

Ilya G Shenderovich

List of Publications by Year in descending order

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81743

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102
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102
times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	Surface characterization of flax, hemp and cellulose fibers; Surface properties and the water uptake behavior. <i>Polymer Composites</i> , 2002, 23, 872-894.	2.3	350
2	Hydrogen Bonding of Water Confined in Mesoporous Silica MCM-41 and SBA-15 Studied by ^1H Solid-State NMR. <i>Chemistry - A European Journal</i> , 2004, 10, 5689-5696.	1.7	340
3	Pyridine- ^{15}N A Mobile NMR Sensor for Surface Acidity and Surface Defects of Mesoporous Silica. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11924-11939.	1.2	246
4	Nuclear Scalar Spin-Spin Coupling Reveals Novel Properties of Low-Barrier Hydrogen Bonds in a Polar Environment. <i>Chemistry - A European Journal</i> , 1999, 5, 492-497.	1.7	190
5	Nuclear Scalar Spin-Spin Couplings and Geometries of Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2000, 122, 1979-1988.	6.6	188
6	Low-Temperature NMR Studies of the Structure and Dynamics of a Novel Series of Acid-Base Complexes of HF with Collidine Exhibiting Scalar Couplings Across Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2003, 125, 11710-11720.	6.6	170
7	Structural and dynamical properties of guest molecules confined in mesoporous silica materials revealed by NMR. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4843.	1.3	145
8	OHO Hydrogen Bond Geometries and NMR Chemical Shifts: From Equilibrium Structures to Geometric H/D Isotope Effects, with Applications for Water, Protonated Water, and Compressed Ice. <i>Israel Journal of Chemistry</i> , 2009, 49, 199-216.	1.0	143
9	$^1\text{H}/^{15}\text{N}$ NMR chemical shielding, dipolar $^{15}\text{N}, ^2\text{H}$ coupling and hydrogen bond geometry correlations in a novel series of hydrogen-bonded acid-base complexes of collidine with carboxylic acids. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S18-S29.	1.1	141
10	Influence of the temperature-dependent dielectric constant on the H/D isotope effects on the NMR chemical shifts and the hydrogen bond geometry of the collidine-HF complex in CDF ₃ /CDF ₂ Cl ₂ solution. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S91-S99.	1.1	137
11	^2H -Solid-State NMR Study of Benzene- d_6 Confined in Mesoporous Silica SBA-15. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1977-1984.	1.2	121
12	H/D isotope effects on the low-temperature NMR parameters and hydrogen bond geometries of (FH) ₂ F ⁺ and (FH) ₃ F ⁺ dissolved in CDF ₃ /CDF ₂ Cl ₂ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5488-5497.	1.3	103
13	Hexagonal Molybdenum Trioxide Known for 100 Years and Still a Fount of New Discoveries. <i>Inorganic Chemistry</i> , 2010, 49, 9400-9408.	1.9	102
14	Hydrogen/Deuterium-Isotope Effects on NMR Chemical Shifts and Symmetry of Homoconjugated Hydrogen-Bonded Ions in Polar Solution. <i>Journal of the American Chemical Society</i> , 2000, 122, 12878-12879.	6.6	100
15	NMR Parameters and Geometries of OHN and ODN Hydrogen Bonds of Pyridine-Acid Complexes. <i>Chemistry - A European Journal</i> , 2004, 10, 5195-5204.	1.7	97
16	Attenuation of London Dispersion in Dichloromethane Solutions. <i>Journal of the American Chemical Society</i> , 2017, 139, 13126-13140.	6.6	93
17	NMR studies of solid state solvent and H/D isotope effects on hydrogen bond geometries of 1:1 complexes of collidine with carboxylic acids. <i>Journal of Molecular Structure</i> , 2004, 700, 19-27.	1.8	70
18	NMR Studies of Protonation and Hydrogen Bond States of Internal Aldimines of Pyridoxal 5-Phosphate Acid-Base in Alanine Racemase, Aspartate Aminotransferase, and Poly-L-lysine. <i>Journal of the American Chemical Society</i> , 2013, 135, 18160-18175.	6.6	67

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19	NMR Localization of Protons in Critical Enzyme Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2007, 129, 9558-9559.	6.6	66
20	NMR Provides Checklist of Generic Properties for Atomic-Scale Models of Periodic Mesoporous Silicas. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12088-12096.	1.2	62
21	Acidity of Sulfonic and Phosphonic Acid-Functionalized SBA-15 under Almost Water-Free Conditions. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19185-19192.	1.5	62
22	Amine-Borane Dehydrogenation and Transfer Hydrogenation Catalyzed by Diimine Cobaltates. <i>Chemistry - A European Journal</i> , 2019, 25, 238-245.	1.7	58
23	Critical hydrogen bonds and protonation states of pyridoxal 5-phosphate revealed by NMR. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1426-1437.	1.1	57
24	Synthesis and Characterization of Chiral Benzylic Ether-Bridged Periodic Mesoporous Organosilicas. <i>Chemistry - A European Journal</i> , 2008, 14, 5935-5940.	1.7	55
25	P=O Moiety as an Ambidextrous Hydrogen Bond Acceptor. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1711-1720.	1.5	52
26	Geometrical Features of Hydrogen Bonded Complexes Involving Sterically Hindered Pyridines. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10872-10879.	1.1	51
27	Mutable Lewis and Brønsted Acidity of Aluminated SBA-15 as Revealed by NMR of Adsorbed Pyridine- ¹⁵ N. <i>Langmuir</i> , 2011, 27, 12115-12123.	1.6	50
28	Selective P ₄ Activation by a Highly Reduced Cobaltate: Synthesis of Dicobalt Tetraphosphido Complexes. <i>Chemistry - A European Journal</i> , 2017, 23, 6094-6102.	1.7	50
29	Symmetrization of Cationic Hydrogen Bridges of Protonated Sponges Induced by Solvent and Counteranion Interactions as Revealed by NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2010, 16, 1679-1690.	1.7	49
30	NMR Studies of Solid Pentachlorophenol-4-Methylpyridine Complexes Exhibiting Strong OHN Hydrogen Bonds: Geometric H/D Isotope Effects and Hydrogen Bond Coupling Cause Isotopic Polymorphism. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11370-11387.	1.1	48
31	Carboxylic Acid-Doped SBA-15 Silica as a Host for Metallo-supramolecular Coordination Polymers. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14637-14647.	1.2	46
32	Geometry and Spectral Properties of the Protonated Homodimer of Pyridine in the Liquid and Solid States. A Combined NMR, X-ray Diffraction and Inelastic Neutron Scattering Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8041-8048.	1.1	46
33	Hydrogen Bonding of Water Confined in Controlled-Pore Glass 10-75 Studied by ¹ H-Solid State NMR. <i>Zeitschrift Fur Physikalische Chemie</i> , 2007, 221, 155-168.	1.4	45
34	² H-solid state NMR and DSC study of isobutyric acid in mesoporous silica materials. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2249.	1.3	44
35	A DFT and AIM analysis of the spin-spin couplings across the hydrogen bond in the fluorobenzamide and related compounds. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 585-592.	1.1	44
36	Difference between ¹ H NMR signals of primary amide protons as a simple spectral index of the amide intramolecular hydrogen bond strength. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 287-295.	0.9	44

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37	Nuclear Magnetic Resonance and ab Initio Studies of Small Complexes Formed between Water and Pyridine Derivatives in Solid and Liquid Phases. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6084-6093.	1.1	43
38	Density Functional Study of the Proton Transfer Effect on Vibrations of Strong (Short) Intermolecular O-H...N/O...N Hydrogen Bonds in Aprotic Solvents. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2393-2399.	1.1	42
39	Interpretation of Hydrogen/Deuterium Isotope Effects on NMR Chemical Shifts of [FHF] ⁻ Ion Based on Calculations of Nuclear Magnetic Shielding Tensor Surface. <i>Zeitschrift Fur Physikalische Chemie</i> , 2003, 217, 1549-1564.	1.4	41
40	Counteranion-dependent mechanisms of intramolecular proton transfer in aprotic solution. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10373.	1.3	39
41	Stray field gradient NMR reveals effects of hydrogen bonding on diffusion coefficients of pyridine in mesoporous silica. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S149-S157.	1.1	36
42	Solid-State NMR Studies of Aminocarboxylic Salt Bridges in Lysine Modified Cellulose. <i>Journal of Physical Chemistry B</i> , 2009, 113, 934-940.	1.2	31
43	Effect of Hydrogen Bonding to Water on the ³¹ P Chemical Shift Tensor of Phenyl- and Trialkylphosphine Oxides and \pm -Amino Phosphonates. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8717-8729.	1.5	31
44	Evidence of microphase separation in controlled pore glasses. <i>Solid State Nuclear Magnetic Resonance</i> , 2005, 28, 117-124.	1.5	28
45	Cyclic trimers of phosphinic acids in polar aprotic solvent: symmetry, chirality and H/D isotope effects on NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4901-4910.	1.3	28
46	Intrinsic Proton-Donating Power of Zinc-Bound Water in a Carbonic Anhydrase Active Site Model Estimated by NMR. <i>Journal of the American Chemical Society</i> , 2011, 133, 11331-11338.	6.6	27
47	FTIR study of the hydrogen bond symmetry in protonated homodimers of pyridine and collidine in solution. <i>Journal of Molecular Structure</i> , 2012, 1018, 39-44.	1.8	27
48	Correlations of NHN hydrogen bond energy with geometry and ¹ H NMR chemical shift difference of NH protons for aniline complexes. <i>Journal of Chemical Physics</i> , 2019, 150, 114305.	1.2	25
49	Does Water Affect the Acidity of Surfaces? The Proton-Donating Ability of Silanol and Carboxylic Acid Groups at Mesoporous Silica. <i>ChemPhysChem</i> , 2012, 13, 2282-2285.	1.0	24
50	How Short is the Strongest Hydrogen Bond in the Proton-Bound Homodimers of Pyridine Derivatives?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10804-10812.	1.1	24
51	Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 14281-14288.	7.2	24
52	Effect of Noncovalent Interactions on the ³¹ P Chemical Shift Tensor of Phosphine Oxides, Phosphinic, Phosphonic, and Phosphoric Acids, and Their Complexes with Lead(II). <i>Journal of Physical Chemistry C</i> , 2013, 117, 26689-26702.	1.5	23
53	NMR study of proton transfer to strong bases on inner surfaces of MCM-41. <i>Microporous and Mesoporous Materials</i> , 2010, 134, 22-28.	2.2	22
54	A qualitative study of the effect of a counterion and polar environment on the structure and spectroscopic signatures of a hydrated hydroxyl anion. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	22

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55	NMR Study of Solvation Effect on the Geometry of Proton-Bound Homodimers of Increasing Size. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8697-8705.	1.1	21
56	Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. <i>Journal of Chemical Physics</i> , 2018, 148, 124313.	1.2	21
57	NMR Studies of Active Site Properties of Human Carbonic Anhydrase...II by Using ¹⁵ N-Labeled 4-Methylimidazole as a Local Probe and Histidine Hydrogen Bond Correlations. <i>Chemistry - A European Journal</i> , 2015, 21, 2915-2929.	1.7	20
58	For Whom a Puddle Is the Sea? Adsorption of Organic Guests on Hydrated MCM-41 Silica. <i>Langmuir</i> , 2020, 36, 11383-11392.	1.6	19
59	Adduct under Field – A Qualitative Approach to Account for Solvent Effect on Hydrogen Bonding. <i>Molecules</i> , 2020, 25, 436.	1.7	19
60	Local-structure effects on 31P NMR chemical shift tensors in solid state. <i>Journal of Chemical Physics</i> , 2019, 150, 144706.	1.2	18
61	Solid State NMR for Nonexperts: An Overview of Simple but General Practical Methods. <i>Solids</i> , 2021, 2, 139-154.	1.1	18
62	NMR and EPR Study of the Nitroxide Radical Tempo Interaction with Phenols. <i>Spectroscopy Letters</i> , 1997, 30, 1515-1523.	0.5	17
63	Photoinduced Proton Transfer in a Pyridine Based Polymer Gel. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10728-10733.	1.2	17
64	Solvent effects on acid-base complexes. What is more important: A macroscopic reaction field or solute-solvent interactions?. <i>Journal of Chemical Physics</i> , 2019, 150, 204505.	1.2	17
65	H/D isotope effects on NMR chemical shifts of nuclei involved in a hydrogen bridge of hydrogen isocyanide complexes with fluoride anion. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5154.	1.3	16
66	The Partner Does Matter: The Structure of Heteroaggregates of Acridine Orange in Water. <i>Molecules</i> , 2019, 24, 2816.	1.7	16
67	Electric field effect on 31P NMR magnetic shielding. <i>Journal of Chemical Physics</i> , 2020, 153, 184501.	1.2	16
68	NMR Study of Intercalates and Grafted Organic Derivatives of H ₂ La ₂ Ti ₃ O ₁₀ . <i>Molecules</i> , 2020, 25, 5229.	1.7	14
69	NMR Study of Blue-Shifting Hydrogen Bonds Formed by Fluoroform in Solution. <i>Zeitschrift Fur Physikalische Chemie</i> , 2008, 222, 1225-1245.	1.4	13
70	Inter- vs. Intramolecular Hydrogen Bond Patterns and Proton Dynamics in Nitrophthalic Acid Associates. <i>Molecules</i> , 2020, 25, 4720.	1.7	13
71	Experimentally Established Benchmark Calculations of ³¹ P NMR Quantities. <i>Chemistry Methods</i> , 2021, 1, 61-70.	1.8	13
72	Maximum value of the chemical shift in the 1H NMR spectrum of a hydrogen-bonded complex. <i>Russian Journal of General Chemistry</i> , 2006, 76, 501-506.	0.3	11

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73	Qualitative analysis of the geometry of the hydrogen bond in the homoconjugated pyridine ion. Russian Journal of General Chemistry, 2007, 77, 620-624.	0.3	10
74	Studies of adsorption of 2,2'-bipyridyl on the surface of highly regulated silica matrix of the MCM-41 type by means of ¹⁵ N NMR spectroscopy. Russian Journal of General Chemistry, 2010, 80, 2027-2031.	0.3	10
75	Synthesis of a carborane-substituted bis(phosphanido) cobaltate(³⁻), ligand substitution, and unusual P ₄ fragmentation. Chemical Science, 2021, 12, 11225-11235.	3.7	10
76	Solvent induced temperature dependencies of NMR parameters of hydrogen bonded anionic clusters. Journal of Molecular Structure, 2004, 697, 9-15.	1.8	9
77	Energy Analysis of Competing Non-Covalent Interaction in 1:1 and 1:2 Adducts of Collidine with Benzoic Acids by Means of X-Ray Diffraction. Zeitschrift Fur Physikalische Chemie, 2013, 227, 775-790.	1.4	9
78	Efficiency and lead uptake mechanism of a phosphonate functionalized mesoporous silica through P/Pb association ratio. Materials Chemistry and Physics, 2020, 239, 122037.	2.0	9
79	Modeling of Solute-Solvent Interactions Using an External Electric Field From Tautomeric Equilibrium in Nonpolar Solvents to the Dissociation of Alkali Metal Halides. Molecules, 2021, 26, 1283.	1.7	9
80	1,3,5-Triaza-7-Phosphaadamantane (PTA) as a ³¹ P NMR Probe for Organometallic Transition Metal Complexes in Solution. Molecules, 2021, 26, 1390.	1.7	9
81	Spectroscopic Signatures of [H ₉ O ₄] ⁺ and [H ₁₃ O ₆] ⁺ Ions in a Polar Aprotic Environment Revealed Under DFT-PCM Approximation. Acta Chimica Slovenica, 2011, 58, 402-10.	0.2	9
82	Actual Symmetry of Symmetric Molecular Adducts in the Gas Phase, Solution and in the Solid State. Symmetry, 2021, 13, 756.	1.1	8
83	Photochemistry of deprotonated rhenium(I) (3,3'-dihydroxy-2,2'-bipyridine) tricarbonyl chloride. Photoisomerization at the chelate in basic solution. Inorganica Chimica Acta, 2014, 421, 496-499.	1.2	7
84	Halide-Substituted Phosphacyclohexadienyl Iron Complexes: Covalent Structures vs. Ion Pairs. European Journal of Inorganic Chemistry, 2019, 2019, 1567-1574.	1.0	7
85	NMR-Detected Host-Guest Proton Exchange as a Tool to Explore Surface/Volume Ratios and Fluid Filling of Internal and External Spaces of Porous Solids Containing Surface OH Groups. Journal of Physical Chemistry C, 2020, 124, 22082-22095.	1.5	6
86	Complexation behaviour of LiCl and LiPF ₆ model studies in the solid-state and in solution using a bidentate picolyl-based ligand. Chemical Communications, 2020, 56, 13335-13338.	2.2	5
87	Investigations on Tetragonally Distorted Sodium Thallide NaTl ₈ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 82-87.	0.6	5
88	Novel Silica Hybrid Adsorbent Functionalized with ¹⁻ -Glutathione Used for the Uptake of As(V) from Aqueous Media. Industrial & Engineering Chemistry Research, 2022, 61, 4348-4362.	1.8	5
89	Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. Angewandte Chemie, 2019, 131, 14419-14426.	1.6	4
90	Spectrophotometric investigations of protonated forms of heterocyclic compounds. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2012, 113, 275-278.	0.2	3

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91	NMR Properties of the Cyanide Anion, a Quasisymmetric Two-Faced Hydrogen Bonding Acceptor. <i>Symmetry</i> , 2021, 13, 1298.	1.1	2
92	NMR Spectroscopic Detection of an Elusive Protonated and Coinage Metalated Silicide [NHC ^{Dipp} Cu(I ⁴)Si ⁹]H ²⁺ in Solution. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3684-3690.	1.0	2
93	Modeling of the Response of Hydrogen Bond Properties on an External Electric Field: Geometry, NMR Chemical Shift, Spin-Spin Scalar Coupling. <i>Molecules</i> , 2021, 26, 4967.	1.7	2
94	Acridine – a Promising Fluorescence Probe of Non-Covalent Molecular Interactions. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013, 227, 857-868.	1.4	1
95	The Effects of Alkaline Earth Metals on the Structure of Sodium Borosilicate Glasses: ¹¹ B and ²⁹ Si NMR Study. <i>Materials Science Forum</i> , 2020, 989, 192-198.	0.3	1
96	Editorial to the Special Issue – Gulliver in the Country of Lilliput: An Interplay of Noncovalent Interactions. <i>Molecules</i> , 2021, 26, 158.	1.7	1
97	Halide-Substituted Phosphacyclohexadienyl Iron Complexes: Covalent Structures vs. Ion Pairs. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1434-1434.	1.0	0