Raymond J Abraham

List of Publications by Year
in descending order

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98 papers	2,052 citations	257450 24 h-index	302126 39 g-index
102 all docs	102 docs citations	102 times ranked	1862 citing authors

#	Article	IF	Citations
1	The use of MM/QM calculations of 13C chemical shifts in the conformational analysis of some monosaccharides and sucrose. New Journal of Chemistry, 2021, 45, 2001-2009.	2.8	3
2	The use of MM/QM calculations of 13 C and 15 N chemical shifts in the conformational analysis of alkyl substituted anilines. Magnetic Resonance in Chemistry, 2020, 58, 520-531.	1.9	3
3	The use of chemical shift calculations in the conformational analysis of substituted benzenes. New Journal of Chemistry, 2019, 43, 5382-5394.	2.8	5
4	A convenient and accurate method for predicting¹³C chemical shifts in organic molecules. New Journal of Chemistry, 2018, 42, 5024-5036.	2.8	8
5	A molecular mechanics and ab initio prediction of the ¹<scp>H</scp> chemical shifts of pinanes. Magnetic Resonance in Chemistry, 2017, 55, 837-845.	1.9	4
6	A simple and facile NMR method for the determination of hydrogen bonding by amide Nâ€“H protons in protein models and other compounds. New Journal of Chemistry, 2017, 41, 6064-6066.	2.8	18
7	A theoretical and NMR lanthanideâ€induced shift (LIS) investigation of the conformations of lactams.. Magnetic Resonance in Chemistry, 2017, 55, 1059-1072.	1.9	6
8	A re-investigation of ⁴J_{FF} and ⁵J_{FF} nuclear spinâ€“spin couplings in substituted benzenes, a novel conformational tool. Physical Chemistry Chemical Physics, 2016, 18, 15822-15827.	2.8	5
9	Tautomerism in 8-Nitroguanosine Studied by NMR and Theoretical Calculations. Nucleosides, Nucleotides and Nucleic Acids, 2016, 35, 53-63.	1.1	2
10	Conformational analysis, part 43. A theoretical and LIS/NMR investigation of the conformations of substituted benzamides. Magnetic Resonance in Chemistry, 2015, 53, 498-508.	1.9	6
11	Experimental and theoretical evaluation of trans-3-halo-2-hydroxy-tetrahydropyran conformational preferences. Beyond anomeric interaction. RSC Advances, 2015, 5, 35412-35420.	3.6	14
12	Is there an intramolecular hydrogen bond in 2-halophenols? A theoretical and spectroscopic investigation. Physical Chemistry Chemical Physics, 2015, 17, 25151-25159.	2.8	30
13	An NMR Method for the Quantitative Assessment of Intramolecular Hydrogen Bonding: Application to Physicochemical, Environmental, and Biochemical Properties. Journal of Organic Chemistry, 2014, 79, 11075-11083.	3.2	83
14	¹H NMR spectra part 31: ¹H chemical shifts of amides in DMSO solvent. Magnetic Resonance in Chemistry, 2014, 52, 395-408.	1.9	26
15	¹H NMR spectra. Part 29Â§: proton chemical shifts and couplings in estersâ€”the conformational analysis of methyl Î³â€butyrolactones. Magnetic Resonance in Chemistry, 2013, 51, 9-15.	1.9	3
16	¹H NMR spectra. Part 30: ¹H chemical shifts in amides and the magnetic anisotropy, electric field and steric effects of the amide group. Magnetic Resonance in Chemistry, 2013, 51, 143-155.	1.9	29
17	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.	1.9	20
18	A ¹H NMR and theoretical investigation of the conformations of some monosubstituted cyclobutanes. Magnetic Resonance in Chemistry, 2011, 49, 23-29.	1.9	8

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19	Conformational analysis: Part 42. A modelling and LIS/NMR investigation of the conformations of some aromatic SO compounds. Journal of Physical Organic Chemistry, 2010, 23, 544-550.	1.9	2
20	The hydrogen bond acidity and other descriptors for oximes. New Journal of Chemistry, 2009, 33, 76-81.	2.8	16
21	The role of stereoelectronic interactions in the conformational isomerism of some phosphorusâ€containing model compounds. Journal of Physical Organic Chemistry, 2008, 21, 505-509.	1.9	4
22	¹H chemical shifts in NMR. Part 27: proton chemical shifts in sulfoxides and sulfones and the magnetic anisotropy, electric field and steric effects of the SO bond. Magnetic Resonance in Chemistry, 2008, 46, 667-675.	1.9	21
23	The prediction of ¹H chemical shifts in amines: a semiempirical and ab initio investigation. Magnetic Resonance in Chemistry, 2007, 45, 749-757.	1.9	11
24	An NMR, IR and theoretical investigation of ¹H Chemical Shifts and hydrogen bonding in phenols. Magnetic Resonance in Chemistry, 2007, 45, 865-877.	1.9	78
25	Conformational analysis, Part 41. A modelling and LIS/NMR investigation of the conformations ofÎ±,Î²-unsaturated carbonyl compounds. Journal of Physical Organic Chemistry, 2006, 19, 384-392.	1.9	16
26	1H chemical shifts in NMR. Part 24â€"proton chemical shifts in somegem-difunctional compounds: 3-endo- and 3-exo-substituted norbornanones. Journal of Physical Organic Chemistry, 2006, 19, 376-383.	1.9	1
27	1H chemical shifts in NMR: Part 23, the effect of dimethyl sulphoxideversus chloroform solvent on1H chemical shifts. Magnetic Resonance in Chemistry, 2006, 44, 491-509.	1.9	109
28	1H chemical shifts in NMR. Part 21?Prediction of the1H chemical shifts of molecules containing the ester group: a modelling andab initio investigation. Magnetic Resonance in Chemistry, 2005, 43, 3-15.	1.9	19
29	â€˜Objectiveâ€™ determination of coupling constants and conformational equilibria by solvent variation: a comment. Magnetic Resonance in Chemistry, 2005, 43, 424-426.	1.9	0
30	1H chemical shifts in NMR: Part 22â€"Prediction of the1H chemical shifts of alcohols, diols and inositols in solution, a conformational and solvation investigation. Magnetic Resonance in Chemistry, 2005, 43, 611-624.	1.9	55
31	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.	1.9	14
32	1H chemical shifts in NMR. Part 20â€" Anisotropic and steric effects in halogen substituent chemical shifts(SCS), a modelling andab initio investigation. Magnetic Resonance in Chemistry, 2004, 42, 436-444.	1.9	14
33	Conformational behaviour of methyl 2-fluoroesters through theoretical calculations, NMR and IR spectroscopy. Physical Chemistry Chemical Physics, 2004, 6, 1152.	2.8	10
34	1H chemical shifts in NMR: Part 19. Carbonyl anisotropies and steric effects in aromatic aldehydes and ketones. Magnetic Resonance in Chemistry, 2003, 41, 26-36.	1.9	81
35	Conformational analysis. Part 40: a theoretical and NMR investigation of the conformations ofcis-andtrans-cyclopentane-1,3-diol. Magnetic Resonance in Chemistry, 2003, 41, 1000-1008.	1.9	17
36	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.	1.9	20

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37	Conformational analysis in N-methylfluoroamides. A theoretical, NMR and IR investigation. Perkin Transactions II RSC, 2002, , 773-778.	1.1	19
38	1H chemical shifts in NMR. Part 18.1 Ring currents and Ï€-electron effects in hetero-aromatics. Perkin Transactions II RSC, 2002, , 1081-1091.	1.1	51
39	Conformational analysis.. Perkin Transactions II RSC, 2002, , 2025-2030.	1.1	22
40	Conformational analysis of 2-halocyclohexanones: an NMR, theoretical and solvation study. Perkin Transactions II RSC, 2002, , 1494-1498.	1.1	46
41	A1H NMR and molecular modelling investigation of diastereotopic methylene hydrogen atoms. Magnetic Resonance in Chemistry, 2002, 40, 279-283.	1.9	14
42	Substituent effects on1H and13C NMR chemical shifts in ?-monosubstituted ethyl acetates: principal component analysis and1H chemical shift calculations. Magnetic Resonance in Chemistry, 2002, 40, 449-454.	1.9	13
43	Conformational analysis: Part 37. A13C and1H NMR and theoretical investigation of the conformational equilibrium of 2-methylcyclohexanone oxime and of itsO-methyl ether. Magnetic Resonance in Chemistry, 2002, 40, 49-56.	1.9	8
44	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.	1.9	17
45	Proton chemical shifts in NMR. Part 16.1 Proton chemical shifts in acetylenes and the anisotropic and steric effects of the acetylene group. Perkin Transactions II RSC, 2001, , 1195-1204.	1.1	11
46	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
47	Conformational analysis. Part 36. A variable temperature 13C NMR study of conformational equilibria in methyl substituted cycloalkanes. Perkin Transactions II RSC, 2001, , 302-307.	1.1	30
48	Conformational analysis of 2-bromocyclohexanone. A combined NMR, IR, solvation and theoretical approach. Journal of Physical Organic Chemistry, 2001, 14, 317-322.	1.9	25
49	Proton chemical shifts in NMR: Part 17. Chemical shifts in alkenes and anisotropic and steric effects of the double bond. Magnetic Resonance in Chemistry, 2001, 39, 421-431.	1.9	37
50	Complete analysis of the1H NMR spectra of bicyclo[3.2.0]hept-2-en-6-one and the 7,7-dimethyl, 7,7-dichloro and 7-endo-chloro derivatives. Magnetic Resonance in Chemistry, 2001, 39, 759-761.	1.9	0
51	Proton chemical shifts in NMR. Part 15?proton chemical shifts in nitriles and the electric field and ?-electron effects of the cyano group. Magnetic Resonance in Chemistry, 2000, 38, 570-579.	1.9	17
52	Proton chemical shifts in NMR. Part 14. Proton chemical shifts, ring currents and Ï€ electron effects in condensed aromatic hydrocarbons and substituted benzenes. Perkin Transactions II RSC, 2000, , 803-812.	1.1	44
53	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
54	Conformational analysis. Part 34. An NMR investigation of the conformational equilibrium and intramolecular hydrogen bonding in nipecotic acid derivatives. Perkin Transactions II RSC, 2000, , 2382-2392.	1.1	15

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55	A model for the calculation of proton chemical shifts in non-conjugated organic compounds. Progress in Nuclear Magnetic Resonance Spectroscopy, 1999, 35, 85-152.	7.5	51
56	Conformational analysis, Part 31.1 A theoretical and lanthanide induced shift (LIS) investigation of the conformations of some epoxides. Journal of the Chemical Society Perkin Transactions II, 1999, , 99-106.	0.9	18
57	Substituent chemical shifts in NMR spectroscopy. Part 11. Does Câ€”C bond anisotropy contribute to proton chemical shifts?. Magnetic Resonance in Chemistry, 1998, 36, S179-S188.	1.9	15
58	Conformational analysis. Part 30.1 The conformational analysis of some lactones by the lanthanide induced shift (LIS) technique. Journal of the Chemical Society Perkin Transactions II, 1997, , 1279-1286.	0.9	20
59	Proton chemical shifts in NMR spectroscopy. Part 7.1 Câ€“C anisotropy and the methyl effect. Journal of the Chemical Society Perkin Transactions II, 1997, , 31-40.	0.9	22
60	Conformational Analysis Part 26â€”An Objective Method for Determining Conformer Populations and Coupling Constants in NMR Spectroscopy. Magnetic Resonance in Chemistry, 1996, 34, 71-77.	1.9	20
61	Conformational analysis. Part 25. The evaluation of molecular geometries by the lanthanide induced shift (LIS) technique. Journal of the Chemical Society Perkin Transactions II, 1995, , 1973.	0.9	17
62	Conformational analysis. Part 24. A lanthanide-induced-shift (LIS) NMR investigation of aromatic ketones. Lutetium versus lanthanum reagents in probing diamagnetic complexation shifts. Journal of the Chemical Society Perkin Transactions II, 1995, , 1965.	0.9	11
63	Conformational analysis. Part 20â€”conformational analysis of 4-deoxy-4-fluoro-D-glucose and 6-deoxy-6-fluoro-D-galactose in solution. Magnetic Resonance in Chemistry, 1994, 32, 248-254.	1.9	18
64	Conformational analysis. Part 23. A lanthanide-induced shift investigation of some cyclic and acyclic sulfoxides. Journal of the Chemical Society Perkin Transactions II, 1994, , 2329.	0.9	25
65	Conformational analysis 18â€”lanthanide-induced shift (LIS) investigation of some 2-substituted 1,3-dioxanes. Magnetic Resonance in Chemistry, 1992, 30, 1019-1024.	1.9	5
66	Conformational analysis. Part 19â€”conformational analysis of 6-deoxy-6-fluoro-D-glucose (6DFG) in solution. Magnetic Resonance in Chemistry, 1992, 30, S60-S65.	1.9	19
67	NMR spectra of the porphyrins. Part 39. Paramagnetic shifts in cobalt(II) porphyrins. Magnetic Resonance in Chemistry, 1990, 28, 1051-1057.	1.9	8
68	A theoretical study of the Si-O bond in disiloxane and related molecules. Journal of Computer-Aided Molecular Design, 1989, 2, 267-280.	2.9	6
69	Substituent chemical shifts in NMR. Part 4â€”1H SCS in some 2-substituted norbornanes and bornanes. Magnetic Resonance in Chemistry, 1989, 27, 1074-1084.	1.9	39
70	13â€”Lanthanide-induced shift (LIS) investigation of the conformation of aryl sulphones using a novel lanthanide-sulphone complexation model. Magnetic Resonance in Chemistry, 1988, 26, 252-259.	1.9	18
71	Conformational analysis. 15â€”Lanthanide-induced shift investigation of 2-exo-norborneol using tailored models of lanthanide complexation. Magnetic Resonance in Chemistry, 1988, 26, 1027-1035.	1.9	3
72	Charge calculations in molecular mechanics. V. Silicon compounds and ? bonding. Journal of Computational Chemistry, 1988, 9, 244-256.	3.3	23

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73	Charge calculations in molecular mechanics IV: A general method for conjugated systems. Journal of Computational Chemistry, 1988, 9, 288-297.	3.3	78
74	A molecular mechanics study of the Si?O bond and alkyl-silanes. Journal of Computational Chemistry, 1988, 9, 709-718.	3.3	10
75	Substituent chemical shifts in NMR. 3â€"Carbonitrile SCS in rigid molecules. Magnetic Resonance in Chemistry, 1986, 24, 451-459.	1.9	20
76	Charge calculations in molecular mechanics. III: Amino acids and peptides. Journal of Computational Chemistry, 1985, 6, 173-181.	3.3	56
77	Substituent chemical shifts in NMR. 1â€"Proton resonance spectra and geometries of norbornene, norbornane and adamantane. Magnetic Resonance in Chemistry, 1985, 23, 856-861.	1.9	44
78	Substituent chemical shifts in NMR. 2â€"Bromine SCS in rigid molecules. Magnetic Resonance in Chemistry, 1985, 23, 862-871.	1.9	23
79	A novel use of cobalt(III)meso-tetraphenylporphyrin as a chiral shift reagent. Magnetic Resonance in Chemistry, 1984, 22, 57-60.	0.7	12
80	Tetraphenylporphyrin molecules containing heteroatoms other than nitrogen: 8â€"A carbon-13 NMR study. Magnetic Resonance in Chemistry, 1984, 22, 561-564.	0.7	9
81	NMR spectra of porphyrins. 26â€"conjugation versus steric repulsions in a planar chiralmeso-Aminoporphyrin. Magnetic Resonance in Chemistry, 1984, 22, 771-774.	0.7	3
82	The NMR spectra of porphyrins. 27â€"proton NMR spectra of chlorophyll-a and pheophytin-a. Magnetic Resonance in Chemistry, 1984, 22, 779-783.	0.7	30
83	An NMR and solvation study of rotational isomerism in epihalohydrins. Tetrahedron, 1983, 39, 4201-4208.	1.9	4
84	Conformational analysis. Part 6. A lanthanide-induced shift nuclear magnetic resonance investigation of steric effects in mesitaldehyde and 2,4,6-trimethylacetophenone. Journal of the Chemical Society Perkin Transactions II, 1983, , 1161.	0.9	6
85	Conformational analysis-V.. Tetrahedron, 1982, 38, 3245-3254.	1.9	28
86	Conformational analysisâ€"III. Tetrahedron, 1982, 38, 1485-1491.	1.9	33
87	Conformational analysisâ€"II. Tetrahedron, 1981, 37, 1081-1090.	1.9	21
88	The fixed conformation of the leucyl side-chain in a tripeptide. Magnetic Resonance in Chemistry, 1980, 14, 543-544.	0.7	4
89	The NMR spectra and conformations of cyclic compounds: IXâ€"conformational studies of bicyclo(3,1,0)hexane derivatives by13C NMR. Magnetic Resonance in Chemistry, 1974, 6, 184-189.	0.7	17
90	The determination of conformational effects in some fluorobenzenes by a combined mo/coupling constant treatment. Magnetic Resonance in Chemistry, 1974, 6, 612-613.	0.7	6

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91	Nuclear magnetic resonance spectra of fluorobenzenes. II. Effect of substituents on the meta and para fluorine-fluorine coupling constants. Journal of the American Chemical Society, 1968, 90, 147-153.	13.7	75
92	Modelling1H Chemical Shifts, Hydrocarbons. , 0, , 85-132.		0
93	Chemical Shift Calculations and Molecular Structure. , 0, , 67-83.		1
94	A Practical Approach to1H NMR Calculation and Prediction. , 0, , 349-368.		1
95	Introduction to1H NMR Chemical Shifts. , 0, , 1-21.		0
96	Interpretation of1H NMR Coupling Patterns. , 0, , 23-65.		0
97	Modelling1H Chemical Shifts, Divalent Substituents. , 0, , 247-301.		0
98	1H Chemical Shifts and Structural Chemistry. , 0, , 303-347.		0