Claudio F Tormena

List of Publications by Year
in descending order

166	2,618	218592	345118
papers	citations	26 h-index	36 g-index

171	171	171	2336
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stereoelectronic interactions: A booster for ⁴J_{HF} transmission. Magnetic Resonance in Chemistry, 2022, 60, 481-488.	1.1	1
2	Mechanistic investigation of enolate/stabilized vinylogous carbanion-mediated organocatalytic azide (3 + 2) cycloaddition reactions for the synthesis of 1,2,3-triazoles. Organic and Biomolecular Chemistry, 2022, 20, 6019-6026.	1.5	4
3	Proteomic characterization of the fibroin-based silk fibers produced by weaver ant Camponotus textor. Journal of Proteomics, 2022, , 104579.	1.2	0
4	Inverse halogen dependence in anion ¹³C NMR. Physical Chemistry Chemical Physics, 2021, 23, 3019-3030.	1.3	3
5	Ionomics and lipidomics for evaluating the transgenic (cp4-EPSPS gene) and non-transgenic soybean seed generations. Microchemical Journal, 2021, 165, 106130.	2.3	2
6	Evaluation of the cytotoxicity on breast cancer cell of extracts and compounds isolated from Hyptis pectinata (L.) poit. Natural Product Research, 2020, 34, 102-109.	1.0	9
7	Counterintuitive deshielding on the ¹³C NMR chemical shift for the trifluoromethyl anion. Magnetic Resonance in Chemistry, 2020, 58, 540-547.	1.1	2
8	Improving the Sensitivity of FESTA Methods for the Analysis of Fluorinated Mixtures. Analytical Chemistry, 2020, 92, 2224-2228.	3.2	9
9	Selective Nuclear Magnetic Resonance Experiments for Sign-Sensitive Determination of Heteronuclear Couplings: Expanding the Analysis of Crude Reaction Mixtures. Analytical Chemistry, 2020, 92, 14047-14053.	3.2	9
10	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.	1.1	9
11	¹J_{CH} Coupling in Benzaldehyde Derivatives: Ortho Substitution Effect. ACS Omega, 2019, 4, 1494-1503.	1.6	5
12	Dealing with supramolecular structure for ionic liquids: a DOSY NMR approach. Physical Chemistry Chemical Physics, 2019, 21, 2567-2571.	1.3	25
13	Enantiodiscrimination by matrix-assisted DOSY NMR. Chemical Communications, 2019, 55, 8611-8614.	2.2	5
14	Unexpected behavior of the ³J_{CH} coupling constant in unsaturated compounds. Magnetic Resonance in Chemistry, 2019, 57, 939-945.	1.1	3
15	Probing the Formation of Wormlike Micelles Formed by Cationic Surfactant with Chlorobenzoate Derivatives. Langmuir, 2019, 35, 17046-17053.	1.6	10
16	Intramolecular hydrogen bonding and conformational preferences on 2-fluoro-phenylaminocyclohexanol. Revista Dos Trabalhos De IniciaÃ§Ã£o CientÃfica Da UNICAMP, 2019, , .	0.0	0
17	Revealing the Conformational Preferences of Proteinogenic Glutamic Acid Derivatives in Solution by ¹H NMR Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry A, 2018, 122, 4555-4561.	1.1	2
18	The Antagonist Effect of Nitrogen Lone Pair: 3 J HF versus 5 J HF. ChemPhysChem, 2018, 19, 1358-1362.	1.0	7

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19	The halogen effect on the ¹³C NMR chemical shift in substituted benzenes. Physical Chemistry Chemical Physics, 2018, 20, 11247-11259.	1.3	34
20	FESTA: An Efficient Nuclear Magnetic Resonance Approach for the Structural Analysis of Mixtures Containing Fluorinated Species. Analytical Chemistry, 2018, 90, 5445-5450.	3.2	19
21	Revisiting the Long-Range Perlin Effect in a Conformationally Constrained Oxocane. Journal of Organic Chemistry, 2018, 83, 10501-10504.	1.7	6
22	Cobalt-Catalyzed Stereoselective Synthesis of 2,5-trans-THF Nitrile Derivatives as a Platform for Diversification: Development and Mechanistic Studies. Journal of Organic Chemistry, 2018, 83, 7694-7713.	1.7	16
23	Predicting Counterion Effects Using a Gold Affinity Index and a Hydrogen Bonding Basicity Index. Organic Letters, 2017, 19, 5848-5851.	2.4	70
24	pH influences hydrolysis of sodium polyphosphate in dairy matrices and the structure of processed cheese. Journal of Dairy Science, 2017, 100, 8735-8743.	1.4	18
25	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.	3.7	39
26	1H and 19F NMR in drug stress testing: the case of voriconazole. RSC Advances, 2017, 7, 34000-34004.	1.7	7
27	¹⁹F NMR matrixâ€assisted DOSY: a versatile tool for differentiating fluorinated species in mixtures. Magnetic Resonance in Chemistry, 2017, 55, 323-328.	1.1	12
28	Trends of intramolecular hydrogen bonding in substituted alcohols: a deeper investigation. Physical Chemistry Chemical Physics, 2017, 19, 16904-16913.	1.3	30
29	Ultrahighâ€Resolution Diffusionâ€Ordered Spectroscopy. Angewandte Chemie, 2016, 128, 15808-15811.	1.6	13
30	Effects of novel acylhydrazones derived from 4-quinolone on the acetylcholinesterase activity and AÎ²42 peptide fibrils formation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1464-1470.	2.5	10
31	Conformational analysis of small molecules: NMR and quantum mechanics calculations. Progress in Nuclear Magnetic Resonance Spectroscopy, 2016, 96, 73-88.	3.9	47
32	Convection in liquid-state NMR: expect the unexpected. RSC Advances, 2016, 6, 95173-95176.	1.7	39
33	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.	1.3	14
34	Ultrahighâ€Resolution Diffusionâ€Ordered Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 15579-15582.	7.2	59
35	Achieving regio- and stereo-control in the fluorination of aziridines under acidic conditions. Chemical Communications, 2016, 52, 13353-13356.	2.2	40
36	Experimental and theoretical evaluation of trans-3-halo-2-hydroxy-tetrahydropyran conformational preferences. Beyond anomeric interaction. RSC Advances, 2015, 5, 35412-35420.	1.7	14

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37	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.	1.3	18
38	Is there an intramolecular hydrogen bond in 2-halophenols? A theoretical and spectroscopic investigation. Physical Chemistry Chemical Physics, 2015, 17, 25151-25159.	1.3	30
39	1H chemical shift differences of Prelogâ€“Djerassi lactone derivatives: DFT and NMR conformational studies. Organic and Biomolecular Chemistry, 2015, 13, 2140-2145.	1.5	5
40	¹⁹F DOSY NMR analysis for spin systems with ⁿJ_{FF} couplings. Magnetic Resonance in Chemistry, 2014, 52, 172-177.	1.1	26
41	Experimental and Theoretical Studies of Intramolecular Hydrogen Bonding in 3-Hydroxytetrahydropyran: Beyond AIM Analysis. Journal of Physical Chemistry A, 2014, 118, 2794-2800.	1.1	18
42	An asymmetric substrate-controlled Moritaâ€“Baylisâ€“Hillman reaction as approach for the synthesis of pyrrolizidinones and pyrrolizidines. Tetrahedron, 2014, 70, 3319-3326.	1.0	11
43	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.	2.0	10
44	Gauche Preference of Î²-Fluoroalkyl Ammonium Salts. Journal of Physical Chemistry A, 2014, 118, 503-507.	1.1	15
45	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.	1.1	18
46	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.	1.1	16
47	The Dielsâ€“Alder reactions of para-benzoquinone nitrogen-derivatives: an experimental and theoretical study. Tetrahedron, 2014, 70, 6963-6973.	1.0	16
48	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.	1.8	6
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	Chemical Shift Trends in Light Atoms. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, , 315-345.	0.6	0
51	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.	2.0	6
52	Synthesis and spectroscopic analysis of substituted 2-aminothiazolines. Journal of Molecular Structure, 2013, 1037, 186-190.	1.8	3
53	The electronic origin of unusually large ⁿJ_{FN} coupling constants in some fluoroximes. Magnetic Resonance in Chemistry, 2013, 51, 334-338.	1.1	5
54	Heterocycles from Moritaâ€“Baylisâ€“Hillman adducts: synthesis of 5-oxopyrazolidines, arylidene-5-oxopyrazolidines, and oxo-2,5-dihydro-pyrazols. Tetrahedron, 2013, 69, 826-832.	1.0	10

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55	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.	2.0	11
56	Unusual Through-Space, TS, Pathway for the Transmission of J_{FHf} Coupling: 2-Fluorobenzaldehyde Study Case. Journal of Physical Chemistry A, 2013, 117, 7939-7945.	1.1	8
57	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.	0.9	16
58	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.	0.9	7
59	Unexpected Geometrical Effects on Paramagnetic Spinâ€“Orbit and Spinâ€“Dipolar ²J_{FF} Couplings. Journal of Physical Chemistry A, 2012, 116, 4930-4933.	1.1	8
60	Stereoelectronic Interactions and the One-Bond Câ€“F Coupling Constant in Sevoflurane. Journal of Physical Chemistry A, 2012, 116, 1677-1682.	1.1	26
61	Kinetic resolution of Î±-bromophenylacetamides using quinine or Cinchona alkaloid salts. Tetrahedron: Asymmetry, 2012, 23, 748-753.	1.8	4
62	The Fâ‹¯HO intramolecular hydrogen bond forming five-membered rings hardly appear in monocyclic organofluorine compounds. RSC Advances, 2012, 2, 4169.	1.7	48
63	The Role of Î²-Bulky Substituents in Aldol Reactions of Boron Enolates of Methylketones with Aldehydes: Experimental and Theoretical Studies by DFT Analysis. Journal of Organic Chemistry, 2012, 77, 1765-1788.	1.7	17
64	1,5-Stereoinduction in Boron-Mediated Aldol Reactions of Î²,Î³-Bisalkoxy Methylketones Containing Cyclic Protecting Groups. Journal of Organic Chemistry, 2012, 77, 3766-3792.	1.7	19
65	Computational evidence for intramolecular hydrogen bonding and nonbonding XÂ·Â·Â·O interactions in 2'-haloflavonols. Beilstein Journal of Organic Chemistry, 2012, 8, 112-117.	1.3	20
66	Critical analysis of the throughâ€space transmission of NMR J_{FH} spinâ€“spin coupling constants. International Journal of Quantum Chemistry, 2012, 112, 3158-3163.	1.0	15
67	¹H NMR Spectra. Part 28: Proton chemical shifts and couplings in threeâ€membered rings. A ring current model for cyclopropane and a novel dihedral angle dependence for ³J_{HH} couplings involving the epoxy proton. Magnetic Resonance in Chemistry, 2012, 50, 305-313.	1.1	20
68	Matrixâ€assisted diffusionâ€ordered spectroscopy: application of surfactant solutions to the resolution of isomer spectra. Magnetic Resonance in Chemistry, 2012, 50, 458-465.	1.1	20
69	Theoretical and infrared studies on the conformations of monofluorophenols. Journal of Molecular Structure, 2012, 1009, 11-15.	1.8	14
70	Experimental, SOPPA(CCSD), and DFT Analysis of Substitutent Effects on NMR1JCFCoupling Constants in Fluorobenzene Derivatives. Journal of Physical Chemistry A, 2011, 115, 1272-1279.	1.1	32
71	Alkyl Group Effect on the Conformational Isomerism of trans-2-Bromoalkoxycyclohexanes Analyzed by NMR Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry A, 2011, 115, 10122-10127.	1.1	7
72	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.	1.1	5

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73	Effect of Electronic Interactions on NMR1JCFand2JCFCouplings incis-andtrans-4-t-Butyl-2-fluorocyclohexanones and Their Alcohol Derivatives. Journal of Physical Chemistry A, 2011, 115, 5684-5692.	1.1	22
74	Nigriventrine: A low molecular mass neuroactive compound from the venom of the spider Phoneutria nigriventer. Toxicon, 2011, 57, 266-274.	0.8	16
75	Structural investigations of 5-hydroxy-4,5-dihydroisoxazoles. Journal of Molecular Structure, 2011, 1006, 462-468.	1.8	4
76	Theoretical and infrared studies on the conformational isomerism of trans-2-bromo-alkoxycyclohexanes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 359-362.	2.0	4
77	A ¹H NMR and theoretical investigation of the conformations of some monosubstituted cyclobutanes. Magnetic Resonance in Chemistry, 2011, 49, 23-29.	1.1	8
78	¹⁹F chemical shifts, coupling constants and conformational preferences in monosubstituted perfluoroparacyclophanes. Magnetic Resonance in Chemistry, 2011, 49, 93-105.	1.1	15
79	^{1h}J_{FH}coupling in 2â€fluorophenol revisited: Is intramolecular hydrogen bond responsible for this longâ€range coupling?. Magnetic Resonance in Chemistry, 2011, 49, 763-767.	1.1	49
80	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.	2.0	28
81	Heck Reaction on Morita-Baylis-Hillman Adducts: Diastereoselective Synthesis of Pyrrolizidinones and Pyrrolizidines. Synlett, 2011, 2011, 2059-2063.	1.0	3
82	The case of infrared carbonyl stretching intensities of 2-bromocyclohexanone: Conformational and intermolecular interaction insights. Chemical Physics Letters, 2010, 494, 26-30.	1.2	14
83	Matrixâ€assisted diffusionâ€ordered spectroscopy: mixture resolution by NMR using SDS micelles. Magnetic Resonance in Chemistry, 2010, 48, 550-553.	1.1	71
84	Difference between 2JC2H3 and 2JC3H2 spin-spin couplings in heterocyclic five- and six-membered rings as a probe for studying Ïƒ-ring currents: a quantum chemical analysis. Magnetic Resonance in Chemistry, 2010, 48, S151-S158.	1.1	8
85	Revisiting the stability of endo/exo Diels-Alder adducts between cyclopentadiene and 1,4-benzoquinone. Journal of the Brazilian Chemical Society, 2010, 21, 112-118.	0.6	5
86	Polybioside, a Neuroactive Compound from the Venom of the Social WaspPolybia paulista. Journal of Natural Products, 2010, 73, 527-531.	1.5	15
87	Influence of Î²-Substituents in Aldol Reactions of Boron Enolates of Î²-Alkoxy Methylketones. Organic Letters, 2010, 12, 5056-5059.	2.4	14
88	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.	1.1	23
89	Stereochemical dependence of NMR geminal spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2009, 47, 113-120.	1.1	16
90	On the 4 J HH long-range coupling in 2-bromocyclohexanone: conformational insights. Magnetic Resonance in Chemistry, 2009, 47, 348-351.	1.1	7

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91	Addition of kinetic boron enolates generated from Î²-alkoxy methyl ketones to aldehydes. Density functional theory calculations on the transition structures. Tetrahedron, 2009, 65, 8714-8721.	1.0	17
92	Spectroscopic and theoretical studies of some N-methoxy-N-methyl-2-[(4â€²-substituted) phenylthio]propanamides. Journal of Molecular Structure, 2009, 920, 393-400.	1.8	14
93	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.	2.0	4
94	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.	2.3	32
95	Effect of Sulfur Oxidation on the Transmission Mechanism of ⁴J_{HH} NMR Coupling Constants in 1,3-Dithiane. Journal of Physical Chemistry A, 2009, 113, 2647-2651.	1.1	10
96	Monoamine oxidase inhibitory activities of indolylalkaloid toxins from the venom of the colonial spider Parawixia bistriata: Functional characterization of PwTX-I. Toxicon, 2009, 54, 717-724.	0.8	24
97	Qualitative Study of Substituent Effects on NMR 15N and 17O Chemical Shifts. Journal of Physical Chemistry A, 2009, 113, 9874-9880.	1.1	11
98	Theoretical and Experimental Investigation on the Rotational Isomerism in Î±-Fluoroacetophenones. Journal of Physical Chemistry A, 2009, 113, 2906-2913.	1.1	8
99	Conformational and electronic interaction studies of some p-substituted Î±-methylsulfonyl-Î±-diethoxyphosphorylacetophenones. Journal of Molecular Structure, 2008, 892, 300-304.	1.8	2
100	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
101	The role of stereoelectronic interactions in the conformational isomerism of some phosphorusâ€containing model compounds. Journal of Physical Organic Chemistry, 2008, 21, 505-509.	0.9	4
102	The effect of carbonyl group in the asymmetry of ^{3, 4}J_{CH} coupling constants in norbornanones. Magnetic Resonance in Chemistry, 2008, 46, 107-109.	1.1	15
103	NMR spinâ€spin couplings involving nuclei in the neighborhood of a carbonyl group. ³J_{CH} couplings in Î±â€substituted acetamides. Magnetic Resonance in Chemistry, 2008, 46, 202-205.	1.1	9
104	Density functionals for calculating NMR 1JCH coupling constants in electron-rich systems. Chemical Physics Letters, 2008, 454, 129-132.	1.2	7
105	Solvent effects in the conformational stability of Î±-substituted acetamides through theoretical and experimental data. Journal of Molecular Structure, 2008, 875, 235-243.	1.8	18
106	Stereochemical behavior of 1JCH and 2JCH NMR coupling constants in Î±-substituted acetamides. Journal of Molecular Structure, 2008, 891, 508-513.	1.8	7
107	Stereoelectronic Interaction and Their Effects on Conformational Preference for 2-Substituted Methylenecyclohexane: An Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2008, 112, 8785-8789.	1.1	13
108	Analysis of the Electronic Origin of the 1JCH Spinâ"Spin Coupling Trend in 1-X-Cyclopropanes: Experimental and DFT Study. Journal of Physical Chemistry A, 2008, 112, 11956-11959.	1.1	14

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109	Intra- and Intermolecular Hydrogen Bonds in Alkyl and Silyl Ethers:â€‰ Experimental and Theoretical Analysis. Journal of Physical Chemistry A, 2008, 112, 232-237.	1.1	17
110	Electronic Interactions and Their Influence on the Conformational Stability of trans-2-Halocyclopentanol. Journal of Physical Chemistry A, 2007, 111, 295-298.	1.1	5
111	Lone-Pair Orientation Effect of an Î±-Oxygen Atom on 1JCC NMR Spinâ^'Spin Coupling Constants in o-Substituted Phenols. Experimental and DFT Study. Journal of Chemical Theory and Computation, 2007, 3, 1284-1294.	2.3	9
112	Long-rangeJCH heteronuclear coupling constants in cyclopentane derivatives. Part II. Magnetic Resonance in Chemistry, 2007, 45, 82-86.	1.1	8
113	Experimental and DFT studies on the transmission mechanisms of analogous NMRJCH andJCC couplings in 1-X- and 1-X-3-methylbicyclo[1.1.1]-pentanes. Magnetic Resonance in Chemistry, 2007, 45, 572-577.	1.1	8
114	Experimental and theoretical investigation of NMR2JHH coupling constant on six-membered ring systems containing oxygen or sulfur atoms. Magnetic Resonance in Chemistry, 2007, 45, 590-594.	1.1	11
115	NMR and theoretical investigation of the ketoâ€“enol tautomerism in cyclohexane-1,3-diones. Journal of Molecular Structure, 2007, 828, 54-58.	1.8	20
116	Structural determination of Zn and Cdâ€“DTPA complexes: MS, infrared, 13C NMR and theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 1197-1200.	2.0	30
117	Conformational Preferences of 2-Methoxy, 2-Methylthio, and 2-Methylselenocyclohexyl-N,N-dimethylcarbamate:â€‰ A Theoretical and Experimental Investigation. Journal of Physical Chemistry A, 2007, 111, 11701-11705.	1.1	7
118	Spectrometric and theoretical investigation of the structures of Cu and Pb/DTPA complexes. Structural Chemistry, 2007, 18, 605-609.	1.0	21
119	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
120	Experimental and Theoretical Study of Hyperconjugative Interaction Effects on NMR1JCHScalar Couplings. Journal of Physical Chemistry A, 2006, 110, 4266-4275.	1.1	48
121	Conformational Behavior ofcis-2-Methoxy,cis-2-Methylthio, andcis-2-Methylselenocyclohexanol:Â A Theoretical and Experimental Investigation. Journal of Physical Chemistry A, 2006, 110, 9438-9442.	1.1	8
122	Stereoelectronic interactions and their effects on conformational preference for 1,3-dithiane-1-oxide and 1,4-dithiane-1-oxide. A theoretical and experimental study. Chemical Physics Letters, 2006, 426, 176-179.	1.2	8
123	Conformational influence on intramolecular cyclization for a Î²-ketoester containing oxirane ring: A theoretical and experimental study. Journal of Molecular Structure, 2006, 794, 221-224.	1.8	0
124	Spectroscopic and theoretical studies of some p-substituted Î±-methylthio-Î±-diethoxyphosphorylacetophenones. Journal of Molecular Structure, 2006, 798, 57-63.	1.8	5
125	Conformational and stereoelectronic investigation of chloromethyl methyl sulfide and its sulfinyl and sulfonyl analogs. Journal of Molecular Structure, 2006, 800, 45-50.	1.8	12
126	Conformational preferences and orbital interactions for methyl haloacetates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 511-517.	2.0	6

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127	Solvent effects in the 2JHH, 3JHH, 1JNC and 2JNC coupling constants in the NMR spectrum of acetylcholine chloride. Journal of Molecular Structure, 2006, 797, 44-48.	1.8	8
128	Orbital interactions and their effects on the conformational stability in six-membered rings containing nitrogen atoms. Computational and Theoretical Chemistry, 2006, 763, 145-148.	1.5	10
129	The Venomous Secrets of the Web Droplets from the Viscid Spiral of the Orb-Weaver SpiderNephila clavipes (Araneae, Tetragnatidae). Chemistry and Biodiversity, 2006, 3, 727-741.	1.0	21
130	Long-rangeJCH heteronuclear coupling constants in cyclopentane derivatives. Magnetic Resonance in Chemistry, 2006, 44, 95-98.	1.1	24
131	Conformational analysis and stereoelectronic effects in trans-1,2-dihalocyclohexanes: 1H NMR and theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1771-1776.	2.0	13
132	13C NMR, infrared, solvation and theoretical investigation of the conformational isomerism in 1-haloacetones (X = Cl, Br and I). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2221-2230.	2.0	11
133	Conformational properties of trans-2-halo-acetoxycyclohexanes: 1H NMR, solvation and theoretical investigation. Journal of Molecular Structure, 2005, 734, 211-217.	1.8	6
134	Conformational preferences for N,N-dimethyl-2-haloacetamides (halo=F, Cl, Br and I) through theoretical and experimental studies: An unexpected orbital interaction. Computational and Theoretical Chemistry, 2005, 728, 79-84.	1.5	26
135	Structure Determination of Hydroxytrypargine: A New Tetrahydro-?-Carboline Toxin from the Venom of the SpiderParawixia bistriata. Helvetica Chimica Acta, 2005, 88, 796-801.	1.0	19
136	Structure Determination of a Tetrahydro-?-carboline of Arthropod Origin: A Novel Alkaloid-Toxin Subclass from the Web of SpiderNephila clavipes. Chemistry and Biodiversity, 2005, 2, 525-534.	1.0	28
137	Stereochemical and Electronic Interaction Studies of Some Meta- andPara-Substituted Î±-Methylsulfinyl-Î±-Diethoxyphosphoryl Acetophenones. Phosphorus, Sulfur and Silicon and the Related Elements, 2005, 180, 1425-1426.	0.8	0
138	Isolation and chemical characterization of PwTx-II: A novel alkaloid toxin from the venom of the spider Parawixia bistriata (Araneidae, Araneae). Toxicon, 2005, 46, 786-796.	0.8	18
139	Orbital Interactions and Their Effects on13C NMR Chemical Shifts for 4,6-Disubstituted-2,2-dimethyl-1,3-dioxanes. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 6077-6082.	1.1	21
140	Conformational analysis of fluoroacetoxime and of itsO-methyl ether by1H,13C and15N NMR and theoretical calculations. Journal of Physical Organic Chemistry, 2004, 17, 42-48.	0.9	14
141	Structure Determination of an Organometallic 1-(Diazenylaryl)ethanol: A Novel Toxin Subclass from the Web of the SpiderNephila clavipes. Chemistry and Biodiversity, 2004, 1, 830-838.	1.0	14
142	Stereochemical and electronic interaction studies of some meta- and para-substituted Î±-methylsulfinyl-Î±-diethoxyphosphorylacetophenones. Journal of Molecular Structure, 2004, 707, 199-210.	1.8	4
143	Chemical shifts calculations on aromatic systems: a comparison of models and basis sets. Chemical Physics Letters, 2004, 398, 466-470.	1.2	34
144	Conformational behaviour in S-methyl halothioacetates through NMR, FT-IR, and theoretical calculations. Canadian Journal of Chemistry, 2004, 82, 418-426.	0.6	4

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145	Theoretical and Infrared Investigation of the Conformations of 1,3-Dihaloacetones. Journal of Physical Chemistry A, 2004, 108, 5161-5168.	1.1	16
146	Anomeric Effect on Geminal and VicinalJHHNMR Coupling Constants. Journal of Physical Chemistry A, 2004, 108, 7762-7768.	1.1	31
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