Ilya G Shenderovich

List of Publications by Year
in descending order

97	4,714	81743 39	98622 67
papers	citations	h-index	g-index

102	102	102	4003
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Novel Silica Hybrid Adsorbent Functionalized with <scp>l</scp>-Glutathione Used for the Uptake of As(V) from Aqueous Media. Industrial & Engineering Chemistry Research, 2022, 61, 4348-4362.	1.8	5
2	Experimentally Established Benchmark Calculations of ³¹P NMR Quantities. Chemistry Methods, 2021, 1, 61-70.	1.8	13
3	Synthesis of a carborane-substituted bis(phosphanido) cobaltate(<scp>i</scp>), ligand substitution, and unusual P₄fragmentation. Chemical Science, 2021, 12, 11225-11235.	3.7	10
4	Modeling of Solute-Solvent Interactions Using an External Electric Fieldâ€"From Tautomeric Equilibrium in Nonpolar Solvents to the Dissociation of Alkali Metal Halides. Molecules, 2021, 26, 1283.	1.7	9
5	1,3,5-Triaza-7-Phosphaadamantane (PTA) as a 31P NMR Probe for Organometallic Transition Metal Complexes in Solution. Molecules, 2021, 26, 1390.	1.7	9
6	Solid State NMR for Nonexperts: An Overview of Simple but General Practical Methods. Solids, 2021, 2, 139-154.	1.1	18
7	Actual Symmetry of Symmetric Molecular Adducts in the Gas Phase, Solution and in the Solid State. Symmetry, 2021, 13, 756.	1.1	8
8	NMR Properties of the Cyanide Anion, a Quasisymmetric Two-Faced Hydrogen Bonding Acceptor. Symmetry, 2021, 13, 1298.	1.1	2
9	NMRâ€Spectroscopic Detection of an Elusive Protonated and Coinage Metalated Silicide [NHC^{Dipp}Cu(Î·⁴â€Si₉)H]^{2â^'} in Solution. European Journal of Inorganic Chemistry, 2021, 2021, 3684-3690.	1.0	2
10	Modeling of the Response of Hydrogen Bond Properties on an External Electric Field: Geometry, NMR Chemical Shift, Spin-Spin Scalar Coupling. Molecules, 2021, 26, 4967.	1.7	2
11	Editorial to the Special Issue â€œGulliver in the Country of Lilliput: An Interplay of Noncovalent Interactionsâ€. Molecules, 2021, 26, 158.	1.7	1
12	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
13	Complexation behaviour of LiCl and LiPF₆â€“ model studies in the solid-state and in solution using a bidentate picolyl-based ligand. Chemical Communications, 2020, 56, 13335-13338.	2.2	5
14	NMR Study of Intercalates and Grafted Organic Derivatives of H2La2Ti3O10. Molecules, 2020, 25, 5229.	1.7	14
15	Electric field effect on 31P NMR magnetic shielding. Journal of Chemical Physics, 2020, 153, 184501.	1.2	16
16	Inter- vs. Intramolecular Hydrogen Bond Patterns and Proton Dynamics in Nitrophthalic Acid Associates. Molecules, 2020, 25, 4720.	1.7	13
17	For Whom a Puddle Is the Sea? Adsorption of Organic Guests on Hydrated MCM-41 Silica. Langmuir, 2020, 36, 11383-11392.	1.6	19
18	NMR-Detected Hostâ€“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

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19	The Effects of Alkaline Earth Metals on the Structure of Sodium Borosilicate Glasses: ¹¹B and ²⁹Si NMR Study. Materials Science Forum, 2020, 989, 192-198.	0.3	1
20	Investigations on Tetragonally Distorted Sodium Thallide NaTlâ€tI8. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 82-87.	0.6	5
21	Adduct under Fieldâ€"A Qualitative Approach to Account for Solvent Effect on Hydrogen Bonding. Molecules, 2020, 25, 436.	1.7	19
22	Solvent effects on acid-base complexes. What is more important: A macroscopic reaction field or solute-solvent interactions?. Journal of Chemical Physics, 2019, 150, 204505.	1.2	17
23	Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. Angewandte Chemie - International Edition, 2019, 58, 14281-14288.	7.2	24
24	Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. Angewandte Chemie, 2019, 131, 14419-14426.	1.6	4
25	The Partner Does Matter: The Structure of Heteroaggregates of Acridine Orange in Water. Molecules, 2019, 24, 2816.	1.7	16
26	Local-structure effects on 31P NMR chemical shift tensors in solid state. Journal of Chemical Physics, 2019, 150, 144706.	1.2	18
27	Halideâ€Substituted Phosphacyclohexadienyl Iron Complexes: Covalent Structures vs. Ion Pairs. European Journal of Inorganic Chemistry, 2019, 2019, 1434-1434.	1.0	0
28	Correlations of NHN hydrogen bond energy with geometry and1H NMR chemical shift difference of NH protons for aniline complexes. Journal of Chemical Physics, 2019, 150, 114305.	1.2	25
29	Halideâ€Substituted Phosphacyclohexadienyl Iron Complexes: Covalent Structures vs. Ion Pairs. European Journal of Inorganic Chemistry, 2019, 2019, 1567-1574.	1.0	7
30	Amineâ€Borane Dehydrogenation and Transfer Hydrogenation Catalyzed by Î±â€Diimine Cobaltates. Chemistry - A European Journal, 2019, 25, 238-245.	1.7	58
31	Cyclic trimers of phosphinic acids in polar aprotic solvent: symmetry, chirality and H/D isotope effects on NMR chemical shifts. Physical Chemistry Chemical Physics, 2018, 20, 4901-4910.	1.3	28
32	Pâ•O Moiety as an Ambidextrous Hydrogen Bond Acceptor. Journal of Physical Chemistry C, 2018, 122, 1711-1720.	1.5	52
33	Simplified calculation approaches designed to reproduce the geometry of hydrogen bonds in molecular complexes in aprotic solvents. Journal of Chemical Physics, 2018, 148, 124313.	1.2	21
34	NMR Study of Solvation Effect on the Geometry of Proton-Bound Homodimers of Increasing Size. Journal of Physical Chemistry A, 2017, 121, 8697-8705.	1.1	21
35	Attenuation of London Dispersion in Dichloromethane Solutions. Journal of the American Chemical Society, 2017, 139, 13126-13140.	6.6	93
36	Selective P₄ Activation by a Highly Reduced Cobaltate: Synthesis of Dicobalt Tetraphosphido Complexes. Chemistry - A European Journal, 2017, 23, 6094-6102.	1.7	50

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37	Effect of Hydrogen Bonding to Water on the ³¹P Chemical Shift Tensor of Phenyl- and Trialkylphosphine Oxides and Î±-Amino Phosphonates. Journal of Physical Chemistry C, 2016, 120, 8717-8729.	1.5	31
38	NMR Studies of Activeâ€Site Properties of Human Carbonic Anhydraseâ€...II by Using ¹⁵Nâ€Labeled 4â€Methylimidazole as a Local Probe and Histidine Hydrogenâ€Bond Correlations. Chemistry - A European Journal, 2015, 21, 2915-2929.	1.7	20
39	How Short is the Strongest Hydrogen Bond in the Proton-Bound Homodimers of Pyridine Derivatives?. Journal of Physical Chemistry A, 2014, 118, 10804-10812.	1.1	24
40	Photochemistry of deprotonated rhenium(I) (3,3â€²-dihydroxy-2,2â€²-bipyridine) tricarbonyl chloride. Photoisomerization at the chelate in basic solution. Inorganica Chimica Acta, 2014, 421, 496-499.	1.2	7
41	NMR Studies of Protonation and Hydrogen Bond States of Internal Aldimines of Pyridoxal 5â€²-Phosphate Acidâ€“Base in Alanine Racemase, Aspartate Aminotransferase, and Poly-<scp>l</scp>-lysine. Journal of the American Chemical Society, 2013, 135, 18160-18175.	6.6	67
42	Effect of Noncovalent Interactions on the ³¹P Chemical Shift Tensor of Phosphine Oxides, Phosphinic, Phosphonic, and Phosphoric Acids, and Their Complexes with Lead(II). Journal of Physical Chemistry C, 2013, 117, 26689-26702.	1.5	23
43	A qualitative study of the effect of a counterion and polar environment on the structure and spectroscopic signatures of a hydrated hydroxyl anion. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	22
44	Acridine â€“ a Promising Fluorescence Probe of Non-Covalent Molecular Interactions. Zeitschrift Fur Physikalische Chemie, 2013, 227, 857-868.	1.4	1
45	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
46	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. Journal of Physical Chemistry A, 2012, 116, 11370-11387.	1.1	48
47	FTIR study of the hydrogen bond symmetry in protonated homodimers of pyridine and collidine in solution. Journal of Molecular Structure, 2012, 1018, 39-44.	1.8	27
48	Spectrophotometric investigations of protonated forms of heterocyclic compounds. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2012, 113, 275-278.	0.2	3
49	Difference between ¹H NMR signals of primary amide protons as a simple spectral index of the amide intramolecular hydrogen bond strength. Journal of Physical Organic Chemistry, 2012, 25, 287-295.	0.9	44
50	Does Water Affect the Acidity of Surfaces? The Protonâ€Donating Ability of Silanol and Carboxylic Acid Groups at Mesoporous Silica. ChemPhysChem, 2012, 13, 2282-2285.	1.0	24
51	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. Journal of Physical Chemistry A, 2011, 115, 8041-8048.	1.1	46
52	Mutable Lewis and BrÃ¸nsted Acidity of Aluminated SBA-15 as Revealed by NMR of Adsorbed Pyridine-¹⁵N. Langmuir, 2011, 27, 12115-12123.	1.6	50
53	Intrinsic Proton-Donating Power of Zinc-Bound Water in a Carbonic Anhydrase Active Site Model Estimated by NMR. Journal of the American Chemical Society, 2011, 133, 11331-11338.	6.6	27
54	Critical hydrogen bonds and protonation states of pyridoxal 5â€²-phosphate revealed by NMR. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1426-1437.	1.1	57

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55	Spectroscopic Signatures of [H9O4]+ and [H13O6]+ Ions in a Polar Aprotic Environment Revealed Under DFT-PCM Approximation. Acta Chimica Slovenica, 2011, 58, 402-10.	0.2	9
56	Studies of adsorption of 2,2â€²-bipyridyl on the surface of highly regulated silica matrix of the MCM-41 type by means of 15N NMR spectroscopy. Russian Journal of General Chemistry, 2010, 80, 2027-2031.	0.3	10
57	Symmetrization of Cationic Hydrogen Bridges of Protonated Sponges Induced by Solvent and Counteranion Interactions as Revealed by NMR Spectroscopy. Chemistry - A European Journal, 2010, 16, 1679-1690.	1.7	49
58	NMR study of proton transfer to strong bases on inner surfaces of MCM-41. Microporous and Mesoporous Materials, 2010, 134, 22-28.	2.2	22
59	Density Functional Study of the Proton Transfer Effect on Vibrations of Strong (Short) Intermolecular Oâ^'HÂ·Â·Â·N/O^{â^'}Â·Â·Â·Hâ^'N⁺Hydrogen Bonds in Aprotic Solvents. Journal of Physical Chemistry A, 2010, 114, 2393-2399.	1.1	42
60	â€œHexagonal Molybdenum Trioxideâ€â€”Known for 100 Years and Still a Fount of New Discoveries. Inorganic Chemistry, 2010, 49, 9400-9408.	1.9	102
61	Photoinduced Proton Transfer in a Pyridine Based Polymer Gel. Journal of Physical Chemistry B, 2010, 114, 10728-10733.	1.2	17
62	Counteranion-dependent mechanisms of intramolecular proton transfer in aprotic solution. Physical Chemistry Chemical Physics, 2010, 12, 10373.	1.3	39
63	A DFT and AIM analysis of the spinâ€“spin couplings across the hydrogen bond in the 2â€fluorobenzamide and related compounds. Magnetic Resonance in Chemistry, 2009, 47, 585-592.	1.1	44
64	Solid-State NMR Studies of Aminocarboxylic Salt Bridges in <scp>l</scp>-Lysine Modified Cellulose. Journal of Physical Chemistry B, 2009, 113, 934-940.	1.2	31
65	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. Israel Journal of Chemistry, 2009, 49, 199-216.	1.0	143
66	H/D isotope effects on NMR chemical shifts of nuclei involved in a hydrogen bridge of hydrogen isocyanide complexes with fluoride anion. Physical Chemistry Chemical Physics, 2009, 11, 5154.	1.3	16
67	Acidity of Sulfonic and Phosphonic Acid-Functionalized SBA-15 under Almost Water-Free Conditions. Journal of Physical Chemistry C, 2009, 113, 19185-19192.	1.5	62
68	Synthesis and Characterization of Chiral Benzylic Etherâ€Bridged Periodic Mesoporous Organosilicas. Chemistry - A European Journal, 2008, 14, 5935-5940.	1.7	55
69	Carboxylic Acid-Doped SBA-15 Silica as a Host for Metallo-supramolecular Coordination Polymers. Journal of Physical Chemistry B, 2008, 112, 14637-14647.	1.2	46
70	NMR Study of Blue-Shifting Hydrogen Bonds Formed by Fluoroform in Solution. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1225-1245.	1.4	13
71	NMR Localization of Protons in Critical Enzyme Hydrogen Bonds. Journal of the American Chemical Society, 2007, 129, 9558-9559.	6.6	66
72	NMR Provides Checklist of Generic Properties for Atomic-Scale Models of Periodic Mesoporous Silicas. Journal of Physical Chemistry B, 2007, 111, 12088-12096.	1.2	62

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73	Nuclear Magnetic Resonance and ab Initio Studies of Small Complexes Formed between Water and Pyridine Derivatives in Solid and Liquid Phases. Journal of Physical Chemistry A, 2007, 111, 6084-6093.	1.1	43
74	2H-solid state NMR and DSC study of isobutyric acid in mesoporous silica materials. Physical Chemistry Chemical Physics, 2007, 9, 2249.	1.3	44
75	Hydrogen Bonding of Water Confined in Controlled-Pore Glass 10-75 Studied by1H-Solid State NMR. Zeitschrift Fur Physikalische Chemie, 2007, 221, 155-168.	1.4	45
76	Structural and dynamical properties of guest molecules confined in mesoporous silica materials revealed by NMR. Physical Chemistry Chemical Physics, 2007, 9, 4843.	1.3	145
77	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
78	Geometrical Features of Hydrogen Bonded Complexes Involving Sterically Hindered Pyridines. Journal of Physical Chemistry A, 2006, 110, 10872-10879.	1.1	51
79	Maximum value of the chemical shift in the 1H NMR spectrum of a hydrogen-bonded complex. Russian Journal of General Chemistry, 2006, 76, 501-506.	0.3	11
80	Evidence of microphase separation in controlled pore glasses. Solid State Nuclear Magnetic Resonance, 2005, 28, 117-124.	1.5	28
81	Solvent induced temperature dependencies of NMR parameters of hydrogen bonded anionic clusters. Journal of Molecular Structure, 2004, 697, 9-15.	1.8	9
82	NMR Parameters and Geometries of OHN and ODN Hydrogen Bonds of Pyridineâ€“Acid Complexes. Chemistry - A European Journal, 2004, 10, 5195-5204.	1.7	97
83	Hydrogen Bonding of Water Confined in Mesoporous Silica MCM-41 and SBA-15 Studied by1H Solid-State NMR. Chemistry - A European Journal, 2004, 10, 5689-5696.	1.7	340
84	NMR studies of solid stateâ€”solvent and H/D isotope effects on hydrogen bond geometries of 1:1 complexes of collidine with carboxylic acids. Journal of Molecular Structure, 2004, 700, 19-27.	1.8	70
85	Pyridine-15N A Mobile NMR Sensor for Surface Acidity and Surface Defects of Mesoporous Silica. Journal of Physical Chemistry B, 2003, 107, 11924-11939.	1.2	246
86	Low-Temperature NMR Studies of the Structure and Dynamics of a Novel Series of Acidâ^'Base Complexes of HF with Collidine Exhibiting Scalar Couplings Across Hydrogen Bondsâ€. Journal of the American Chemical Society, 2003, 125, 11710-11720.	6.6	170
87	Interpretation of Hydrogen/Deuterium Isotope Effects on NMR Chemical Shifts of [FHF]â^' Ion Based on Calculations of Nuclear Magnetic Shielding Tensor Surface. Zeitschrift Fur Physikalische Chemie, 2003, 217, 1549-1564.	1.4	41
88	2H-Solid-State NMR Study of Benzene-d6Confined in Mesoporous Silica SBA-15. Journal of Physical Chemistry B, 2002, 106, 1977-1984.	1.2	121
89	H/D isotope effects on the low-temperature NMR parameters and hydrogen bond geometries of (FH)2Fâ^'and (FH)3Fâ^'dissolved in CDF3/CDF2Cl. Physical Chemistry Chemical Physics, 2002, 4, 5488-5497.	1.3	103
90	Surface characterization of flax, hemp and cellulose fibers; Surface properties and the water uptake behavior. Polymer Composites, 2002, 23, 872-894.	2.3	350

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91	Stray field gradient NMR reveals effects of hydrogen bonding on diffusion coefficients of pyridine in mesoporous silica. Magnetic Resonance in Chemistry, 2001, 39, S149-S157.	1.1	36
92	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 CDF3/CDClF2 solution. Magnetic Resonance in Chemistry, 2001, 39, S91-S99.	1.1	137
93	1H/15N NMR chemical shielding, dipolar15N,2H coupling and hydrogen bond geometry correlations in a novel series of hydrogen-bonded acid-base complexes of collidine with carboxylic acids. Magnetic Resonance in Chemistry, 2001, 39, S18-S29.	1.1	141
94	Nuclear Scalar Spinâ^'Spin Couplings and Geometries of Hydrogen Bonds. Journal of the American Chemical Society, 2000, 122, 1979-1988.	6.6	188
95	Hydrogen/Deuterium-Isotope Effects on NMR Chemical Shifts and Symmetry of Homoconjugated Hydrogen-Bonded Ions in Polar Solution. Journal of the American Chemical Society, 2000, 122, 12878-12879.	6.6	100
96	Nuclear Scalar Spin-Spin Coupling Reveals Novel Properties of Low-Barrier Hydrogen Bonds in a Polar Environment. Chemistry - A European Journal, 1999, 5, 492-497.	1.7	190
97	NMR and EPR Study of the Nitroxide Radical Tempo Interaction with Phenols. Spectroscopy Letters, 1997, 30, 1515-1523.	0.5	17