothiocyanates: Influencing Charge Transfer Bands with Supramolecular Structure. Inorganic Chemistry, 2018, 57, 2455-2471.	4.0	19
13	Revisiting NMR Through-Space J_{FF} Spinâ€“Spin Coupling Constants for Getting Insight into Proximate F---F Interactions. Journal of Physical Chemistry A, 2014, 118, 5068-5075.	2.5	18
14	Effects of stereoelectronic interactions on the relativistic spinâ€“orbit and paramagnetic components of the ¹³C NMR shielding tensors of dihaloethenes. Physical Chemistry Chemical Physics, 2015, 17, 19315-19324.	2.8	18
15	Ionic Liquid Solvation versus Catalysis: Computational Insight from a Multisubstituted Imidazole Synthesis in [Et 2 NH 2][HSO 4]. ChemistryOpen, 2016, 5, 460-469.	1.9	18
16	A study of the rotational barriers for some organic compounds using the G3 and G3CEP theories. Journal of Molecular Modeling, 2014, 20, 2199.	1.8	17
17	Quadrupolar ¹⁴N NMR Relaxation from Force-Field and Ab Initio Molecular Dynamics in Different Solvents. Journal of Chemical Theory and Computation, 2019, 15, 509-519.	5.3	17
18	A theoretical investigation of the dictating forces in small amino acid conformational preferences: The case of glycine, sarcosine and N,N-dimethylglycine. Chemical Physics, 2013, 421, 32-38.	1.9	16

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19	Conformational Analysis and Intramolecular Interactions of <scp>l</scp>-Proline Methyl Ester and Its N-Acetylated Derivative through Spectroscopic and Theoretical Studies. Journal of Physical Chemistry A, 2014, 118, 1748-1758.	2.5	16
20	Critical analysis of the throughâ€space transmission of NMR J_{FH} spinâ€“spin coupling constants. International Journal of Quantum Chemistry, 2012, 112, 3158-3163.	2.0	15
21	NMR spinâ€“spin coupling constants: bond angle dependence of the sign and magnitude of the vicinal³J_{HF}coupling. Physical Chemistry Chemical Physics, 2016, 18, 24119-24128.	2.8	14
22	NMR J-Coupling Constants of Tlâ€“Pt Bonded Metal Complexes in Aqueous Solution: Ab Initio Molecular Dynamics and Localized Orbital Analysis. Inorganic Chemistry, 2016, 55, 12011-12023.	4.0	14
23	The lack of intramolecular hydrogen bonding and the side chain effect in alanine conformers. Journal of Molecular Structure, 2012, 1014, 12-16.	3.6	13
24	p-Aminobenzoic acid protonation dynamics in an evaporating droplet by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2021, 23, 19659-19672.	2.8	13
25	Conformational and stereoelectronic investigation of chloromethyl methyl sulfide and its sulfinyl and sulfonyl analogs. Journal of Molecular Structure, 2006, 800, 45-50.	3.6	12
26	Studies on the s-cisâ€“trans isomerism for some furan derivatives through IR and NMR spectroscopies and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 84-89.	3.9	11
27	The case of intramolecular hydrogen bonding, hyperconjugation and classical effects on the conformational isomerism of substituted carbonyl and thiocarbonyl compounds. Computational and Theoretical Chemistry, 2008, 851, 147-157.	1.5	10
28	Phenylalanine and tyrosine methyl ester intramolecular interactions and conformational analysis by 1H NMR and infrared spectroscopies and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 482-489.	3.9	10
29	Probing the geometry reorganization from solution to gas-phase in putrescine derivatives by IRMPD, ¹H-NMR and theoretical calculations. Physical Chemistry Chemical Physics, 2017, 19, 24330-24340.	2.8	10
30	A new Pu(<scp>iii</scp>) coordination geometry in (C₅H₅NBr)₂[PuCl₃(H₂O)₅]Â·2ClÂ·2H₂O as obtained via supramolecular assembly in aqueous, high chloride media. Chemical Communications, 2017, 53, 10816-10819.	4.1	10
31	Dealing with Hydrogen Bonding on the Conformational Preference of 1,3-Aminopropanols: Experimental and Molecular Dynamics Approaches. Journal of Physical Chemistry A, 2019, 123, 8583-8594.	2.5	9
32	Solvent effect on the ¹⁹⁵Pt NMR properties in pyridonate-bridged Pt^{III} dinuclear complex derivatives investigated by ab initio molecular dynamics and localized orbital analysis. Physical Chemistry Chemical Physics, 2021, 23, 12864-12880.	2.8	9
33	Influence of tetralkylammonium cations on the formation of silicoaluminophosphates CAL-2. Microporous and Mesoporous Materials, 2009, 120, 187-194.	4.4	8
34	Difference between 2JC2H3 and 2JC3H2 spin-spin couplings in heterocyclic five- and six-membered rings as a probe for studying Ï*f*-ring currents: a quantum chemical analysis. Magnetic Resonance in Chemistry, 2010, 48, S151-S158.	1.9	8
35	Unexpected Geometrical Effects on Paramagnetic Spinâ€“Orbit and Spinâ€“Dipolar ²J_{FF} Couplings. Journal of Physical Chemistry A, 2012, 116, 4930-4933.	2.5	8
36	Exploring the G3 method in the study of rotational barrier of some simple molecules. International Journal of Quantum Chemistry, 2010, 110, 2006-2014.	2.0	7

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37	1H NMR and theoretical studies on the conformational equilibrium of tryptophan methyl ester. Journal of Molecular Structure, 2013, 1050, 174-179.	3.6	7
38	A theoretical and experimental ¹H NMR spectroscopy study of the stereoelectronic interactions that rule the conformational energies of alanine and valine methyl ester. Journal of Physical Organic Chemistry, 2013, 26, 849-857.	1.9	7
39	Experimental and theoretical evaluation on the conformational behavior of <scp>l</scp>-aspartic acid dimethyl ester and its N-acetylated derivative. RSC Advances, 2015, 5, 18013-18024.	3.6	7
40	Plutonium chlorido nitrato complexes: ligand competition and computational metrics for assembly and bonding. Chemical Communications, 2018, 54, 12014-12017.	4.1	7
41	A critical evaluation of the s-cisâ€“trans isomerism of 2-acetylpyrrole and its N-methyl derivative through infrared and NMR spectroscopies and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 196-203.	3.9	6
42	13C NMR: nJCH and 1JCC scalar spinâ€“spin coupling constants (SSCCs) for some 3-monosubstituted 2-methylpropenes. Journal of Molecular Structure, 2014, 1068, 170-175.	3.6	6
43	Formation of isomers of anionic hemiesters of sugars and carbonic acid in aqueous medium. Carbohydrate Research, 2016, 428, 18-22.	2.3	6
44	Analyzing the Nâ€“H+â€¦Ï€ interactions of protonated tryptophan and phenylalkylamines using QTAIM, NCI, and NBO. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
45	Stereochemical Dependence of ³J_{CH} Coupling Constants in 2-Substituted 4-t-Butyl-cyclohexanone and Their Alcohol Derivatives. Journal of Physical Chemistry A, 2011, 115, 14539-14545.	2.5	5
46	Conformational Analysis and Electronic Interactions of Some 4â€²-Substituted-2-ethylthio-phenylacetates. Journal of Physical Chemistry A, 2015, 119, 3823-3832.	2.5	5
47	Conformational analysis of 2-halocyclopentanones by NMR and IR spectroscopies and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 1089-1096.	3.9	4
48	Structural investigations of 5-hydroxy-4,5-dihydroisoxazoles. Journal of Molecular Structure, 2011, 1006, 462-468.	3.6	4
49	Transmission Mechanisms of the Fermi-Contact Term of Spinâ€“Spin Couplings. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, 3, 245-284.	0.6	4
50	Spinâ€“spin coupling constants in linear substituted HCN clusters. Molecular Physics, 2019, 117, 693-704.	1.7	3
51	Flow Synthesis of 2â€[Methyl(pyridinâ€2â€yl)amino]ethanol: An Experimental and Computational Study. Chemical Engineering and Technology, 2021, 44, 283-290.	1.5	3
52	Efeito das interaÃ§Ãµes hiperconjugativas na constante de acoplamento Â¹J CH da hexametilenotetramina e do adamantano: estudo teÃ³rico e experimental. Quimica Nova, 2007, 30, 1681-1685.	0.3	3
53	Conformational isomerism and electronic interactions in some Î±-aminoketones. Computational and Theoretical Chemistry, 2006, 766, 177-183.	1.5	2
54	An investigation of the electronic structure of some 3-monosubstituted-2-methylpropenes through computational chemistry and photoelectron spectroscopy. Chemical Physics, 2008, 349, 263-268.	1.9	2

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55	Conformational and stereoeletronic investigations of muscarinic agonists of acetylcholine by NMR and theoretical calculations. Journal of Molecular Structure, 2012, 1015, 33-40.	3.6	2
56	Synthesis and Dielsâ€“Alder Reactions of a Benzo[5]radialene Derivative. Organic Letters, 2014, 16, 4020-4023.	4.6	2
57	Conformational analysis and electronic interactions of some 2-[2â€²-(4â€²-sustituted-phenylsulfanyl)-acetyl]-5-substituted furans and 2-[2â€²-(phenylselanyl)-acetyl]-5-methylfuran. Journal of Molecular Structure, 2021, 1225, 129088.	3.6	2
58	On the intermolecular interaction of N-benzylquininium chloride or quinine with some carbonyl group containing compounds. Tetrahedron Letters, 2016, 57, 2152-2157.	1.4	1
59	Spectroscopic and theoretical studies of some 2-(2â€²-ethylsulfanyl)acetyl-5-substituted furans and thiophenes. Journal of Molecular Structure, 2022, 1261, 132895.	3.6	1
60	Chemical Shift Trends in Light Atoms. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, , 315-345.	0.6	0