

# Lyubov P Safonova

## List of Publications by Year in descending order

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papers

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citations

516215

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89  
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89  
docs citations

89  
times ranked

593  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	Triethanolamine-based protic ionic liquids with various sulfonic acids: Synthesis and properties. Journal of Molecular Liquids, 2017, 242, 838-844.	2.3	32
4	The physicochemical properties and structure of alkylammonium protic ionic liquids of RnH4-nNX (n=1-3) family. A mini-review. Journal of Molecular Liquids, 2021, 321, 114350.	2.3	31
5	Conductance studies of 1-1 electrolytes in N,N-dimethylformamide at various temperatures. Physical Chemistry Chemical Physics, 2001, 3, 819-823.	1.3	28
6	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
7	Orthophosphoric Acid-N,N-Dimethylformamide System: IR Study. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2003, 29, 515-518.	0.3	26
8	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
9	Conductometry of electrolyte solutions. Russian Chemical Reviews, 1992, 61, 959-973.	2.5	25
10	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
11	Triethylamine-Based Salts: Protic Ionic Liquids or Molecular Complexes?. Journal of Physical Chemistry B, 2019, 123, 10794-10806.	1.2	23
12	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
13	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
14	Physico-chemical characterization of alkyl-imidazolium protic ionic liquids. Journal of Molecular Liquids, 2020, 297, 111305.	2.3	19
15	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
16	Structure of orthophosphoric Acid-N,N-dimethylformamide complexes. Russian Journal of Physical Chemistry A, 2006, 80, S7-S13.	0.1	16
17	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
18	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

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19	Proton conducting gel electrolytes based on polymethylmethacrylate doped with sulfuric acid solutions in N,N-dimethylformamide. <i>Journal of Polymer Research</i> , 2012, 19, 1.	1.2	15
20	Influence of Cation Size on the Structural Features and Interactions in Tertiary Alkylammonium Trifluoroacetates: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5878-5885.	1.1	15
21	Ion Pair Structures and Hydrogen Bonding in R <sub>n</sub> NH <sub>4</sub> <sup>+</sup> Alkylammonium Ionic Liquids with Hydrogen Sulfate and Mesylate Anions by DFT Computations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3170-3179.	1.1	15
22	Physico-chemical and structural characterization of the binary system phosphoric acid–N,N-dimethylformamide. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8977.	1.3	14
23	Dissociation Constant of Acetic Acid in (N,N-Dimethylformamide+Water) Mixtures at the Temperature 298.15 K. <i>Journal of Solution Chemistry</i> , 2011, 40, 980-988.	0.6	13
24	Polymer electrolytes based on PVdF-HFP doped with protic ionic liquids containing different cations. <i>Journal of Molecular Liquids</i> , 2019, 283, 338-345.	2.3	13
25	Thermodynamic investigation of the orthophosphoric acid–N,N-dimethylformamide system. <i>Journal of Molecular Liquids</i> , 2005, 121, 53-57.	2.3	12
26	Quantum-chemical studies of dimethylformamide 1 : 1 complexes with phosphoric acid. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1847-1854.	0.1	12
27	Physicochemical Properties of the H <sub>3</sub> PO <sub>4</sub> -Dimethylformamide System. <i>Russian Journal of General Chemistry</i> , 2004, 74, 174-178.	0.3	11
28	The intermolecular structure of phosphoric acid–N,N-dimethylformamide mixtures as studied by computer simulation. <i>Journal of Chemical Physics</i> , 2011, 134, 174506.	1.2	11
29	Solvent effect on proton transfer in the complexes of N,N-dimethylformamide with sulfuric and phosphoric acid: A DFT investigation. <i>Journal of Molecular Structure</i> , 2016, 1106, 424-429.	1.8	11
30	The calorimetric investigation of phosphoric acid–N,N-dimethylformamide system. <i>Thermochimica Acta</i> , 2003, 405, 117-122.	1.2	10
31	Partial Molar Volumes of Tetraalkylammonium Ions in N, N-Dimethylformamide. <i>Journal of Solution Chemistry</i> , 2005, 34, 529-536.	0.6	10
32	A molecular dynamics simulation of H <sub>3</sub> PO <sub>4</sub> , H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> , and the protonated form of N,N-dimethylformamide in liquid N,N-dimethylformamide. <i>Russian Journal of Physical Chemistry A</i> , 2009, 83, 2103-2109.	0.1	10
33	Simulating the proton transfer reaction in the phosphoric acid-N,N-dimethylformamide system by means of the AM1 semiempirical method. <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 1917-1922.	0.1	10
34	Hydrogen bonds in complexes of phosphonic and methylphosphonic acids with dimethylformamide. <i>Russian Journal of Physical Chemistry A</i> , 2015, 89, 2248-2253.	0.1	10
35	Influence of solvent environment using the CPCM model on the H-bond geometry in the complexes of phosphorus acids with DMSO. <i>Structural Chemistry</i> , 2016, 27, 1189-1198.	1.0	9
36	Quantum Chemical Modeling of the Structure and H Bonding in Triethanolammonium-Based Protic Ionic Liquids with Sulfonic Acids. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3735-3742.	1.1	9

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37	Structure and ion-ion interactions in trifluoroacetate-based ionic liquids: Quantum chemical and molecular dynamics simulation studies. <i>Journal of Molecular Liquids</i> , 2021, 328, 115449.	2.3	9
38	Intermolecular interactions in orthophosphoric acid-N,N-dimethylformamide system according to viscometric data. <i>Russian Chemical Bulletin</i> , 2005, 54, 2325-2329.	0.4	8
39	The Thermal Diffusion of Hydrogen Chloride in Water-Monoatomic Alcohol Mixtures at 298 K. <i>Journal of Solution Chemistry</i> , 2006, 35, 1621-1630.	0.6	8
40	Diethylamine-based ionic liquids: quantum chemical calculations and experiment. <i>Russian Chemical Bulletin</i> , 2019, 68, 2009-2019.	0.4	8
41	Volumetric Properties of Protic Ionic Liquids Based on Alkylammonium Cations at $T = (293.15 \text{--} 353.15) \text{ K}$ and Atmospheric Pressure. <i>Journal of Chemical &amp; Engineering Data</i> , 2019, 64, 211-217.	1.0	8
42	Thermodynamic characteristics of solvation of individual ions in ethanol at 25 to 55°C. <i>Journal of Solution Chemistry</i> , 1990, 19, 975-994.	0.6	7
43	Ab initio calculations of proton transfer in dimethylformamide-phosphoric acid complexes of 1 : 1 composition. <i>Russian Journal of Physical Chemistry A</i> , 2015, 89, 608-615.	0.1	7
44	Membranes based on polybenzimidazole and protic ionic liquid: preparation and properties. <i>Russian Chemical Bulletin</i> , 2021, 70, 56-61.	0.4	7
45	Alkylimidazolium Protic Ionic Liquids: Structural Features and Physicochemical Properties. <i>ChemPhysChem</i> , 2021, , .	1.0	7
46	Partial molar volumes of ions in ethanol from 233 to 313 K. <i>Journal of Solution Chemistry</i> , 1988, 17, 569-580.	0.6	6
47	Analysis of the thermodynamic characteristics of the solvation of ions in protic solvents at various temperatures using model concepts. <i>Thermochimica Acta</i> , 1990, 169, 347-352.	1.2	6
48	Conductivity and thermal stability of proton-conducting electrolytes at confined geometry of polymeric gel. <i>Ionics</i> , 2013, 19, 701-707.	1.2	6
49	The Hammett acidity function $H_0$ of phosphoric acid solutions in N,N-dimethylformamide at 298.15K. <i>Journal of Molecular Liquids</i> , 2014, 193, 1-5.	2.3	6
50	Complexes of sulfuric acid with N,N-dimethylformamide: An ab initio investigation. <i>Pure and Applied Chemistry</i> , 2012, 85, 225-236.	0.9	5
51	Conductivity of gel polymer electrolytes doped with solutions of phosphonic acid or protic ionic liquids. <i>Chemical Physics Letters</i> , 2018, 697, 1-6.	1.2	5
52	Imidazolium zwitterion-based protic ionic liquids: from monomers to polymer membranes. <i>Polymer International</i> , 2021, 70, 1582-1589.	1.6	5
53	Title is missing!. <i>Journal of Structural Chemistry</i> , 2002, 43, 284-292.	0.3	4
54	Proton-conducting gel electrolytes based on poly(methyl methacrylate) doped with phosphoric acid in N,N-dimethylformamide. <i>Polymer Science - Series A</i> , 2011, 53, 44-51.	0.4	4

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55	Conductivity and intermolecular interactions in proton-conducting gel electrolytes. <i>Journal of Applied Polymer Science</i> , 2014, 131, .	1.3	4
56	Hydrogen bonding analysis of phosphoric acid-N,N-dimethylformamide mixtures. <i>Journal of Molecular Modeling</i> , 2014, 20, 2349.	0.8	4
57	C-PCM based calculation of energy profiles for proton transfer in phosphorus-containing acid-N,N-dimethylformamide complexes. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 293-299.	0.1	4
58	Proton transfer in the molecular complexes of phosphorus acids with DMSO. <i>Structural Chemistry</i> , 2016, 27, 1561-1567.	1.0	4
59	Densities, Viscosities, and Conductivities of Phosphonic Acid Solutions in N,N-Dimethylformamide and Water. <i>Journal of Chemical &amp; Engineering Data</i> , 2017, 62, 80-86.	1.0	4
60	Thermal properties of protic ionic liquids derivatives triethanolamine-based salts of mineral and organic acids. <i>Journal of Thermal Analysis and Calorimetry</i> , 2019, 138, 703-712.	2.0	4
61	Comparisons of NH <sub>2</sub> -O and OH <sub>2</sub> -O hydrogen bonds in various ethanolammonium <sup>+</sup> -based protic ionic liquids. <i>Structural Chemistry</i> , 2021, 32, 2061-2073.	1.0	4
62	Analysis of the thermodynamic characteristics of solvation of individual ions in ethanol using model concepts. <i>Journal of Solution Chemistry</i> , 1992, 21, 533-543.	0.6	3
63	Thermodynamics of ionic solvation in n-propanol from 25 to 50°C. <i>Journal of Solution Chemistry</i> , 1994, 23, 379-397.	0.6	3
64	NMR studies of N,N-dimethylformamide mixtures with acetic acid and ethanol. <i>Russian Journal of General Chemistry</i> , 2009, 79, 246-251.	0.3	3
65	Computer simulation study of the intermolecular structure of phosphoric acid-N,N-dimethylformamide mixtures. <i>Journal of Molecular Modeling</i> , 2015, 21, 17.	0.8	3
66	Ab initio molecular dynamics study of H-bonding and proton transfer in the phosphoric acid-N,N-Dimethylformamide system. <i>Journal of Chemical Physics</i> , 2016, 145, 124507.	1.2	3
67	Volumetric properties of ammonium-based salts in N,N-Dimethylformamide over the temperature range 298.15 K to 348.15 K. <i>Journal of Chemical Thermodynamics</i> , 2021, 155, 106371.	1.0	3
68	The physicochemical properties of the LiCl-CeCl <sub>3</sub> -H <sub>2</sub> O ternary system. <i>Russian Journal of Physical Chemistry A</i> , 2006, 80, 345-347.	0.1	2
69	Entropy characteristic of solvation and thermal diffusion of hydrogen chloride in water-1-propanol solutions: A thermoelectrochemical determination. <i>Russian Journal of Electrochemistry</i> , 2006, 42, 969-973.	0.3	2
70	Molecular dynamics simulation of the structure of ion solvation shells in N,N-dimethylformamide. <i>Journal of Molecular Liquids</i> , 2007, 131-132, 124-130.	2.3	2
71	Molecular dynamics simulation of Bu <sub>4</sub> N <sup>+</sup> in dimethylformamide: Solvation-induced volume changes. <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 961-966.	0.1	2
72	Structure of bilirubin and its anion according to quantum chemical calculations and molecular dynamics simulation. <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 2165-2170.	0.1	2

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73	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
74	Conductometric study of diclofenac salts in water at different temperatures. Journal of Molecular Liquids, 2015, 208, 16-20.	2.3	2
75	Thermochemical investigation of the (phosphonic acid+N,N-dimethylformamide) system at T=(298.15 to) Tj ETQq1_1.0.784314 rgBT / 1.0	1.0	2
76	Ab initio study of hydrogen bonding in the H <sub>3</sub> PO <sub>2</sub> dimer and H <sub>3</sub> PO <sub>2</sub> â€“DMF complex. Journal of Molecular Modeling, 2017, 23, 220.	0.8	2
77	Possibility of Protic Ionic Liquids Formation From Triethanolamine with Sulfonamides. Journal of Physical Chemistry B, 2018, 122, 6586-6594.	1.2	2
78	Structural characterization of H <sub>3</sub> PO <sub>3</sub> and H <sub>3</sub> PO <sub>4</sub> acids solutions in DMF: Spectral analysis and CPMD simulation. Journal of Molecular Liquids, 2020, 300, 112342.	2.3	2
79	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
80	The thermodynamic characteristics of solutions of Bu <sub>4</sub> NI in dimethylsulfoxide over a wide concentration range. Russian Journal of Physical Chemistry A, 2008, 82, 740-745.	0.1	1
81	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
82	Evaluation of Acid Dissociation Constants in DMSO and DMF by Quantum-Chemical Methods. Journal of Solution Chemistry, 2018, 47, 140-149.	0.6	1
83	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
84	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
85	The thermal diffusion of hydrogen chloride in aqueous solutions of acetonitrile. Russian Journal of Physical Chemistry A, 2006, 80, 1433-1437.	0.1	0
86	The dynamics of ions in dimethylformamide. Russian Journal of Physical Chemistry A, 2006, 80, 1438-1444.	0.1	0
87	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
88	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
89	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