

Alessandro Bagno

List of Publications by Year in descending order

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126
papers

4,400
citations

81900

39
h-index

133252

59
g-index

139
all docs

139
docs citations

139
times ranked

4265
citing authors

#	ARTICLE	IF	CITATIONS
1	Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021). <i>Pure and Applied Chemistry</i> , 2022, 94, 353-534.	1.9	17
2	Bioactive Phloroglucinyl Heterodimers: The Tautomeric and Rotameric Equilibria of Arzanol. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 4810-4816.	2.4	0
3	Unraveling the Key Features of the Reactive State of Decatungstate Anion in Hydrogen Atom Transfer (HAT) Photocatalysis. <i>ACS Catalysis</i> , 2016, 6, 7174-7182.	11.2	124
4	Insights into the cytotoxic activity of the phosphane copper(I) complex [Cu(thp) ₄][PF ₆]. <i>Journal of Inorganic Biochemistry</i> , 2016, 165, 80-91.	3.5	38
5	Direct Detection of ¹⁷ O in [Gd(DOTA)] ³⁺ by NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2015, 21, 1955-1960.	3.3	8
6	Characterization of Paramagnetic Reactive Intermediates: Predicting the NMR Spectra of Iron(IV)â€“Oxo Complexes by DFT. <i>Chemistry - A European Journal</i> , 2015, 21, 12960-12970.	3.3	15
7	Fourâ€“Component Relativistic DFT Calculations of ¹³ C Chemical Shifts of Halogenated Natural Substances. <i>Chemistry - A European Journal</i> , 2015, 21, 18834-18840.	3.3	27
8	Multinuclear Solid-State NMR and DFT Studies on Phosphanido-Bridged Diplatinum Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 5855-5863.	4.0	18
9	Addressing the stereochemistry of complex organic molecules by density functional theoryâ€“NMR. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015, 5, 228-240.	14.6	59
10	Insights on the Isotropic-to-Smectic A Transition in Ionic Liquid Crystals from Coarse-Grained Molecular Dynamics Simulations: The Role of Microphase Segregation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3829-3836.	2.6	49
11	MD simulation of xenon in ionic liquids: Disentangling the cationic and anionic cage effects on the structural and dynamic properties. <i>Journal of Molecular Liquids</i> , 2015, 210, 272-278.	4.9	7
12	Oxygenation by Ruthenium Monosubstituted Polyoxotungstates in Aqueous Solution: Experimental and Computational Dissection of a Ru(III)â€“Ru(V) Catalytic Cycle. <i>Chemistry - A European Journal</i> , 2014, 20, 10932-10943.	3.3	11
13	Understanding Cage Effects in Imidazolium Ionic Liquids by ¹²⁹ Xe NMR: MD Simulations and Relativistic DFT Calculations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13963-13968.	2.6	24
14	Computational ¹⁹ F NMR. 2. Organic compounds. <i>RSC Advances</i> , 2014, 4, 41605-41611.	3.6	21
15	Predicting the spin state of paramagnetic iron complexes by DFT calculation of proton NMR spectra. <i>Dalton Transactions</i> , 2014, 43, 9486-9496.	3.3	33
16	A DFT study of the vicinal 3J(119Sn,13C) and 3J(119Sn,1H) coupling constants in trimethyl- and chlorodimethylstannyl propanoates. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 139-146.	1.8	8
17	Electronic and EPR spectra of the species involved in [W10O32]4+ photocatalysis. A relativistic DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2890.	2.8	28
18	Longâ€“Range Diastereoselectivity in an Ugi Reaction: Stereocontrolled and Diversityâ€“Oriented Synthesis of Tetrahydrobenzoxazepines. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5064-5075.	2.4	25

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19	Spectroscopic signatures of the carbon buckyonions C60@C180 and C60@C240: a dispersion-corrected DFT study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18030.	2.8	19
20	Reactivity of Auranofin with Selenols and Thiols – Implications for the Anticancer Activity of Gold(I) Compounds. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2718-2727.	2.0	25
21	Probing the C ₆₀ triplet state coupling to nuclear spins inside and out. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2013, 371, 20120475.	3.4	13
22	Predicting the paramagnet-enhanced NMR relaxation of H ₂ encapsulated in endofullerene nitroxides by density-functional theory calculations. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2013, 371, 20110634.	3.4	5
23	Computational 19F NMR. 1. General features. <i>Highlights in Theoretical Chemistry</i> , 2013, , 41-52.	0.0	0
24	Observation of scalar nuclear spin–spin coupling in van der Waals complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 12393-12397.	7.1	28
25	Counterion effects on the 183W NMR spectra of the lacunary Keggin polyoxotungstate [PW11O39]7–. Relativistic DFT calculations. <i>Comptes Rendus Chimie</i> , 2012, 15, 118-123.	0.5	4
26	Understanding the Extraordinary Deshielding of ¹²⁹ Xe in a Permetallated Cryptophane by Relativistic DFT. <i>Chemistry - A European Journal</i> , 2012, 18, 7341-7345.	3.3	20
27	Computational 19F NMR. 1. General features. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	19
28	Thermo-induced lipid oxidation of a culinary oil: The effect of materials used in common food processing on the evolution of oxidised species. <i>Food Chemistry</i> , 2012, 133, 754-759.	8.2	11
29	Addressing the Stereochemistry of Complex Organic Molecules by Density Functional Theory-NMR: Vannusal B in Retrospective. <i>Journal of the American Chemical Society</i> , 2011, 133, 6072-6077.	13.7	118
30	Relativistic DFT calculations of the NMR properties and reactivity of transition metal methane η^5 -complexes: insights on C–H bond activation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4285.	2.8	19
31	Predicting the UV spectrum of polyoxometalates by TD–DFT. <i>Journal of Computational Chemistry</i> , 2011, 32, 2983-2987.	3.3	31
32	NMR Spectra of Terminal Oxo Gold and Platinum Complexes: Relativistic DFT Predictions. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1083-1086.	13.8	40
33	Predicting the 1H and 13C NMR spectra of paramagnetic Ru(III) complexes by DFT. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S132-S141.	1.9	40
34	Computing the NMR spectra of the sponge metabolite arsenicin A: when simple becomes difficult. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 1016-1021.	1.9	9
35	Thermoinduced Lipid Oxidation of a Culinary Oil: A Kinetic Study of the Oxidation Products by Magnetic Resonance Spectroscopies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10059-10065.	2.5	26
36	Preferential solvation of glucose and talose in water–acetonitrile mixtures: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2981.	2.8	24

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37	Predicting the NMR Spectra of Paramagnetic Molecules by DFT: Application to Organic Free Radicals and Transition-Metal Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 7990-8004.	3.3	97
38	NMR quantification of trace components in complex matrices by band-selective excitation with adiabatic pulses. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 868-872.	1.9	29
39	Can Two Molecules Have the Same NMR Spectrum? Hexacyclinol Revisited. <i>Organic Letters</i> , 2009, 11, 1409-1412.	4.6	49
40	H ₂ O ₂ activation by heteropolyacids with defect structures: the case of $\text{H}^+\text{[(XO)}_4\text{]}_n\text{W}_{10}\text{O}_{32}$ (X = Si, Ge, n = 8; X = P, n = 12).	1.9	17
41	Formylation of activated arenes by phenyl formate: implications for the mechanism of the Fries rearrangement of aryl formates. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 682-687.	1.9	4
42	Predicting the NMR spectra of nucleotides by DFT calculations: cyclic uridine monophosphate. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 518-524.	1.9	17
43	Computational NMR Spectroscopy of Organoarsenicals and the Natural Polyarsenic Compound Arsenicin. <i>Chemistry - A European Journal</i> , 2008, 14, 10445-10452.	3.3	27
44	Prediction of the ¹ H and ¹³ C NMR Spectra of D-Glucose in Water by DFT Methods and MD Simulations. <i>Journal of Organic Chemistry</i> , 2007, 72, 7373-7381.	3.2	100
45	Metal-Mediated Coupling in DNA Base Pairs: A Relativistic DFT Predictions. <i>Journal of the American Chemical Society</i> , 2007, 129, 11360-11361.	13.7	48
46	Asymmetric Tetraprotonation of $\text{H}^+\text{[(SiO)}_4\text{]}_n\text{W}_{10}\text{O}_{32}$ Triggers a Catalytic Epoxidation Reaction: Perspectives in the Assignment of the Active Catalyst. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3255-3258.	13.8	72
47	Computing the ¹ H NMR Spectrum of a Bulk Ionic Liquid from Snapshots of Carboxymethylchitosan Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2007, 8, 873-881.	2.1	51
48	Computer simulation of diffusion coefficients of the room-temperature ionic liquid [bmim][BF ₄]: Problems with classical simulation techniques. <i>Journal of Molecular Liquids</i> , 2007, 131-132, 17-23.	4.9	69
49	Computational NMR spectroscopy: reversing the information flow. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 603-619.	1.4	109
50	Nuclear Spin Relaxation Driven by Intermolecular Dipolar Interactions: The Role of Solute-Solvent Pair Correlations in the Modeling of Spectral Density Functions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5676-5689.	2.6	35
51	Relativistic DFT Calculation of ¹¹⁹ Sn Chemical Shifts and Coupling Constants in Tin Compounds. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 37-46.	5.3	83
52	Fries Rearrangement of Aryl Formates: A Mechanistic Study by Means of ¹ H, ² H, and ¹¹ B NMR Spectroscopy and DFT Calculations. <i>Journal of Organic Chemistry</i> , 2006, 71, 9331-9340.	3.2	26
53	Computing the NMR Spectrum of a Bulk Ionic Liquid Phase by QM/MM Methods. <i>Journal of Physical Chemistry B</i> , 2006, 110, 23004-23006.	2.6	46
54	Structure of D-ribonic acid-dimethyltin(IV) in coordinating solvents: an experimental and DFT ¹¹⁹ Sn NMR study. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 874-883.	1.9	9

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55	Selective J-resolved spectra: A double pulsed field gradient spin-echo approach. <i>Journal of Magnetic Resonance</i> , 2006, 182, 29-37.	2.1	11
56	Toward the Complete Prediction of the ^1H and ^{13}C NMR Spectra of Complex Organic Molecules by DFT Methods: Application to Natural Substances. <i>Chemistry - A European Journal</i> , 2006, 12, 5514-5525.	3.3	189
57	Computational Modeling of Polyoxotungstates by Relativistic DFT Calculations of ^{183}W NMR Chemical Shifts. <i>Chemistry - A European Journal</i> , 2006, 12, 8460-8471.	3.3	53
58	NMR techniques for the investigation of solvation phenomena and non-covalent interactions. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2005, 47, 41-93.	7.5	105
59	Solvation of Tetraalkylammonium Chlorides in Acetonitrile-Water Mixtures: Mass Spectrometry and Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2005, 6, 1307-1315.	2.1	22
60	Vicinal Tungsten-Tungsten Coupling Constants in Polyoxotungstates: DFT Calculations Challenge an Empirical Rule. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2023-2026.	13.8	38
61	Calculation of NMR Parameters in Van Der Waals Complexes Involving Organic Systems and Xenon. <i>ChemInform</i> , 2005, 36, no.	0.0	0
62	Vicinal Tungsten-Tungsten Coupling Constants in Polyoxotungstates: DFT Calculations Challenge an Empirical Rule.. <i>ChemInform</i> , 2005, 36, no.	0.0	0
63	The effect of the anion on the physical properties of trihalide-based N,N-dialkylimidazolium ionic liquids. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 1624.	2.8	75
64	Fries Rearrangement of Aryl Formates Promoted by BCl_3 . Mechanistic Evidence from ^{11}B NMR Spectra and DFT Calculations. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2004, 59, 386-397.	0.7	6
65	Detecting intermolecular NOEs by means of a novel DPGSE pulse sequence. Application to the solvation of carbohydrates in binary mixtures. <i>Journal of Magnetic Resonance</i> , 2004, 167, 31-35.	2.1	17
66	Calculation of NMR parameters in van der Waals complexes involving organic systems and xenon. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 945-950.	1.9	9
67	Photooxidation in Water by New Hybrid Molecular Photocatalysts Integrating an Organic Sensitizer with a Polyoxometalate Core. <i>Advanced Synthesis and Catalysis</i> , 2004, 346, 648-654.	4.3	96
68	Conformational Analysis of Saturated trans-Fused 1,3,2-Benzoxazaphosphinine 2-Oxides $\hat{\wedge}$ DFT Calculation of NMRJ(P,H) Coupling Constants. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 4921-4930.	2.4	11
69	Relativistic DFT calculation of ^{99}Ru NMR parameters: chemical shifts and spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, S79-S87.	1.9	41
70	Preferential Solvation and Self-Association in Alcohol-Acetonitrile Mixtures Observed through Mass Spectrometric Analysis of Clusters: Influence of Alkyl Chain Length. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3479-3487.	2.6	24
71	Relativistic DFT Calculations of Polyoxotungstate ^{183}W NMR Spectra: Insight into their Solution Structure. <i>ChemPhysChem</i> , 2003, 4, 517-519.	2.1	37
72	DFT Study of the NMR Properties of Xenon in Covalent Compounds and van der Waals Complexes-Implications for the Use of ^{129}Xe as a Molecular Probe. <i>Chemistry - A European Journal</i> , 2003, 9, 1486-1495.	3.3	51

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73	Predicting ¹³ C NMR Spectra by DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9964-9973.	2.5	121
74	Modeling NMR Parameters by DFT Methods as an Aid to the Conformational Analysis of cis-Fused 7a(8a)-Methyl Octa(hexa)hydrocyclopenta[d][1,3]oxazines and [3,1]benzoxazines. <i>Journal of the American Chemical Society</i> , 2003, 125, 4609-4618.	13.7	115
75	Through-Space Spin-Spin Coupling In Acetylenic Systems. Ab Initio and DFT Calculations. <i>International Journal of Molecular Sciences</i> , 2003, 4, 193-202.	4.1	8
76	[60]Fullerene as a Substituent. <i>Chemistry - A European Journal</i> , 2002, 8, 1015.	3.3	53
77	Through-Space Spin-Spin Coupling in van der Waals Dimers and CH/π Interacting Systems. An Ab Initio and DFT Study. <i>Chemistry - A European Journal</i> , 2002, 8, 2047.	3.3	49
78	DFT Calculations of ⁹⁹ Ru Chemical Shifts with All-Electron and Effective Core Potential Basis Sets. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 1475-1483.	2.0	30
79	Probing the solvation shell of organic molecules by intermolecular ¹ H NOESY. <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 790-795.	1.9	40
80	DFT Calculations of ⁹⁹ Ru Chemical Shifts with All-Electron and Effective Core Potential Basis Sets. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 1475-1483.	2.0	1
81	Substituent effects on the through-space nuclear magnetic spin-spin coupling in van der Waals dimers. <i>Arkivoc</i> , 2002, 2002, 38-44.	0.5	9
82	Carbon and Nitrogen Basicity of Aminothiophenes and Anilines. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6537-6542.	2.5	25
83	NMR properties (chemical shift and relaxation rate) of acceptor and hydrogen bridge nuclei in hydrogen-bonded complexes. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S59-S66.	1.9	3
84	New Formylating Agents ^η Preparative Procedures and Mechanistic Investigations. <i>European Journal of Organic Chemistry</i> , 2001, 2001, 2947.	2.4	18
85	Complete Prediction of the ¹ H NMR Spectrum of Organic Molecules by DFT Calculations of Chemical Shifts and Spin-Spin Coupling Constants. <i>Chemistry - A European Journal</i> , 2001, 7, 1652-1661.	3.3	107
86	DFT Calculation of Intermolecular Nuclear Spin-Spin Coupling in van der Waals Dimers. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2532-2534.	13.8	34
87	DFT Calculation of Intermolecular Nuclear Spin-Spin Coupling in van der Waals Dimers The authors wish to thank V. G. Malkin and O. L. Malkina for providing the deMon-NMR program and for helpful discussions.. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2532-2534.	13.8	0
88	Microwave-Assisted Rapid Incorporation of Ruthenium into Lacunary Keggin-Type Polyoxotungstates: One-Step Synthesis, ⁹⁹ Ru, ¹⁸³ W NMR Characterization and Catalytic Activity of [PW ₁₁ O ₃₉ Ru _{II} (DMSO)] ⁵⁻ . <i>European Journal of Inorganic Chemistry</i> , 2000, 2000, 17-20.	2.0	73
89	Investigation of Cation-Anion Interactions in 2-Propanol Solutions of Sodium Alkoxides and Thiolates by ²³ Na-NMR Spectroscopy. <i>European Journal of Organic Chemistry</i> , 2000, 2000, 1953-1957.	2.4	2
90	Detecting Hydrogen Bonding by NMR Relaxation of the Acceptor Nuclei. <i>Chemistry - A European Journal</i> , 2000, 6, 2915-2924.	3.3	11

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91	Quantum Chemical Modeling of Through-Hydrogen Bond Spin-Spin Coupling in Amides and Ubiquitin. <i>Chemistry - A European Journal</i> , 2000, 6, 2925-2930.	3.3	49
92	Acyl group vs nitrogen protonation of carboxylic and $\frac{1}{2}$ non-carboxylic amides in the gas phase and water. <i>Journal of Physical Organic Chemistry</i> , 2000, 13, 574-578.	1.9	17
93	Effective core potential DFT calculations of nuclear shielding as a tool for the prediction and assignment of the tungsten chemical shift in mono- and polynuclear complexes. <i>Chemical Physics Letters</i> , 2000, 317, 123-128.	2.6	38
94	Selectivity in Proton Transfer, Hydrogen Bonding, and Solvation. <i>Accounts of Chemical Research</i> , 2000, 33, 609-616.	15.6	58
95	Deprotonation of Amides and Polyfunctional Imides Probed by Heteronuclear NMR and Quantum Chemical Calculations. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 287-295.	2.4	23
96	Steric Effects on the Proton-Transfer Equilibria of Ketones, Sulfoxides, and Phenols. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 1507-1515.	2.4	7
97	Solvent Effect on the Protonation of Acetylene and Ethylene $\hat{=}$ Continuum Solvent Quantum Chemical Calculations. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 2893-2897.	2.4	8
98	Site of Protonation of Carboxylic and Non-Carboxylic Amides in the Gas Phase and in Water. <i>Chemistry - A European Journal</i> , 1999, 5, 523-536.	3.3	51
99	Preferential Solvation of Organic Species in Binary Solvent Mixtures Probed by Intermolecular ^1H NOESY NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 1999, 5, 1291-1300.	3.3	45
100	Experimental and theoretical investigation of gas phase complexes between chloride ion and some chloroethenes. <i>International Journal of Mass Spectrometry</i> , 1998, 179-180, 349-357.	1.5	5
101	Site of Protonation of Alkyl- and Arylhydrazines Probed by ^{14}N , ^{15}N , and ^{13}C NMR Relaxation and Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2888-2892.	2.5	23
102	The ab initio neon $\hat{=}$ water potential-energy surface and its relationship with the hydrophobic hydration shell. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 2501-2504.	1.7	30
103	Reactive Intermediates in Peptide Synthesis: $\hat{=}$ First Crystal Structures and ab Initio Calculations of 2-Alkoxy-5(4H)-oxazolones from Urethane-Protected Amino Acids. <i>Journal of the American Chemical Society</i> , 1997, 119, 4136-4142.	13.7	19
104	Preferential Solvation of Neutral Species in Binary Solvent Mixtures Characterized by ^1H NOESY NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 1997, 119, 2299-2300.	13.7	30
105	Ab Initio Calculations on Water $\hat{=}$ Peroxovanadium Clusters, $\text{VO}(\text{O}_2)(\text{H}_2\text{O})_{n+}$ ($n = 1 \hat{=}$ 5). Implications for the Structure in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4637-4640.	2.5	23
106	Ab initio calculation of NMR properties (shielding and electric field gradient) of ^{33}S in sulfur compounds. <i>Computational and Theoretical Chemistry</i> , 1997, 418, 243-255.	1.5	11
107	Site of Ionization of Polyfunctional Bases and Acids. 1. Ab Initio Proton Affinities. <i>The Journal of Physical Chemistry</i> , 1996, 100, 1536-1544.	2.9	62
108	Solvent effect on relative N- and O-acidity. Inversion of the deprotonation site of 2- and 4-[(2,4,6-trinitrophenyl)amino]benzoic acids. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 2163.	0.9	8

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109	Site of Ionization of Polyfunctional Bases and Acids. 2. Ab Initio Electric Field Gradients at Nitrogen, Oxygen, Phosphorus, and Sulfur in Neutral and Ionized Forms. <i>The Journal of Physical Chemistry</i> , 1996, 100, 1545-1553.	2.9	24
110	Steric effects on the solvation of protonated di-tert-butyl ketone and phenyl tert-butyl ketone. <i>Journal of the Chemical Society Chemical Communications</i> , 1995, , 2053.	2.0	5
111	Relative basicity of nitrogen, oxygen, and sulfur bases. The site of protonation in sulfenamides and sulfenamides determined by nitrogen-14 NMR relaxation. <i>Journal of Organic Chemistry</i> , 1994, 59, 232-233.	3.2	23
112	Site of Ionization of Hydroxamic Acids Probed by Heteronuclear NMR Relaxation Rate and NOE Measurements. An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 1994, 116, 916-924.	13.7	99
113	Thermodynamics of protonation and hydration of aliphatic amides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 1091.	0.9	21
114	A novel method for the determination of ionization sites in polyfunctional acids and bases by NMR relaxation rate measurements. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 283.	0.9	15
115	Solvation of nonelectrolytes in water probed by oxygen-17 NMR relaxation of the solvent. <i>The Journal of Physical Chemistry</i> , 1993, 97, 4601-4607.	2.9	36
116	A program for interconverting concentration units in binary mixtures. <i>Computers & Chemistry</i> , 1992, 16, 267-268.	1.2	0
117	A pulse sequence for T1 measurement by inversion-recovery in the presence of acoustic ringing. <i>Magnetic Resonance in Chemistry</i> , 1992, 30, 1164-1168.	1.9	4
118	Kinetics of nucleophilic aromatic substitution in concentrated solutions of alkali metal methoxides in methanol. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1991, , 651.	0.9	4
119	Thermodynamics of protonation of ketones and esters and energies of hydration of their conjugate acids. <i>The Journal of Physical Chemistry</i> , 1991, 95, 345-352.	2.9	48
120	Levelling of substituent effects on acidities in the gas phase compared with those in solution. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1991, , 1601.	0.9	3
121	Copper(II) Chloride Catalyzed Carboxydiazoniation of Arenediazonium Tetrafluoroborates with Carbon Monoxide in Aqueous Dioxane Solution to Arenecarboxylic Acids. <i>Synlett</i> , 1990, 1990, 596-598.	1.8	3
122	The excess basicity of alkali metal methoxides in methanol. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1990, , 1017.	0.9	12
123	Thermodynamics of protonation of N,N-dimethylthioamides in aqueous sulfuric acid. <i>Canadian Journal of Chemistry</i> , 1990, 68, 1746-1749.	1.1	7
124	Chemistry in superacids. 8. Superacid-catalyzed carbonylation of methane, methyl halides, methyl alcohol, and dimethyl ether to methyl acetate and acetic acid. <i>Journal of Organic Chemistry</i> , 1990, 55, 4284-4289.	3.2	60
125	Acid-base properties of organic solvents. <i>Journal of the American Chemical Society</i> , 1988, 110, 4577-4582.	13.7	61
126	Stability and solvation of organic cations. <i>Reviews of Chemical Intermediates</i> , 1987, 7, 313-352.	1.1	78