Alessandro Bagno

List of Publications by Year
in descending order

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126	4,400	81900	133252
papers	citations	39 h-index	59 g-index

139	139	139	4265
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Toward the Complete Prediction of the1H and13C NMR Spectra of Complex Organic Molecules by DFT Methods: Application to Natural Substances. Chemistry - A European Journal, 2006, 12, 5514-5525.	3.3	189
2	Unraveling the Key Features of the Reactive State of Decatungstate Anion in Hydrogen Atom Transfer (HAT) Photocatalysis. ACS Catalysis, 2016, 6, 7174-7182.	11.2	124
3	Predicting 13C NMR Spectra by DFT Calculations. Journal of Physical Chemistry A, 2003, 107, 9964-9973.	2.5	121
4	Addressing the Stereochemistry of Complex Organic Molecules by Density Functional Theory-NMR: Vannusal B in Retrospective. Journal of the American Chemical Society, 2011, 133, 6072-6077.	13.7	118
5	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. Journal of the American Chemical Society, 2003, 125, 4609-4618.	13.7	115
6	Computational NMR spectroscopy: reversing the information flow. Theoretical Chemistry Accounts, 2007, 117, 603-619.	1.4	109
7	Complete Prediction of the1H NMR Spectrum of Organic Molecules by DFT Calculations of Chemical Shifts and Spin-Spin Coupling Constants. Chemistry - A European Journal, 2001, 7, 1652-1661.	3.3	107
8	NMR techniques for the investigation of solvation phenomena and non-covalent interactions. Progress in Nuclear Magnetic Resonance Spectroscopy, 2005, 47, 41-93.	7.5	105
9	Prediction of the ¹H and ¹³C NMR Spectra of Î±-<scp>d</scp>-Glucose in Water by DFT Methods and MD Simulations. Journal of Organic Chemistry, 2007, 72, 7373-7381.	3.2	100
10	Site of Ionization of Hydroxamic Acids Probed by Heteronuclear NMR Relaxation Rate and NOE Measurements. An Experimental and Theoretical Study. Journal of the American Chemical Society, 1994, 116, 916-924.	13.7	99
11	Predicting the NMR Spectra of Paramagnetic Molecules by DFT: Application to Organic Free Radicals and Transitionâ€Metal Complexes. Chemistry - A European Journal, 2009, 15, 7990-8004.	3.3	97
12	Photooxidation in Water by New Hybrid Molecular Photocatalysts Integrating an Organic Sensitizer with a Polyoxometalate Core. Advanced Synthesis and Catalysis, 2004, 346, 648-654.	4.3	96
13	Relativistic DFT Calculation of 119Sn Chemical Shifts and Coupling Constants in Tin Compounds. Journal of Chemical Theory and Computation, 2006, 2, 37-46.	5.3	83
14	Stability and solvation of organic cations. Reviews of Chemical Intermediates, 1987, 7, 313-352.	1.1	78
15	The effect of the anion on the physical properties of trihalide-based N,N-dialkylimidazolium ionic liquids. Organic and Biomolecular Chemistry, 2005, 3, 1624.	2.8	75
16	Microwaveâ€Assisted Rapid Incorporation of Ruthenium into Lacunary Keggināâ€Type Polyoxotungstates: Oneâ€Step Synthesis, ⁹⁹ Ru, ¹⁸³ W NMR Characterization and Catalytic Activity of [PW ₁₁ O ₃₉ Ru ^{II} (DMSO)] ^{5â€“}. European Journal of Inorganic Chemistry, 2000, 2000, 17-20.	2.0	73
17	Asymmetric Tetraprotonation of Î³-[(SiO4)W10O32]8â¯ Triggers a Catalytic Epoxidation Reaction: Perspectives in the Assignment of the Active Catalyst. Angewandte Chemie - International Edition, 2007, 46, 3255-3258.	13.8	72
18	Computer simulation of diffusion coefficients of the room-temperature ionic liquid [bmim][BF4]: Problems with classical simulation techniques. Journal of Molecular Liquids, 2007, 131-132, 17-23.	4.9	69

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19	Site of Ionization of Polyfunctional Bases and Acids. 1.Ab InitioProton Affinities. The Journal of Physical Chemistry, 1996, 100, 1536-1544.	2.9	62
20	Acid-base properties of organic solvents. Journal of the American Chemical Society, 1988, 110, 4577-4582.	13.7	61
21	Chemistry in superacids. 8. Superacid-catalyzed carbonylation of methane, methyl halides, methyl alcohol, and dimethyl ether to methyl acetate and acetic acid. Journal of Organic Chemistry, 1990, 55, 4284-4289.	3.2	60
22	Addressing the stereochemistry of complex organic molecules by density functional theoryâ€‹scp›NMR‹/scp›. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 228-240.	14.6	59
23	Selectivity in Proton Transfer, Hydrogen Bonding, and Solvation. Accounts of Chemical Research, 2000, 33, 609-616.	15.6	58
24	[60]Fullerene as a Substituent. Chemistry - A European Journal, 2002, 8, 1015.	3.3	53
25	Computational Modeling of Polyoxotungstates by Relativistic DFT Calculations of183W NMR Chemical Shifts. Chemistry - A European Journal, 2006, 12, 8460-8471.	3.3	53
26	Site of Protonation of Carboxylic and Non-Carboxylic Amides in the Gas Phase and in Water. Chemistry - A European Journal, 1999, 5, 523-536.	3.3	51
27	DFT Study of the NMR Properties of Xenon in Covalent Compounds and van der Waals Complexesâ€”Implications for the Use of 129Xe as a Molecular Probe. Chemistry - A European Journal, 2003, 9, 1486-1495.	3.3	51
28	Computing the1H NMR Spectrum of a Bulk Ionic Liquid from Snapshots of Carâ€“Parrinello Molecular Dynamics Simulations. ChemPhysChem, 2007, 8, 873-881.	2.1	51
29	Quantum Chemical Modeling of Through-Hydrogen Bond Spin-Spin Coupling in Amides and Ubiquitin. Chemistry - A European Journal, 2000, 6, 2925-2930.	3.3	49
30	Through-Space Spinâ€“Spin Coupling in van der Waals Dimers and CH/Ï€ Interacting Systems. An Ab Initio and DFT Study. Chemistry - A European Journal, 2002, 8, 2047.	3.3	49
31	Can Two Molecules Have the Same NMR Spectrum? Hexacyclinol Revisited. Organic Letters, 2009, 11, 1409-1412.	4.6	49
32	Insights on the Isotropic-to-Smectic A Transition in Ionic Liquid Crystals from Coarse-Grained Molecular Dynamics Simulations: The Role of Microphase Segregation. Journal of Physical Chemistry B, 2015, 119, 3829-3836.	2.6	49
33	Thermodynamics of protonation of ketones and esters and energies of hydration of their conjugate acids. The Journal of Physical Chemistry, 1991, 95, 345-352.	2.9	48
34	Metal-MediatedJCoupling in DNA Base Pairs:Â Relativistic DFT Predictions. Journal of the American Chemical Society, 2007, 129, 11360-11361.	13.7	48
35	Computing the NMR Spectrum of a Bulk Ionic Liquid Phase by QM/MM Methods. Journal of Physical Chemistry B, 2006, 110, 23004-23006.	2.6	46
36	Preferential Solvation of Organic Species in Binary Solvent Mixtures Probed by Intermolecular1H NOESY NMR Spectroscopy. Chemistry - A European Journal, 1999, 5, 1291-1300.	3.3	45

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37	Relativistic DFT calculation of99Ru NMR parameters: chemical shifts and spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2004, 42, S79-S87.	1.9	41
38	Probing the solvation shell of organic molecules by intermolecular1H NOESY. Journal of Physical Organic Chemistry, 2002, 15, 790-795.	1.9	40
39	NMR Spectra of Terminal Oxo Gold and Platinum Complexes: Relativistic DFT Predictions. Angewandte Chemie - International Edition, 2010, 49, 1083-1086.	13.8	40
40	Predicting the 1H and 13C NMR spectra of paramagnetic Ru(III) complexes by DFT. Magnetic Resonance in Chemistry, 2010, 48, S132-S141.	1.9	40
41	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. Chemical Physics Letters, 2000, 317, 123-128.	2.6	38
42	Vicinal Tungsten-Tungsten Coupling Constants in Polyoxotungstates: DFT Calculations Challenge an Empirical Rule. Angewandte Chemie - International Edition, 2005, 44, 2023-2026.	13.8	38
43	Insights into the cytotoxic activity of the phosphane copper(I) complex [Cu(thp)4][PF6]. Journal of Inorganic Biochemistry, 2016, 165, 80-91.	3.5	38
44	Relativistic DFT Calculations of Polyoxotungstate 183W NMR Spectra: Insight into their Solution Structure. ChemPhysChem, 2003, 4, 517-519.	2.1	37
45	Solvation of nonelectrolytes in water probed by oxygen-17 NMR relaxation of the solvent. The Journal of Physical Chemistry, 1993, 97, 4601-4607.	2.9	36
46	Nuclear Spin Relaxation Driven by Intermolecular Dipolar Interactions:Â The Role of Soluteâ^'Solvent Pair Correlations in the Modeling of Spectral Density Functions. Journal of Physical Chemistry B, 2006, 110, 5676-5689.	2.6	35
47	DFT Calculation of Intermolecular Nuclear Spin-Spin Coupling in van der Waals Dimers. Angewandte Chemie - International Edition, 2001, 40, 2532-2534.	13.8	34
48	Predicting the spin state of paramagnetic iron complexes by DFT calculation of proton NMR spectra. Dalton Transactions, 2014, 43, 9486-9496.	3.3	33
49	Predicting the UV spectrum of polyoxometalates by TDâ€ÐFT. Journal of Computational Chemistry, 2011, 32, 2983-2987.	3.3	31
50	Preferential Solvation of Neutral Species in Binary Solvent Mixtures Characterized by1H NOESY NMR Spectroscopy. Journal of the American Chemical Society, 1997, 119, 2299-2300.	13.7	30
51	The ab initio neonâ€“water potential-energy surface and its relationship with the hydrophobic hydration shell. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2501-2504.	1.7	30
52	DFT Calculations of99Ru Chemical Shifts with All-Electron and Effective Core Potential Basis Sets. European Journal of Inorganic Chemistry, 2002, 2002, 1475-1483.	2.0	30
53	NMR quantification of trace components in complex matrices by bandâ€selective excitation with adiabatic pulses. Magnetic Resonance in Chemistry, 2009, 47, 868-872.	1.9	29
54	Observation of scalar nuclear spinâ€“spin coupling in van der Waals complexes. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 12393-12397.	7.1	28

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55	Electronic and EPR spectra of the species involved in [W10O32]4â^' photocatalysis. A relativistic DFT investigation. Physical Chemistry Chemical Physics, 2013, 15, 2890.	2.8	28
56	Computational NMR Spectroscopy of Organoarsenicals and the Natural Polyarsenic Compound Arsenicinâ€...A. Chemistry - A European Journal, 2008, 14, 10445-10452.	3.3	27
57	Fourâ€Component Relativistic DFT Calculations of ¹³C Chemical Shifts of Halogenated Natural Substances. Chemistry - A European Journal, 2015, 21, 18834-18840.	3.3	27
58	Fries Rearrangement of Aryl Formates:â€‰ A Mechanistic Study by Means of 1H, 2H, and 11B NMR Spectroscopy and DFT Calculations. Journal of Organic Chemistry, 2006, 71, 9331-9340.	3.2	26
59	Thermoinduced Lipid Oxidation of a Culinary Oil: A Kinetic Study of the Oxidation Products by Magnetic Resonance Spectroscopies. Journal of Physical Chemistry A, 2010, 114, 10059-10065.	2.5	26
60	Carbon and Nitrogen Basicity of Aminothiophenes and Anilines. Journal of Physical Chemistry A, 2001, 105, 6537-6542.	2.5	25
61	Longâ€Range Diastereoselectivity in an Ugi Reaction: Stereocontrolled and Diversityâ€Oriented Synthesis of Tetrahydrobenzoxazepines. European Journal of Organic Chemistry, 2013, 2013, 5064-5075.	2.4	25
62	Reactivity of Auranofin with Selenols and Thiols â€“ Implications for the Anticancer Activity of Gold(I) Compounds. European Journal of Inorganic Chemistry, 2013, 2013, 2718-2727.	2.0	25
63	Site of Ionization of Polyfunctional Bases and Acids. 2.Ab InitioElectric Field Gradients at Nitrogen, Oxygen, Phosphorus, and Sulfur in Neutral and Ionized Forms. The Journal of Physical Chemistry, 1996, 100, 1545-1553.	2.9	24
64	Preferential Solvation and Self-Association in Alcoholâ^'Acetonitrile Mixtures Observed through Mass Spectrometric Analysis of Clusters:Â Influence of Alkyl Chain Length. Journal of Physical Chemistry B, 2004, 108, 3479-3487.	2.6	24
65	Preferential solvation of glucose and talose in waterâ€“acetonitrile mixtures: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2010, 12, 2981.	2.8	24
66	Understanding Cage Effects in Imidazolium Ionic Liquids by ¹²⁹Xe NMR: MD Simulations and Relativistic DFT Calculations. Journal of Physical Chemistry B, 2014, 118, 13963-13968.	2.6	24
67	Relative basicity of nitrogen, oxygen, and sulfur bases. The site of protonation in sulfenamides and sulfinamides determined by nitrogen-14 NMR relaxation. Journal of Organic Chemistry, 1994, 59, 232-233.	3.2	23
68	Ab Initio Calculations on Waterâ^'Peroxovanadium Clusters, VO(O2)(H2O)n+ (n = 1â^'5). Implications for the Structure in Aqueous Solution. Journal of Physical Chemistry A, 1997, 101, 4637-4640.	2.5	23
69	Site of Protonation of Alkyl- and Arylhydrazines Probed by14N,15N, and13C NMR Relaxation and Quantum Chemical Calculations. Journal of Physical Chemistry A, 1998, 102, 2888-2892.	2.5	23
70	Deprotonation of Amides and Polyfunctional Imides Probed by Heteronuclear NMR and Quantum Chemical Calculations. European Journal of Organic Chemistry, 1999, 1999, 287-295.	2.4	23
71	Solvation of Tetraalkylammonium Chlorides in Acetonitrile-Water Mixtures: Mass Spectrometry and Molecular Dynamics Simulations. ChemPhysChem, 2005, 6, 1307-1315.	2.1	22
72	Thermodynamics of protonation and hydration of aliphatic amides. Journal of the Chemical Society Perkin Transactions II, 1993, , 1091.	0.9	21

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73	Computational¹⁹F NMR. 2. Organic compounds. RSC Advances, 2014, 4, 41605-41611.	3.6	21
74	Understanding the Extraordinary Deshielding of ¹²⁹Xe in a Permetallated Cryptophane by Relativistic DFT. Chemistry - A European Journal, 2012, 18, 7341-7345.	3.3	20
75	Reactive Intermediates in Peptide Synthesis:Â First Crystal Structures andab InitioCalculations of 2-Alkoxy-5(4H)-oxazolones from Urethane-Protected Amino Acids. Journal of the American Chemical Society, 1997, 119, 4136-4142.	13.7	19
76	Relativistic DFT calculations of the NMR properties and reactivity of transition metal methane Ïƒ-complexes: insights on Câ€“H bond activation. Physical Chemistry Chemical Physics, 2011, 13, 4285.	2.8	19
77	Computational 19F NMR. 1. General features. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	19
78	Spectroscopic signatures of the carbon buckyonions C60@C180 and C60@C240: a dispersion-corrected DFT study. Physical Chemistry Chemical Physics, 2013, 15, 18030.	2.8	19
79	New Formylating Agents â^' Preparative Procedures and Mechanistic Investigations. European Journal of Organic Chemistry, 2001, 2001, 2947.	2.4	18
80	Multinuclear Solid-State NMR and DFT Studies on Phosphanido-Bridged Diplatinum Complexes. Inorganic Chemistry, 2015, 54, 5855-5863.	4.0	18
81	Acyl group vs nitrogen protonation of carboxylic and ï¿½non-carboxylic amides in the gas phase and water. Journal of Physical Organic Chemistry, 2000, 13, 574-578.	1.9	17
82	Detecting intermolecular NOEs by means of a novel DPFGSE pulse sequence. Application to the solvation of carbohydrates in binary mixtures. Journal of Magnetic Resonance, 2004, 167, 31-35.	2.1	17
83	H₂O₂ activation by heteropolyacids with defect structures: the case of Î³â€[(XO₄)W₁₀O₃₂]^{nâ^'} (Xâ€‰=â€‰Si, Ge, nâ€‰=â€‰8; Xâ€‰=â€‰		
84	Predicting the NMR spectra of nucleotides by DFT calculations: cyclic uridine monophosphate. Magnetic Resonance in Chemistry, 2008, 46, 518-524.	1.9	17
85	Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021). Pure and Applied Chemistry, 2022, 94, 353-534.	1.9	17
86	A novel method for the determination of ionization sites in polyfunctional acids and bases by NMR relaxation rate measurements. Journal of the Chemical Society Perkin Transactions II, 1993, , 283.	0.9	15
87	Characterization of Paramagnetic Reactive Intermediates: Predicting the NMR Spectra of Iron(IV)â€“Oxo Complexes by DFT. Chemistry - A European Journal, 2015, 21, 12960-12970.	3.3	15
88	Probing the C ₆₀ triplet state coupling to nuclear spins inside and out. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20120475.	3.4	13
89	The excess basicity of alkali metal methoxides in methanol. Journal of the Chemical Society Perkin Transactions II, 1990, , 1017.	0.9	12
90	Ab initio calculation of NMR properties (shielding and electric field gradient) of 33S in sulfur compounds. Computational and Theoretical Chemistry, 1997, 418, 243-255.	1.5	11

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91	Detecting Hydrogen Bonding by NMR Relaxation of the Acceptor Nuclei. Chemistry - A European Journal, 2000, 6, 2915-2924.	3.3	11
92	Conformational Analysis of Saturatedtrans-Fused 1,3,2-Benzoxazaphosphinine 2-Oxides â˜' DFT Calculation of NMRJ(P,H) Coupling Constants. European Journal of Organic Chemistry, 2004, 2004, 4921-4930.	2.4	11
93	Selective J-resolved spectra: A double pulsed field gradient spin-echo approach. Journal of Magnetic Resonance, 2006, 182, 29-37.	2.1	11
94	Thermo-induced lipid oxidation of a culinary oil: The effect of materials used in common food processing on the evolution of oxidised species. Food Chemistry, 2012, 133, 754-759.	8.2	11
95	Oxygenation by Ruthenium Monosubstituted Polyoxotungstates in Aqueous Solution: Experimental and Computational Dissection of a Ru(III)â€"Ru(V) Catalytic Cycle. Chemistry - A European Journal, 2014, 20, 10932-10943.	3.3	11
96	Calculation of NMR parameters in van der Waals complexes involving organic systems and xenon. Journal of Physical Organic Chemistry, 2004, 17, 945-950.	1.9	9
97	Structure ofD-ribonic acid-dimethyltin(IV) in coordinating solvents: an experimental and DFT119Sn NMR study. Journal of Physical Organic Chemistry, 2006, 19, 874-883.	1.9	9
98	Computing the NMR spectra of the sponge metabolite arsenicin A: when simple becomes difficult. Journal of Physical Organic Chemistry, 2010, 23, 1016-1021.	1.9	9
99	Substituent effects on the through-space nuclear magnetic spin-spin coupling in van der Waals dimers. Arkivoc, 2002, 2002, 38-44.	0.5	9
100	Solvent effect on relative N- and O-acidity. Inversion of the deprotonation site of 2- and 4-[(2,4,6-trinitrophenyl)amino]benzoic acids. Journal of the Chemical Society Perkin Transactions II, 1996, , 2163.	0.9	8
101	Solvent Effect on the Protonation of Acetylene and Ethylene â€" Continuum Solvent Quantum Chemical Calculations. European Journal of Organic Chemistry, 1999, 1999, 2893-2897.	2.4	8
102	Through-Space Spin-Spin Coupling In Acetylenic Systems. Ab Initio and DFT Calculations. International Journal of Molecular Sciences, 2003, 4, 193-202.	4.1	8
103	A DFT study of the vicinal 3J(119Sn,13C) and 3J(119Sn,1H) coupling constants inÂtrimethyl- and chlorodimethylstannyl propanoates. Journal of Organometallic Chemistry, 2013, 724, 139-146.	1.8	8
104	Direct Detection of ¹⁷O in [Gd(DOTA)]^{â˜'} by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 1955-1960.	3.3	8
105	Thermodynamics of protonation of N,N-dimethylthioamides in aqueous sulfuric acid. Canadian Journal of Chemistry, 1990, 68, 1746-1749.	1.1	7
106	Steric Effects on the Proton-Transfer Equilibria of Ketones, Sulfoxides, and Phenols. European Journal of Organic Chemistry, 1999, 1999, 1507-1515.	2.4	7
107	MD simulation of xenon in ionic liquids: Disentangling the cationic and anionic cage effects on the structural and dynamic properties. Journal of Molecular Liquids, 2015, 210, 272-278.	4.9	7
108	Fries Rearrangement of Aryl Formates Promoted by BCl₃. Mechanistic Evidence from ¹¹B NMR Spectra and DFT Calculations. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2004, 59, 386-397.	0.7	6

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109	Steric effects on the solvation of protonated di-tert-butyl ketone and phenyl tert-butyl ketone. Journal of the Chemical Society Chemical Communications, 1995, , 2053.	2.0	5
110	Experimental and theoretical investigation of gas phase complexes between chloride ion and some chloroethenes. International Journal of Mass Spectrometry, 1998, 179-180, 349-357.	1.5	5
111	Predicting the paramagnet-enhanced NMR relaxation of H₂encapsulated in endofullerene nitroxides by density-functional theory calculations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110634.	3.4	5
112	Kinetics of nucleophilic aromatic substitution in concentrated solutions of alkali metal methoxides in methanol. Journal of the Chemical Society Perkin Transactions II, 1991, , 651.	0.9	4
113	A pulse sequence forT1 measurement by inversion-recovery in the presence of acoustic ringing. Magnetic Resonance in Chemistry, 1992, 30, 1164-1168.	1.9	4
114	Formylation of activated arenes by phenyl formate: implications for the mechanism of the Fries rearrangement of aryl formates. Journal of Physical Organic Chemistry, 2008, 21, 682-687.	1.9	4
115	Counterion effects on the 183W NMR spectra of the lacunary Keggin polyoxotungstate [PW11O39]7â€“. Relativistic DFT calculations. Comptes Rendus Chimie, 2012, 15, 118-123.	0.5	4
116	Copper(II) Chloride Catalyzed Carboxydediazoniation of Arenediazonium Tetrafluoroborates with Carbon Monoxide in Aqueous Dioxane Solution to Arenecarboxylic Acids1. Synlett, 1990, 1990, 596-598.	1.8	3
117	Levelling of substituent effects on acidities in the gas phase compared with those in solution. Journal of the Chemical Society Perkin Transactions II, 1991, , 1601.	0.9	3
118	NMR properties (chemical shift and relaxation rate) of acceptor and hydrogen bridge nuclei in hydrogen-bonded complexes. Magnetic Resonance in Chemistry, 2001, 39, S59-S66.	1.9	3
119	Investigation of Cationâ^'Anion Interactions in 2-Propanol Solutions of Sodium Alkoxides and Thiolates by23Na-NMR Spectroscopy. European Journal of Organic Chemistry, 2000, 2000, 1953-1957.	2.4	2
120	DFT Calculations of 99Ru Chemical Shifts with All-Electron and Effective Core Potential Basis Sets. European Journal of Inorganic Chemistry, 2002, 2002, 1475-1483.	2.0	1
121	A program for interconverting concentration units in binary mixtures. Computers & Chemistry, 1992, 16, 267-268.	1.2	0
122	Calculation of NMR Parameters in Van Der Waals Complexes Involving Organic Systems and Xenon. ChemInform, 2005, 36, no.	0.0	0
123	Vicinal Tungsten?Tungsten Coupling Constants in Polyoxotungstates: DFT Calculations Challenge an Empirical Rule.. ChemInform, 2005, 36, no.	0.0	0
124	Bioactive Phloroglucinyl Heterodimers: The Tautomeric and Rotameric Equlibria of Arzanol. European Journal of Organic Chemistry, 2016, 2016, 4810-4816.	2.4	0
125	Computational 19F NMR. 1. General features. Highlights in Theoretical Chemistry, 2013, , 41-52.	0.0	0
126	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.. Angewandte Chemie - International Edition, 2001, 40, 2532-2534.	13.8	0