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	Matrixâ€assisted diffusionâ€ordered spectroscopy: mixture resolution by NMR using SDS micelles. Magnetic Resonance in Chemistry, 2010, 48, 550-553.	1.1	71
2	Predicting Counterion Effects Using a Gold Affinity Index and a Hydrogen Bonding Basicity Index. Organic Letters, 2017, 19, 5848-5851.	2.4	70
3	Ultrahighâ€Resolution Diffusionâ€Ordered Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 15579-15582.	7.2	59
4	^{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
5	Experimental and Theoretical Study of Hyperconjugative Interaction Effects on NMR1JCHScalar Couplings. Journal of Physical Chemistry A, 2006, 110, 4266-4275.	1.1	48
6	The Fâ‹¯HO intramolecular hydrogen bond forming five-membered rings hardly appear in monocyclic organofluorine compounds. RSC Advances, 2012, 2, 4169.	1.7	48
7	Conformational analysis of small molecules: NMR and quantum mechanics calculations. Progress in Nuclear Magnetic Resonance Spectroscopy, 2016, 96, 73-88.	3.9	47
8	Conformational analysis of 2-halocyclohexanones: an NMR, theoretical and solvation study. Perkin Transactions II RSC, 2002, , 1494-1498.	1.1	46
9	Achieving regio- and stereo-control in the fluorination of aziridines under acidic conditions. Chemical Communications, 2016, 52, 13353-13356.	2.2	40
10	Convection in liquid-state NMR: expect the unexpected. RSC Advances, 2016, 6, 95173-95176.	1.7	39
11	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
12	Conformational analysis. Part 27. NMR, solvation and theoretical investigation of conformational isomerism in fluoro- and 1,1-difluoro-acetone. Journal of the Chemical Society Perkin Transactions II, 1996, , 533.	0.9	38
13	Chemical shifts calculations on aromatic systems: a comparison of models and basis sets. Chemical Physics Letters, 2004, 398, 466-470.	1.2	34
14	The halogen effect on the ¹³C NMR chemical shift in substituted benzenes. Physical Chemistry Chemical Physics, 2018, 20, 11247-11259.	1.3	34
15	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
16	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
17	Photoelectronic and transport properties of polypyrrole doped with a dianionic dye. Electrochimica Acta, 2002, 47, 1351-1357.	2.6	31
18	Anomeric Effect on Geminal and VicinalJHHNMR Coupling Constants. Journal of Physical Chemistry A, 2004, 108, 7762-7768.	1.1	31

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19	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
20	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
21	Trends of intramolecular hydrogen bonding in substituted alcohols: a deeper investigation. Physical Chemistry Chemical Physics, 2017, 19, 16904-16913.	1.3	30
22	Conformational analysis oftrans-2-halocyclohexanols and their methyl ethers: a1H NMR, theoretical and solvation approach. Journal of Physical Organic Chemistry, 2003, 16, 27-33.	0.9	29
23	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
24	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
25	Interaction in trans-2-halocyclohexanols â€" an infrared and theoretical study. Journal of Molecular Structure, 2001, 570, 175-180.	1.8	27
26	Conformational analysis. Part 35. NMR, solvation and theoretical investigation of rotational isomerism in methyl fluoroacetate and methyl difluoroacetate. Perkin Transactions II RSC, 2001, , 815-820.	1.1	26
27	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
28	Stereoelectronic Interactions and the One-Bond Câ€“F Coupling Constant in Sevoflurane. Journal of Physical Chemistry A, 2012, 116, 1677-1682.	1.1	26
29	¹⁹F DOSY NMR analysis for spin systems with ⁿJ_{FF} couplings. Magnetic Resonance in Chemistry, 2014, 52, 172-177.	1.1	26
30	Conformational analysis of 2-bromocyclohexanone. A combined NMR, IR, solvation and theoretical approach. Journal of Physical Organic Chemistry, 2001, 14, 317-322.	0.9	25
31	Dealing with supramolecular structure for ionic liquids: a DOSY NMR approach. Physical Chemistry Chemical Physics, 2019, 21, 2567-2571.	1.3	25
32	Conformational analysis. Part 33.1 An NMR, solvation and theoretical investigation of conformational isomerism in N,N-dimethylfluoroacetamide and N,N-dimethyl-Î±-fluoropropionamide. Perkin Transactions II RSC, 2000, , 2054-2059.	1.1	24
33	Halogenated six-membered rings: a theoretical approach for substituent effects in conformational analysis. Computational and Theoretical Chemistry, 2002, 589-590, 147-151.	1.5	24
34	Long-rangeJCH heteronuclear coupling constants in cyclopentane derivatives. Magnetic Resonance in Chemistry, 2006, 44, 95-98.	1.1	24
35	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
36	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

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37	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
38	Conformational and electronic interaction studies of 2-fluoro-substituted N,N-dimethylacetamides. Journal of Molecular Structure, 2002, 607, 87-99.	1.8	21
39	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
40	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
41	Spectrometric and theoretical investigation of the structures of Cu and Pb/DTPA complexes. Structural Chemistry, 2007, 18, 605-609.	1.0	21
42	NMR, solvation and theoretical investigations of conformational isomerism in 2-X-cyclohexanones (X=NMe2, OMe, SMe and SeMe). Journal of Physical Organic Chemistry, 2003, 16, 833-838.	0.9	20
43	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
44	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
45	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
46	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
47	Conformational analysis in N-methylfluoroamides. A theoretical, NMR and IR investigation. Perkin Transactions II RSC, 2002, , 773-778.	1.1	19
48	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
49	1,5-Stereoinduction in Boron-Mediated Aldol Reactions of Î²,Î´-Bisalkoxy Methylketones Containing Cyclic Protecting Groups. Journal of Organic Chemistry, 2012, 77, 3766-3792.	1.7	19
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	An NMR, IR and theoretical investigation of the methyl effect on conformational isomerism in 3-fluoro-3-methyl-2-butanone and 1-fluoro-3,3-dimethyl-2-butanone. Journal of Physical Organic Chemistry, 2002, 15, 211-217.	0.9	17
58	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
59	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
60	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
61	Theoretical and Infrared Investigation of the Conformations of 1,3-Dihaloacetones. Journal of Physical Chemistry A, 2004, 108, 5161-5168.	1.1	16
62	Stereochemical dependence of NMR geminal spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2009, 47, 113-120.	1.1	16
63	Nigriventrine: A low molecular mass neuroactive compound from the venom of the spider Phoneutria nigriventer. Toxicon, 2011, 57, 266-274.	0.8	16
64	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
65	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
66	The Dielsâ€“Alder reactions of para-benzoquinone nitrogen-derivatives: an experimental and theoretical study. Tetrahedron, 2014, 70, 6963-6973.	1.0	16
67	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
68	Conformational analysis, Part 32.â€ NMR, solvation and theoretical investigation of conformational isomerism in 3-fluorobutan-2-one and 3,3-difluorobutan-2-one. Journal of the Chemical Society Perkin Transactions II, 1999, , 1663-1668.	0.9	15
69	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
70	Polybioside, a Neuroactive Compound from the Venom of the Social WaspPolybia paulista. Journal of Natural Products, 2010, 73, 527-531.	1.5	15
71	¹⁹F chemical shifts, coupling constants and conformational preferences in monosubstituted perfluoroparacyclophanes. Magnetic Resonance in Chemistry, 2011, 49, 93-105.	1.1	15
72	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

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73	Gauche Preference of Î²-Fluoroalkyl Ammonium Salts. Journal of Physical Chemistry A, 2014, 118, 503-507.	1.1	15
74	A1H NMR and molecular modelling investigation of diastereotopic methylene hydrogen atoms. Magnetic Resonance in Chemistry, 2002, 40, 279-283.	1.1	14
75	The utility of infrared spectroscopy for quantitative conformational analysis at a single temperature. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1783-1789.	2.0	14
76	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
77	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
78	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
79	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
80	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
81	Influence of Î²-Substituents in Aldol Reactions of Boron Enolates of Î²-Alkoxy Methylketones. Organic Letters, 2010, 12, 5056-5059.	2.4	14
82	Theoretical and infrared studies on the conformations of monofluorophenols. Journal of Molecular Structure, 2012, 1009, 11-15.	1.8	14
83	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
84	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
85	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
86	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
87	Ultrahighâ€Resolution Diffusionâ€Ordered Spectroscopy. Angewandte Chemie, 2016, 128, 15808-15811.	1.6	13
88	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
89	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
90	Infrared spectroscopy and theoretical calculations as tools for the conformational analysis of 2-methoxycyclohexanone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1177-1182.	2.0	11

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91	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
92	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
93	Qualitative Study of Substituent Effects on NMR 15N and 17O Chemical Shifts. Journal of Physical Chemistry A, 2009, 113, 9874-9880.	1.1	11
94	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
95	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
96	Conformational behaviour of methyl 2-fluoroesters through theoretical calculations, NMR and IR spectroscopy. Physical Chemistry Chemical Physics, 2004, 6, 1152.	1.3	10
97	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
98	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
99	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
100	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
101	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
102	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
103	Probing the Formation of Wormlike Micelles Formed by Cationic Surfactant with Chlorobenzoate Derivatives. Langmuir, 2019, 35, 17046-17053.	1.6	10
104	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
105	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
106	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
107	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
108	Improving the Sensitivity of FESTA Methods for the Analysis of Fluorinated Mixtures. Analytical Chemistry, 2020, 92, 2224-2228.	3.2	9

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109	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
110	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
111	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
112	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
113	Long-rangeJCH heteronuclear coupling constants in cyclopentane derivatives. Part II. Magnetic Resonance in Chemistry, 2007, 45, 82-86.	1.1	8
114	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
115	Theoretical and Experimental Investigation on the Rotational Isomerism in Î±-Fluoroacetophenones. Journal of Physical Chemistry A, 2009, 113, 2906-2913.	1.1	8
116	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
117	A ¹H NMR and theoretical investigation of the conformations of some monosubstituted cyclobutanes. Magnetic Resonance in Chemistry, 2011, 49, 23-29.	1.1	8
118	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
119	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
120	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
121	Density functionals for calculating NMR 1JCH coupling constants in electron-rich systems. Chemical Physics Letters, 2008, 454, 129-132.	1.2	7
122	Stereochemical behavior of 1JCH and 2JCH NMR coupling constants in Î±-substituted acetamides. Journal of Molecular Structure, 2008, 891, 508-513.	1.8	7
123	On the 4 J HH long-range coupling in 2-bromocyclohexanone: conformational insights. Magnetic Resonance in Chemistry, 2009, 47, 348-351.	1.1	7
124	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
125	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
126	1H and 19F NMR in drug stress testing: the case of voriconazole. RSC Advances, 2017, 7, 34000-34004.	1.7	7

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127	The Antagonist Effect of Nitrogen Lone Pair: 3 J HF versus 5 J HF. ChemPhysChem, 2018, 19, 1358-1362.	1.0	7
128	Substituent interactions in trans-2-substituted methoxycyclohexanes: an explanation to the conformational behaviour in a chemometric and theoretical view. Computational and Theoretical Chemistry, 2002, 618, 219-224.	1.5	6
129	Multinuclear magnetic resonance and theoretical calculations in the study of structure and tautomerism of some 2-amino-Nâ€²-(aryl)-benzamidines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 3139-3145.	2.0	6
130	Conformational properties of trans-2-halo-acetoxycyclohexanes: 1H NMR, solvation and theoretical investigation. Journal of Molecular Structure, 2005, 734, 211-217.	1.8	6
131	Conformational preferences and orbital interactions for methyl haloacetates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 511-517.	2.0	6
132	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
133	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
134	Revisiting the Long-Range Perlin Effect in a Conformationally Constrained Oxocane. Journal of Organic Chemistry, 2018, 83, 10501-10504.	1.7	6
135	Spectroscopic and theoretical studies of some p-substituted Î±-methylthio-Î±-diethoxyphosphorylacetophenones. Journal of Molecular Structure, 2006, 798, 57-63.	1.8	5
136	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
137	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
138	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
139	The electronic origin of unusually large ⁿJ_{FN} coupling constants in some fluoroximes. Magnetic Resonance in Chemistry, 2013, 51, 334-338.	1.1	5
140	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
141	¹J_{CH} Coupling in Benzaldehyde Derivatives: Ortho Substitution Effect. ACS Omega, 2019, 4, 1494-1503.	1.6	5
142	Enantiodiscrimination by matrix-assisted DOSY NMR. Chemical Communications, 2019, 55, 8611-8614.	2.2	5
143	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
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	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
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