

Raymond J Abraham

List of Publications by Year in descending order

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1862
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#	ARTICLE	IF	CITATIONS
1	¹ H chemical shifts in NMR: Part 23, the effect of dimethyl sulphoxide versus chloroform solvent on ¹ H chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 491-509.	1.9	109
2	An NMR Method for the Quantitative Assessment of Intramolecular Hydrogen Bonding; Application to Physicochemical, Environmental, and Biochemical Properties. <i>Journal of Organic Chemistry</i> , 2014, 79, 11075-11083.	3.2	83
3	¹ H chemical shifts in NMR: Part 19. Carbonyl anisotropies and steric effects in aromatic aldehydes and ketones. <i>Magnetic Resonance in Chemistry</i> , 2003, 41, 26-36.	1.9	81
4	Charge calculations in molecular mechanics IV: A general method for conjugated systems. <i>Journal of Computational Chemistry</i> , 1988, 9, 288-297.	3.3	78
5	An NMR, IR and theoretical investigation of ¹ H Chemical Shifts and hydrogen bonding in phenols. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 865-877.	1.9	78
6	Nuclear magnetic resonance spectra of fluorobenzenes. II. Effect of substituents on the meta and para fluorine-fluorine coupling constants. <i>Journal of the American Chemical Society</i> , 1968, 90, 147-153.	13.7	75
7	Charge calculations in molecular mechanics. III: Amino acids and peptides. <i>Journal of Computational Chemistry</i> , 1985, 6, 173-181.	3.3	56
8	¹ H chemical shifts in NMR: Part 22 – Prediction of the ¹ H chemical shifts of alcohols, diols and inositols in solution, a conformational and solvation investigation. <i>Magnetic Resonance in Chemistry</i> , 2005, 43, 611-624.	1.9	55
9	A model for the calculation of proton chemical shifts in non-conjugated organic compounds. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1999, 35, 85-152.	7.5	51
10	¹ H chemical shifts in NMR. Part 18.1 Ring currents and π -electron effects in hetero-aromatics. <i>Perkin Transactions II RSC</i> , 2002, , 1081-1091.	1.1	51
11	Conformational analysis of 2-halocyclohexanones: an NMR, theoretical and solvation study. <i>Perkin Transactions II RSC</i> , 2002, , 1494-1498.	1.1	46
12	Substituent chemical shifts in NMR. I – Proton resonance spectra and geometries of norbornene, norbornane and adamantane. <i>Magnetic Resonance in Chemistry</i> , 1985, 23, 856-861.	1.9	44
13	Proton chemical shifts in NMR. Part 14. Proton chemical shifts, ring currents and π electron effects in condensed aromatic hydrocarbons and substituted benzenes. <i>Perkin Transactions II RSC</i> , 2000, , 803-812.	1.1	44
14	Substituent chemical shifts in NMR. Part 4 – ¹ H SCS in some 2-substituted norbornanes and bornanes. <i>Magnetic Resonance in Chemistry</i> , 1989, 27, 1074-1084.	1.9	39
15	Proton chemical shifts in NMR: Part 17. Chemical shifts in alkenes and anisotropic and steric effects of the double bond. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 421-431.	1.9	37
16	Conformational analysis – III. <i>Tetrahedron</i> , 1982, 38, 1485-1491.	1.9	33
17	The NMR spectra of porphyrins. 27 – proton NMR spectra of chlorophyll-a and pheophytin-a. <i>Magnetic Resonance in Chemistry</i> , 1984, 22, 779-783.	0.7	30
18	Conformational analysis. Part 36. A variable temperature ¹³ C NMR study of conformational equilibria in methyl substituted cycloalkanes. <i>Perkin Transactions II RSC</i> , 2001, , 302-307.	1.1	30

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19	Is there an intramolecular hydrogen bond in 2-halophenols? A theoretical and spectroscopic investigation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25151-25159.	2.8	30
20	¹ H NMR spectra. Part 30: ¹ H chemical shifts in amides and the magnetic anisotropy, electric field and steric effects of the amide group. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 143-155.	1.9	29
21	Conformational analysis-V.. <i>Tetrahedron</i> , 1982, 38, 3245-3254.	1.9	28
22	Conformational analysis. Part 35. NMR, solvation and theoretical investigation of rotational isomerism in methyl fluoroacetate and methyl difluoroacetate. <i>Perkin Transactions II RSC</i> , 2001, , 815-820.	1.1	26
23	¹ H NMR spectra part 31: ¹ H chemical shifts of amides in DMSO solvent. <i>Magnetic Resonance in Chemistry</i> , 2014, 52, 395-408.	1.9	26
24	Conformational analysis. Part 23. A lanthanide-induced shift investigation of some cyclic and acyclic sulfoxides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1994, , 2329.	0.9	25
25	Conformational analysis of 2-bromocyclohexanone. A combined NMR, IR, solvation and theoretical approach. <i>Journal of Physical Organic Chemistry</i> , 2001, 14, 317-322.	1.9	25
26	Conformational analysis. Part 33.1 An NMR, solvation and theoretical investigation of conformational isomerism in N,N-dimethylfluoroacetamide and N,N-dimethyl- α -fluoropropionamide. <i>Perkin Transactions II RSC</i> , 2000, , 2054-2059.	1.1	24
27	Substituent chemical shifts in NMR. 29 Bromine SCS in rigid molecules. <i>Magnetic Resonance in Chemistry</i> , 1985, 23, 862-871.	1.9	23
28	Charge calculations in molecular mechanics. V. Silicon compounds and π bonding. <i>Journal of Computational Chemistry</i> , 1988, 9, 244-256.	3.3	23
29	Proton chemical shifts in NMR spectroscopy. Part 7.1 13 C anisotropy and the methyl effect. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 31-40.	0.9	22
30	Conformational analysis.. <i>Perkin Transactions II RSC</i> , 2002, , 2025-2030.	1.1	22
31	Conformational analysis ^{II} . <i>Tetrahedron</i> , 1981, 37, 1081-1090.	1.9	21
32	¹ H 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. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 667-675.	1.9	21
33	Substituent chemical shifts in NMR. 13 Carbonitrile SCS in rigid molecules. <i>Magnetic Resonance in Chemistry</i> , 1986, 24, 451-459.	1.9	20
34	Conformational Analysis Part 26 ^{II} An Objective Method for Determining Conformer Populations and Coupling Constants in NMR Spectroscopy. <i>Magnetic Resonance in Chemistry</i> , 1996, 34, 71-77.	1.9	20
35	Conformational analysis. Part 30.1 The conformational analysis of some lactones by the lanthanide induced shift (LIS) technique. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 1279-1286.	0.9	20
36	NMR, solvation and theoretical investigations of conformational isomerism in 2-X-cyclohexanones (X=NMe ₂ , OMe, SMe and SeMe). <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 833-838.	1.9	20

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37	¹ H NMR Spectra. Part 28: Proton chemical shifts and couplings in three-membered rings. A ring current model for cyclopropane and a novel dihedral angle dependence for ³ J _{HH} couplings involving the epoxy proton. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 305-313.	1.9	20
38	Conformational analysis. Part 19: conformational analysis of 6-deoxy-6-fluoro-D-glucose (6DFG) in solution. <i>Magnetic Resonance in Chemistry</i> , 1992, 30, S60-S65.	1.9	19
39	Conformational analysis in N-methylfluoroamides. A theoretical, NMR and IR investigation. <i>Perkin Transactions II RSC</i> , 2002, , 773-778.	1.1	19
40	¹ H chemical shifts in NMR. Part 21: Prediction of the ¹ H chemical shifts of molecules containing the ester group: a modelling and ab initio investigation. <i>Magnetic Resonance in Chemistry</i> , 2005, 43, 3-15.	1.9	19
41	¹³ C Lanthanide-induced shift (LIS) investigation of the conformation of aryl sulphones using a novel lanthanide-sulphone complexation model. <i>Magnetic Resonance in Chemistry</i> , 1988, 26, 252-259.	1.9	18
42	Conformational analysis. Part 20: conformational analysis of 4-deoxy-4-fluoro-D-glucose and 6-deoxy-6-fluoro-D-galactose in solution. <i>Magnetic Resonance in Chemistry</i> , 1994, 32, 248-254.	1.9	18
43	Conformational analysis, Part 31.1 A theoretical and lanthanide induced shift (LIS) investigation of the conformations of some epoxides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 99-106.	0.9	18
44	A simple and facile NMR method for the determination of hydrogen bonding by amide N-H protons in protein models and other compounds. <i>New Journal of Chemistry</i> , 2017, 41, 6064-6066.	2.8	18
45	The NMR spectra and conformations of cyclic compounds: IX: conformational studies of bicyclo(3,1,0)hexane derivatives by ¹³ C NMR. <i>Magnetic Resonance in Chemistry</i> , 1974, 6, 184-189.	0.7	17
46	Conformational analysis. Part 25. The evaluation of molecular geometries by the lanthanide induced shift (LIS) technique. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 1973.	0.9	17
47	Proton chemical shifts in NMR. Part 15: proton chemical shifts in nitriles and the electric field and π -electron effects of the cyano group. <i>Magnetic Resonance in Chemistry</i> , 2000, 38, 570-579.	1.9	17
48	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. <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 211-217.	1.9	17
49	Conformational analysis. Part 40: a theoretical and NMR investigation of the conformations of cis- and trans-cyclopentane-1,3-diol. <i>Magnetic Resonance in Chemistry</i> , 2003, 41, 1000-1008.	1.9	17
50	Conformational analysis, Part 41. A modelling and LIS/NMR investigation of the conformations of α,β -unsaturated carbonyl compounds. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 384-392.	1.9	16
51	The hydrogen bond acidity and other descriptors for oximes. <i>New Journal of Chemistry</i> , 2009, 33, 76-81.	2.8	16
52	Substituent chemical shifts in NMR spectroscopy. Part 11. Does ¹³ C bond anisotropy contribute to proton chemical shifts?. <i>Magnetic Resonance in Chemistry</i> , 1998, 36, S179-S188.	1.9	15
53	Conformational analysis. Part 34. An NMR investigation of the conformational equilibrium and intramolecular hydrogen bonding in nipecotic acid derivatives. <i>Perkin Transactions II RSC</i> , 2000, , 2382-2392.	1.1	15
54	¹ H NMR and molecular modelling investigation of diastereotopic methylene hydrogen atoms. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 279-283.	1.9	14

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55	Conformational analysis of fluoroacetoxime and of its O-methyl ether by ^1H , ^{13}C and ^{15}N NMR and theoretical calculations. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 42-48.	1.9	14
56	^1H chemical shifts in NMR. Part 20 "Anisotropic and steric effects in halogen substituent chemical shifts (SCS), a modelling and <i>ab initio</i> investigation. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 436-444.	1.9	14
57	Experimental and theoretical evaluation of trans-3-halo-2-hydroxy-tetrahydropyran conformational preferences. Beyond anomeric interaction. <i>RSC Advances</i> , 2015, 5, 35412-35420.	3.6	14
58	Substituent effects on ^1H and ^{13}C NMR chemical shifts in γ -monosubstituted ethyl acetates: principal component analysis and ^1H chemical shift calculations. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 449-454.	1.9	13
59	A novel use of cobalt(III) meso-tetraphenylporphyrin as a chiral shift reagent. <i>Magnetic Resonance in Chemistry</i> , 1984, 22, 57-60.	0.7	12
60	Conformational analysis. Part 24. A lanthanide-induced-shift (LIS) NMR investigation of aromatic ketones. Lutetium versus lanthanum reagents in probing diamagnetic complexation shifts. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 1965.	0.9	11
61	Proton chemical shifts in NMR. Part 16.1 Proton chemical shifts in acetylenes and the anisotropic and steric effects of the acetylene group. <i>Perkin Transactions II RSC</i> , 2001, , 1195-1204.	1.1	11
62	The prediction of ^1H chemical shifts in amines: a semiempirical and <i>ab initio</i> investigation. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 749-757.	1.9	11
63	A molecular mechanics study of the Si-O bond and alkyl-silanes. <i>Journal of Computational Chemistry</i> , 1988, 9, 709-718.	3.3	10
64	Conformational behaviour of methyl 2-fluoroesters through theoretical calculations, NMR and IR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1152.	2.8	10
65	Tetraphenylporphyrin molecules containing heteroatoms other than nitrogen: ^{13}C NMR study. <i>Magnetic Resonance in Chemistry</i> , 1984, 22, 561-564.	0.7	9
66	NMR spectra of the porphyrins. Part 39. Paramagnetic shifts in cobalt(II) porphyrins. <i>Magnetic Resonance in Chemistry</i> , 1990, 28, 1051-1057.	1.9	8
67	Conformational analysis: Part 37. ^{13}C and ^1H NMR and theoretical investigation of the conformational equilibrium of 2-methylcyclohexanone oxime and of its O-methyl ether. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 49-56.	1.9	8
68	A ^1H NMR and theoretical investigation of the conformations of some monosubstituted cyclobutanes. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 23-29.	1.9	8
69	A convenient and accurate method for predicting ^{13}C chemical shifts in organic molecules. <i>New Journal of Chemistry</i> , 2018, 42, 5024-5036.	2.8	8
70	The determination of conformational effects in some fluorobenzenes by a combined J /coupling constant treatment. <i>Magnetic Resonance in Chemistry</i> , 1974, 6, 612-613.	0.7	6
71	Conformational analysis. Part 6. A lanthanide-induced shift nuclear magnetic resonance investigation of steric effects in mesitaldehyde and 2,4,6-trimethylacetophenone. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1983, , 1161.	0.9	6
72	A theoretical study of the Si-O bond in disiloxane and related molecules. <i>Journal of Computer-Aided Molecular Design</i> , 1989, 2, 267-280.	2.9	6

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73	Conformational analysis, part 43. A theoretical and LIS/NMR investigation of the conformations of substituted benzamides. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 498-508.	1.9	6
74	A theoretical and NMR lanthanide-induced shift (LIS) investigation of the conformations of lactams.. <i>Magnetic Resonance in Chemistry</i> , 2017, 55, 1059-1072.	1.9	6
75	Conformational analysis 18 ^W lanthanide-induced shift (LIS) investigation of some 2-substituted 1,3-dioxanes. <i>Magnetic Resonance in Chemistry</i> , 1992, 30, 1019-1024.	1.9	5
76	A re-investigation of ⁴ J _{FF} and ⁵ J _{FF} nuclear spin-spin couplings in substituted benzenes, a novel conformational tool. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15822-15827.	2.8	5
77	The use of chemical shift calculations in the conformational analysis of substituted benzenes. <i>New Journal of Chemistry</i> , 2019, 43, 5382-5394.	2.8	5
78	The fixed conformation of the leucyl side-chain in a tripeptide. <i>Magnetic Resonance in Chemistry</i> , 1980, 14, 543-544.	0.7	4
79	An NMR and solvation study of rotational isomerism in epihalohydrins. <i>Tetrahedron</i> , 1983, 39, 4201-4208.	1.9	4
80	The role of stereoelectronic interactions in the conformational isomerism of some phosphorus-containing model compounds. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 505-509.	1.9	4
81	A molecular mechanics and <i>ab initio</i> prediction of the ¹ H chemical shifts of pinanes. <i>Magnetic Resonance in Chemistry</i> , 2017, 55, 837-845.	1.9	4
82	NMR spectra of porphyrins. 26 ^W conjugation versus steric repulsions in a planar chiral meso-Aminoporphyrin. <i>Magnetic Resonance in Chemistry</i> , 1984, 22, 771-774.	0.7	3
83	Conformational analysis. 15 ^W Lanthanide-induced shift investigation of 2-exo-norborneol using tailored models of lanthanide complexation. <i>Magnetic Resonance in Chemistry</i> , 1988, 26, 1027-1035.	1.9	3
84	¹ H NMR spectra. Part 29 ^W : proton chemical shifts and couplings in esters—the conformational analysis of methyl ¹³ C butyrolactones. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 9-15.	1.9	3
85	The use of MM/QM calculations of ¹³ C and ¹⁵ N chemical shifts in the conformational analysis of alkyl substituted anilines. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 520-531.	1.9	3
86	The use of MM/QM calculations of ¹³ C chemical shifts in the conformational analysis of some monosaccharides and sucrose. <i>New Journal of Chemistry</i> , 2021, 45, 2001-2009.	2.8	3
87	Conformational analysis: Part 42. A modelling and LIS/NMR investigation of the conformations of some aromatic SO compounds. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 544-550.	1.9	2
88	Tautomerism in 8-Nitroguanosine Studied by NMR and Theoretical Calculations. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2016, 35, 53-63.	1.1	2
89	¹ H chemical shifts in NMR. Part 24 ^W proton chemical shifts in some gem-difunctional compounds: 3-endo- and 3-exo-substituted norbornanones. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 376-383.	1.9	1
90	Chemical Shift Calculations and Molecular Structure. , 0, , 67-83.		1

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91	A Practical Approach to ¹ H NMR Calculation and Prediction. , 0, , 349-368.		1
92	Complete analysis of the ¹ H 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
93	â€œObjectiveâ€™™ determination of coupling constants and conformational equilibria by solvent variation: a comment. Magnetic Resonance in Chemistry, 2005, 43, 424-426.	1.9	0
94	Modelling ¹ H Chemical Shifts, Hydrocarbons. , 0, , 85-132.		0
95	Introduction to ¹ H NMR Chemical Shifts. , 0, , 1-21.		0
96	Interpretation of ¹ H NMR Coupling Patterns. , 0, , 23-65.		0
97	Modelling ¹ H Chemical Shifts, Divalent Substituents. , 0, , 247-301.		0
98	¹ H Chemical Shifts and Structural Chemistry. , 0, , 303-347.		0