Lyubov P Safonova

List of Publications by Year
in descending order

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89	839	516215 16	642321 23
papers	citations	h-index	g-index

89	89	89	593
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The physicochemical properties and structure of alkylammonium protic ionic liquids of RnH4-nNX (nâ€¯=â€¯1â€“3) family. A miniâ€“review. Journal of Molecular Liquids, 2021, 321, 114350.	2.3	31
2	Volumetric properties of ammonium-based salts in N,N-Dimethylformamide over the temperature range 298.15ÂK to 348.15ÂK. Journal of Chemical Thermodynamics, 2021, 155, 106371.	1.0	3
3	Membranes based on polybenzimidazole and protic ionic liquid: preparation and properties. Russian Chemical Bulletin, 2021, 70, 56-61.	0.4	7
4	Structure and ion-ion interactions in trifluoroacetate-based ionic liquids: Quantum chemical and molecular dynamics simulation studies. Journal of Molecular Liquids, 2021, 328, 115449.	2.3	9
5	Comparisons of NHâ€¦O and OHâ€¦O hydrogen bonds in various ethanolammoniumâ€“based protic ionic liquids. Structural Chemistry, 2021, 32, 2061-2073.	1.0	4
6	Imidazolium zwitterionâ€based protic ionic liquids: from monomers to polymer membranes. Polymer International, 2021, 70, 1582-1589.	1.6	5
7	Alkylimidazolium Protic Ionic Liquids: Structural Features and Physicochemical Properties. ChemPhysChem, 2021, , .	1.0	7
8	Structural characterization of H3PO3 and H3PO4 acids solutions in DMF: Spectral analysis and CPMD simulation. Journal of Molecular Liquids, 2020, 300, 112342.	2.3	2
9	Physico-chemical characterization of alkyl-imidazolium protic ionic liquids. Journal of Molecular Liquids, 2020, 297, 111305.	2.3	19
10	Ion Pair Structures and Hydrogen Bonding in R_nNH_{4â€“n} Alkylammonium Ionic Liquids with Hydrogen Sulfate and Mesylate Anions by DFT Computations. Journal of Physical Chemistry A, 2020, 124, 3170-3179.	1.1	15
11	Thermal properties of protic ionic liquids derivatives triethanolamine-based salts of mineral and organic acids. Journal of Thermal Analysis and Calorimetry, 2019, 138, 703-712.	2.0	4
12	Polymer electrolytes based on PVdF-HFP doped with protic ionic liquids containing different cations. Journal of Molecular Liquids, 2019, 283, 338-345.	2.3	13
13	Quantum Chemical Modeling of the Structure and H Bonding in Triethanolammonium-Based Protic Ionic Liquids with Sulfonic Acids. Journal of Physical Chemistry A, 2019, 123, 3735-3742.	1.1	9
14	Triethylamine-Based Salts: Protic Ionic Liquids or Molecular Complexes?. Journal of Physical Chemistry B, 2019, 123, 10794-10806.	1.2	23
15	Diethylamine-based ionic liquids: quantum chemical calculations and experiment. Russian Chemical Bulletin, 2019, 68, 2009-2019.	0.4	8
16	Volumetric Properties of Protic Ionic Liquids Based on Alkylammonium Cations at T = (293.15â€“353.15) K and Atmospheric Pressure. Journal of Chemical & Engineering Data, 2019, 64, 211-217.	1.0	8
17	Ab Initio Investigation of the Interionic Interactions in Triethylammonium-Based Protic Ionic Liquids: The Role of Anions in the Formation of Ion Pair and Hydrogen Bonded Structure. Journal of Physical Chemistry A, 2019, 123, 293-300.	1.1	25
18	Conductivity of gel polymer electrolytes doped with solutions of phosphonic acid or protic ionic liquids. Chemical Physics Letters, 2018, 697, 1-6.	1.2	5

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19	The Nature of the Interactions in Triethanolammonium-Based Ionic Liquids. A Quantum Chemical Study. Journal of Physical Chemistry A, 2018, 122, 4562-4570.	1.1	17
20	Evaluation of Acid Dissociation Constants in DMSO and DMF by Quantum-Chemical Methods. Journal of Solution Chemistry, 2018, 47, 140-149.	0.6	1
21	Synthesis and properties of triethanolamine-based salts with mineral and organic acids as protic ionic liquids. Journal of Molecular Liquids, 2018, 249, 825-830.	2.3	27
22	Possibility of Protic Ionic Liquids Formation From Triethanolamine with Sulfonamides. Journal of Physical Chemistry B, 2018, 122, 6586-6594.	1.2	2
23	Influence of Cation Size on the Structural Features and Interactions in Tertiary Alkylammonium Trifluoroacetates: A Density Functional Theory Investigation. Journal of Physical Chemistry A, 2018, 122, 5878-5885.	1.1	15
24	Ab Initio Study of Structural Features and H-Bonding in Alkylammonium-Based Protic Ionic Liquids. Journal of Physical Chemistry A, 2017, 121, 7675-7683.	1.1	26
25	Triethanolamine-based protic ionic liquids with various sulfonic acids: Synthesis and properties. Journal of Molecular Liquids, 2017, 242, 838-844.	2.3	32
26	Ab initio study of hydrogen bonding in the H3PO2 dimer and H3PO2â€“DMF complex. Journal of Molecular Modeling, 2017, 23, 220.	0.8	2
27	Densities, Viscosities, and Conductivities of Phosphonic Acid Solutions in N,N-Dimethylformamide and Water. Journal of Chemical & Engineering Data, 2017, 62, 80-86.	1.0	4
28	Ab initio molecular dynamics study of H-bonding and proton transfer in the phosphoric acidâ€“N,N-Dimethylformamide system. Journal of Chemical Physics, 2016, 145, 124507.	1.2	3
29	Thermochemical investigation of the (phosphonic acid+N,N-dimethylformamide) system at T=(298.15 to) Tj ETQq1 1 0.784314 rgBT /O	1.0	2
30	C-PCM based calculation of energy profiles for proton transfer in phosphorus-containing acidâ€“N,N-dimethylformamide complexes. Russian Journal of Physical Chemistry A, 2016, 90, 293-299.	0.1	4
31	Proton transfer in the molecular complexes of phosphorus acids with DMSO. Structural Chemistry, 2016, 27, 1561-1567.	1.0	4
32	Influence of solvent environment using the CPCM model on the H-bond geometry in the complexes of phosphorus acids with DMSO. Structural Chemistry, 2016, 27, 1189-1198.	1.0	9
33	Solvent effect on proton transfer in the complexes of N,N-dimethylformamide with sulfuric and phosphoric acid: A DFT investigation. Journal of Molecular Structure, 2016, 1106, 424-429.	1.8	11
34	Hydrogen bonds in complexes of phosphonic and metylphosphonic acids with dimethylformamide. Russian Journal of Physical Chemistry A, 2015, 89, 2248-2253.	0.1	10
35	Computer simulation study of the intermolecular structure of phosphoric acidâ€“N,N-dimethylformamide mixtures. Journal of Molecular Modeling, 2015, 21, 17.	0.8	3
36	Conductometric study of diclofenac salts in water at different temperatures. Journal of Molecular Liquids, 2015, 208, 16-20.	2.3	2

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37	Ab initio calculations of proton transfer in dimethylformamide-phosphoric acid complexes of 1 : 1 composition. Russian Journal of Physical Chemistry A, 2015, 89, 608-615.	0.1	7
38	Conductivity and intermolecular interactions in protonâ€conducting gel electrolytes. Journal of Applied Polymer Science, 2014, 131, .	1.3	4
39	The Hammett acidity function H0 of phosphoric acid solutions in N,N-dimethylformamide at 298.15K. Journal of Molecular Liquids, 2014, 193, 1-5.	2.3	6
40	Hydrogen bonding analysis of phosphoric acidâ€“N,N-dimethylformamide mixtures. Journal of Molecular Modeling, 2014, 20, 2349.	0.8	4
41	Conductivity and thermal stability of proton-conducting electrolytes at confined geometry of polymeric gel. Ionics, 2013, 19, 701-707.	1.2	6
42	Quantum-mechanical analysis of the structure of phosphoric acid complexes with methyl methacrylate and methyl trimethylacetate. Russian Journal of Physical Chemistry A, 2013, 87, 2054-2062.	0.1	2
43	Quantum chemical calculations of the structure of hydrogen-bonded sulfuric acid-dimethylformamide complexes. Russian Journal of Physical Chemistry A, 2013, 87, 225-232.	0.1	1
44	Complexes of sulfuric acid with N,N-dimethylformamide: An ab initio investigation. Pure and Applied Chemistry, 2012, 85, 225-236.	0.9	5
45	Quantum-chemical studies of dimethylformamide 1 : 1 complexes with phosphoric acid. Russian Journal of Physical Chemistry A, 2012, 86, 1847-1854.	0.1	12
46	Proton conducting gel electrolytes based on polymethylmethacrylate doped with sulfuric acid solutions in N,N-dimethylformamide. Journal of Polymer Research, 2012, 19, 1.	1.2	15
47	The intermolecular structure of phosphoric acidâ€“N,N-dimethylformamide mixtures as studied by computer simulation. Journal of Chemical Physics, 2011, 134, 174506.	1.2	11
48	Molecular dynamics simulation of Bu4N+ in dimethylformamide: Solvation-induced volume changes. Russian Journal of Physical Chemistry A, 2011, 85, 961-966.	0.1	2
49	Simulating the proton transfer reaction in the phosphoric acid-N,N-dimethylformamide system by means of the AM1 semiempirical method. Russian Journal of Physical Chemistry A, 2011, 85, 1917-1922.	0.1	10
50	Structure of bilirubin and its anion according to quantum chemical calculations and molecular dynamics simulation. Russian Journal of Physical Chemistry A, 2011, 85, 2165-2170.	0.1	2
51	Proton-conducting gel electrolytes based on poly(methyl methacrylate) doped with phosphoric acid in N,N-dimethylformamide. Polymer Science - Series A, 2011, 53, 44-51.	0.4	4
52	Dissociation Constant of Acetic Acid in (N,N-Dimethylformamideâ€‰+â€‰Water) Mixtures at the Temperature 298.15 K. Journal of Solution Chemistry, 2011, 40, 980-988.	0.6	13
53	Calculation of properties of ternary liquid mixtures on the basis of properties of binary solutions. Russian Journal of Applied Chemistry, 2010, 83, 161-164.	0.1	0
54	Partial molar volumes of some drug and pro-drug substances in 1-octanol at T=298.15K. Journal of Chemical Thermodynamics, 2010, 42, 429-435.	1.0	37

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55	Molar heat capacities of the (water+acetonitrile) mixtures at T=(283.15, 298.15, 313.15, and 328.15)K. Journal of Chemical Thermodynamics, 2010, 42, 1209-1212.	1.0	22
56	Physico-chemical and structural characterization of the binary system phosphoric acidâ€“N,N-dimethylformamide. Physical Chemistry Chemical Physics, 2010, 12, 8977.	1.3	14
57	NMR studies of N,N-dimethylformamide mixtures with acetic acid and ethanol. Russian Journal of General Chemistry, 2009, 79, 246-251.	0.3	3
58	Thermal diffusion of hydrogen chloride in aqueous solutions of N,N-dimethylformamide and acetone. Russian Journal of Physical Chemistry A, 2009, 83, 1117-1120.	0.1	0
59	Dissociation constants of phosphoric acid in dimethylformamide-water mixtures at 298.15 K. Russian Journal of Physical Chemistry A, 2009, 83, 1747-1750.	0.1	20
60	A molecular dynamics simulation of H3PO4, H2PO 4 â^' , and the protonated form of N,N-dimethylformamide in liquid N,N-dimethylformamide. Russian Journal of Physical Chemistry A, 2009, 83, 2103-2109.	0.1	10
61	The thermodynamic characteristics of solutions of Bu4NI in dimethylsulfoxide over a wide concentration range. Russian Journal of Physical Chemistry A, 2008, 82, 740-745.	0.1	1
62	Viscosities, Refractive Indexes, and Conductivities of Phosphoric Acid in N,N-Dimethylformamide + Water Mixtures. Journal of Chemical & Engineering Data, 2008, 53, 1381-1386.	1.0	16
63	Molecular dynamics simulation of the structure of ion solvation shells in N,N-dimethylformamide. Journal of Molecular Liquids, 2007, 131-132, 124-130.	2.3	2
64	Change in the volume of orthophosphoric acid solutions in the neutralization with solutions of various bases. Russian Journal of General Chemistry, 2007, 77, 1014-1018.	0.3	0
65	The physicochemical properties of the LiCl-CeCl3-H2O ternary system. Russian Journal of Physical Chemistry A, 2006, 80, 345-347.	0.1	2
66	Standard characteristics of thermodiffusion of hydrogen chloride in the water-2-propanol system at 298.15 K. Russian Journal of Physical Chemistry A, 2006, 80, 1146-1150.	0.1	0
67	The thermal diffusion of hydrogen chloride in aqueous solutions of acetonitrile. Russian Journal of Physical Chemistry A, 2006, 80, 1433-1437.	0.1	0
68	The dynamics of ions in dimethylformamide. Russian Journal of Physical Chemistry A, 2006, 80, 1438-1444.	0.1	0
69	Structure of orthophosphoric Acid-N,N-dimethylformamide complexes. Russian Journal of Physical Chemistry A, 2006, 80, S7-S13.	0.1	16
70	Entropy characteristic of solvation and thermal diffusion of hydrogen chloride in water-1-propanol solutions: A thermoelectrochemical determination. Russian Journal of Electrochemistry, 2006, 42, 969-973.	0.3	2
71	The Thermal Diffusion of Hydrogen Chloride in Waterâ€“Monoatomic Alcohol Mixtures at 298 K. Journal of Solution Chemistry, 2006, 35, 1621-1630.	0.6	8
72	Thermodynamic investigation of the orthophosphoric acidâ€”N,N-dimethylformamide system. Journal of Molecular Liquids, 2005, 121, 53-57.	2.3	12

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73	Partial Molar Volumes of Tetraalkylammonium Ions in N, N-Dimethylformamide. Journal of Solution Chemistry, 2005, 34, 529-536.	0.6	10
74	Intermolecular interactions in orthophosphoric acid-N,N-dimethylformamide system according to viscometric data. Russian Chemical Bulletin, 2005, 54, 2325-2329.	0.4	8
75	Physicochemical Properties of the H3PO4-Dimethylformamide System. Russian Journal of General Chemistry, 2004, 74, 174-178.	0.3	11
76	Orthophosphoric Acid-;N,N-Dimethylformamide System: IR Study. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2003, 29, 515-518.	0.3	26
77	The calorimetric investigation of phosphoric acidâ€“N,N-dimethylformamide system. Thermochimica Acta, 2003, 405, 117-122.	1.2	10
78	Molecular dynamic simulations of a liquid formamide and N,N-dimethylformamide with new quantum mechanical potential. Journal of Molecular Liquids, 2003, 103-104, 15-31.	2.3	36
79	Investigation of the phosphoric acid -N,N-dimethylformamide system as potential solvent for cellulose. Journal of Molecular Liquids, 2003, 103-104, 339-347.	2.3	15
80	Title is missing!. Journal of Structural Chemistry, 2002, 43, 284-292.	0.3	4
81	Conductance studies of 1-1 electrolytes in N,N-dimethylformamide at various temperatures. Physical Chemistry Chemical Physics, 2001, 3, 819-823.	1.3	28
82	Pitzer equation for the enthalpy of solution of electrolytes in N,N-dimethylformamide in a wide temperature range. Theoretical Foundations of Chemical Engineering, 2000, 34, 351-355.	0.2	1
83	Thermodynamics of ionic solvation inn-propanol from ?50 to 50ï¿½C. Journal of Solution Chemistry, 1994, 23, 379-397.	0.6	3
84	Conductometry of electrolyte solutions. Russian Chemical Reviews, 1992, 61, 959-973.	2.5	25
85	Analysis of the thermodynamic characteristics of solvation of individual ions in ethanol using model concepts. Journal of Solution Chemistry, 1992, 21, 533-543.	0.6	3
86	Analysis of interparticle interactions in mixtures of water with amides at various temperatures. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1990, 39, 2289-2295.	0.0	0
87	Thermodynamic characteristics of solvation of individual ions in ethanol at ?50 to 55ï¿½C. Journal of Solution Chemistry, 1990, 19, 975-994.	0.6	7
88	Analysis of the thermodynamic characteristics of the solvation of ions in protic solvents at various temperatures using model concepts. Thermochimica Acta, 1990, 169, 347-352.	1.2	6
89	Partial molar volumes of ions in ethanol from 233 to 313 K. Journal of Solution Chemistry, 1988, 17, 569-580.	0.6	6