

# Mirosław Szafran

## List of Publications by Year in descending order

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docs citations

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times ranked

502  
citing authors

#	ARTICLE	IF	CITATIONS
1	Recent aspects of the proton transfer reaction in H-bonded complexes. Journal of Molecular Structure, 1996, 381, 39-64.	1.8	63
2	Electrostatic Interactions and Conformations of Zwitterionic Pyridinium Alkanoates. Journal of Organic Chemistry, 1998, 63, 2898-2908.	1.7	61
3	Strong hydrogen bonds in 1:1 and 2:1 complexes of pyridine betaine with strong acids. Journal of Molecular Structure, 1994, 322, 297-308.	1.8	48
4	Differences between the N-H...O and O-H...O hydrogen bonds in complexes of 2,6-dichloro-4-nitrophenol with pyridines and pyridine N-oxides. Journal of Molecular Structure, 1996, 381, 107-125.	1.8	33
5	Molecular structures and hydrogen bonding of 1:1 and 2:1 complexes of quinoline betaine with perchloric acid. Journal of Molecular Structure, 2002, 609, 19-28.	1.8	30
6	<sup>1</sup> H and <sup>13</sup> C NMR spectra of betaines, >N+(CH <sub>2</sub> ) <sub>n</sub> COO <sup>-</sup> , and their hydrogen halides. Additivity rules for carbon-13 chemical shifts. Magnetic Resonance in Chemistry, 2000, 38, 43-50.	1.1	29
7	Structure and vibrational spectra of pyridine betaine hydrochloride. Journal of Molecular Structure, 1997, 436-437, 123-142.	1.8	28
8	Influence of Electrostatic Interactions on Complexes with Short O-H...O Hydrogen Bonds in Basic Salts of Pyridine Betaines and Acid Salts of <i>p</i> -Phenylalkanoic Acids. Israel Journal of Chemistry, 1999, 39, 253-260.	1.0	26
9	Hydrogen bonding and proton localization in complexes of carboxybetaines with phenols and carboxylic acids. Journal of Molecular Structure, 1997, 404, 13-23.	1.8	25
10	X-ray, phase transition, IR and Raman studies of the solid complex of bis(pyridine betaine)-sulphuric acid. Journal of Molecular Structure, 1997, 406, 127-135.	1.8	24
11	Crystal structure and vibrational spectrum of N-methylpiperidine betaine hexafluorosilicate. Journal of Molecular Structure, 2001, 598, 267-276.	1.8	24
12	Crystal and molecular structure of N-methylpiperidine betaine hydrobromide. Journal of Molecular Structure, 2002, 605, 319-324.	1.8	24
13	Calculation of the vibrational spectra of pyridine betaine. Journal of Molecular Structure, 1996, 381, 157-167.	1.8	21
14	Bis(N-methylpiperidine betaine) hydrobromide: crystal structure and hydrogen bonding. Journal of Molecular Structure, 2002, 615, 33-43.	1.8	20
15	NH <sup>+</sup> ...O and OH <sup>-</sup> ...O interactions of glycine derivatives with squaric acid. New Journal of Chemistry, 2014, 38, 3556-3568.	1.4	19
16	X-ray, FTIR, <sup>1</sup> H and <sup>13</sup> C NMR, PM3 and AM1 studies of (N <sup>+</sup> ...H <sup>-</sup> N) <sup>+</sup> and (O <sup>-</sup> ...H <sup>+</sup> O) <sup>-</sup> hydrogen bonds in a complex of 1,8-diaminonaphthalene with maleic acid: proton cavity and basicity of proton sponges. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 87-92.	1.7	16
17	Molecular structure and vibrational spectrum of N-methylpyrrolidine betaine hydrogen chloride: experimental and DFT study. Vibrational Spectroscopy, 2000, 23, 1-11.	1.2	16
18	Crystal and molecular structure of 3-(2-amino-pyridinium)-propionate monohydrate. Journal of Molecular Structure, 2006, 786, 25-32.	1.8	16

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19	Structure of the complex of dimethylphenyl betaine with dichloroacetic acid studied by X-ray diffraction, DFT calculations, infrared and Raman spectra. <i>Vibrational Spectroscopy</i> , 2016, 84, 92-100.	1.2	15
20	Crystal structure and vibrational spectra of the 1:1 and 1:2 complexes of pyridine betaine with pentachlorophenol. <i>Journal of Molecular Structure</i> , 1997, 436-437, 143-151.	1.8	14
21	Deprotonation of 1-(carbethoxyalkyl)pyridinium halides with strong N-bases. <i>Journal of Physical Organic Chemistry</i> , 1999, 12, 39-46.	0.9	14
22	Hydrogen bonds in 1:1 complex of piperidine-3-carboxylic acid with salicylic acid. <i>Journal of Molecular Structure</i> , 2009, 920, 68-74.	1.8	14
23	Comparison of low-barrier hydrogen bonds in acid salts of carboxylic acids and basic salts of betaines – FTIR study. <i>Journal of Molecular Structure</i> , 1999, 484, 117-124.	1.8	13
24	FTIR studies of complexes of N-methylmorpholine betaine with phenols. <i>Journal of Molecular Structure</i> , 2002, 614, 189-194.	1.8	13
25	FT-IR, UV-vis and X-ray studies of complexes of pyridine N-oxides with pentachlorophenol. <i>Journal of Molecular Structure</i> , 1995, 356, 169-182.	1.8	11
26	Conformational preferences of isostructural N-methylpiperidine betaine and (1-methylcyclohexyl)acetic acid studied by PM3 and B3LYP calculations. The effect of electrostatic interactions on the rotation barrier. <i>Journal of Molecular Structure</i> , 2001, 598, 251-260.	1.8	10
27	Structural, spectroscopic and theoretical studies of dimethylphenyl betaine complex with two molecules of 2,6-dichloro-4-nitro-phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1216-1226.	2.0	10
28	Structural, vibrational and DFT studies of di-(pipercolinium acid) squarate. <i>Vibrational Spectroscopy</i> , 2017, 88, 106-116.	1.2	10
29	Conformational analysis of 5-piperidinevaleric acid, 5-(N-methylpiperidine)valerate and their hydrogen halides by MO calculations, X-ray diffraction and FTIR spectroscopy. <i>Journal of Molecular Structure</i> , 1999, 484, 125-138.	1.8	9
30	Structural, spectroscopic, and theoretical studies of a very short OHO hydrogen bond in bis(4-(N-methylpiperidinium)butyrate) hydrobromide. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 356-361.	0.9	9
31	Structural, spectroscopic and computational studies of the 2:1 complex of nipecotic acid with squaric acid. <i>Chemical Physics</i> , 2014, 444, 7-14.	0.9	9
32	X-Ray, FTIR and quantum chemical studies of short and asymmetric hydrogen bonds in bis(2,6-dimethylpyridine-N-oxide) sulphate [2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>5</sub> H <sub>3</sub> N <sub>2</sub> -OH] <sub>2</sub> [SO <sub>4</sub> ] <sup>2-</sup> . <i>Journal of Molecular Structure</i> , 1997, 416, 81-90.	1.8	8
33	Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. <i>Vibrational Spectroscopy</i> , 2015, 79, 16-23.	1.2	8
34	Structural and spectroscopic properties of piperidinium-4-carboxylic acid hydrogen squarate. <i>Vibrational Spectroscopy</i> , 2015, 81, 13-21.	1.2	8
35	Spectroscopic studies of the 1:1 complex of piperidine-4-carboxylic acid (isonipecotic acid) with 2,6-dichloro-4-nitrophenol. <i>Vibrational Spectroscopy</i> , 2016, 85, 35-42.	1.2	8
36	Structure, conformation and hydrogen bonding of some pyridiniumpropionate complexes. <i>Journal of Molecular Structure</i> , 1998, 448, 77-89.	1.8	7

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37	Differences in protonâ€“proton coupling constants of N+â€“CH2â€“CH2 protons of some betaines, N+â€“(CH2)2-3â€“COOâ€”, and their complexes in aqueous solution. <i>Journal of Molecular Structure</i> , 2001, 563-564, 555-564.	1.8	7
38	Experimental and theoretical studies of 4-hydroxy-1-methylpiperidinium perchlorate. <i>Journal of Molecular Structure</i> , 2008, 889, 344-351.	1.8	7
39	Cooperative hydrogen bond between piperidine-ethanol and 2,6-dichloro-4- nitrophenol. <i>Journal of Molecular Structure</i> , 2019, 1184, 468-478.	1.8	7
40	Formation of the homoconjugated cation (Ni-Oâ€“Hâ€“Oâ€“-N)+ of N-dodecyl-N,N-dimethylamine oxide in carbon tetrachloride. <i>Journal of Molecular Structure</i> , 1990, 239, 1-11.	1.8	6
41	Conformational Analysis of N-Methylpyrrolidine Betaine Hydrochloride by X-Ray Diffraction and Ab Initio Calculations. <i>Journal of Chemical Research Synopses</i> , 1998, , 296-297.	0.3	6
42	Conformations of, and NHO hydrogen bond in, piperidine-1-valeric acid and its dihydrate. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1967-1971.	0.9	6
43	Disproportional proton tautomers of pipercolic acid and 2,6-dichloro-4-nitrophenol in a 2:3 complex. <i>Chemical Physics</i> , 2016, 477, 88-95.	0.9	6
44	Synthesis, spectroscopic and theoretical studies of (R/S)-piperidinium-3-carboxylic acid 2,6-dichloro-4-nitrophenolate. <i>Vibrational Spectroscopy</i> , 2016, 83, 46-56.	1.2	6
45	Three-component complex of piperidine-ethanol, p-hydroxybenzoic acid and water studied by X-ray, Raman, FTIR and DFT. <i>Vibrational Spectroscopy</i> , 2017, 92, 194-199.	1.2	6
46	Structure and FTIR spectra of 3 : 2 complexes of trimethylamine N-oxide and 4-dimethylamine-2,6-dimethylpyridine N-oxide with perchloric acid. <i>Journal of Molecular Structure</i> , 1996, 375, 197-206.	1.8	5
47	Spectroscopic, structural and theoretical investigation of bis(4-trimethylammoniumbenzoate) hydroiodide hydrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1149-1156.	2.0	5
48	Structures and hydrogen bonding in the 1:1 and 1:2 complexes of trimethylamine Nâ€“oxide with pentachlorophenol. <i>Journal of Molecular Structure</i> , 1999, 477, 49-60.	1.8	4
49	Structure, spectroscopy and DFT calculations of 1,2-di(3-hydroxymethylpyridinium)ethane dibromide. <i>Journal of Molecular Structure</i> , 2016, 1120, 341-350.	1.8	4
50	Tautomers of N -ethyl-3-oxopyridinium and its adduct with squaric acid studied by X-ray, Raman, FTIR, NMR and DFT methods. <i>Vibrational Spectroscopy</i> , 2017, 89, 102-112.	1.2	4
51	Conformational flexibility and pseudosymmetric aggregation in a betinium salt hydrate. <i>Structural Chemistry</i> , 2017, 28, 859-865.	1.0	4
52	Spectroscopic and theoretical studies of the H-bonded complex of quinuclidine with 2,6-dichloro-4-nitrophenol. <i>Vibrational Spectroscopy</i> , 2017, 93, 29-35.	1.2	4
53	Hydrogen-bonding aggregation of N-methylpyrrolidine betaine with p-hydroxybenzoic acid. <i>Journal of Molecular Structure</i> , 2020, 1206, 127695.	1.8	4
54	Crystal and molecular structure of 8-hydroxyquinoline betaine monohydrate studied by X-ray, FTIR, NMR and DFT. <i>Journal of Molecular Structure</i> , 2022, 1248, 131421.	1.8	4

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55	Interactions of pyridoxine (Vitamin B6) with squaric acid and water. Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1251, 131773.	1.8	4
56	Structure of 3-hydroxy-3-phenyl-pyrido[2,1-c][1,4]dihydrooxazinium bromide studied by X-ray, FTIR, <sup>1</sup> H, <sup>13</sup> C and <sup>15</sup> N NMR, and DFT methods. <i>Journal of Molecular Structure</i> , 2006, 792-793, 36-49.	1.8	3
57	THEORETICAL AND EXPERIMENTAL <sup>1</sup> H AND <sup>13</sup> C NMR SPECTRA OF 3-HYDROXYPYRIDINE, 3-METHOXYPYRIDINE, AND N-ETHYL-3-OXYPYRIDINIUM BETAINE*. <i>Computational Methods in Science and Technology</i> , 2004, 10, 47-56.	0.3	3
58	Rare stoichiometry of carboxylate-carboxylate benzbetaine complexes: in vitro versus in silico. <i>CrystEngComm</i> , 2015, 17, 4143-4149.	1.3	2
59	Effects of donor-acceptor groups on structural and spectroscopic properties of hydrogen-bonded complex of 2-(hydroxymethyl)-1-methyl-piperidine with p-hydroxybenzoic acid and water. <i>Vibrational Spectroscopy</i> , 2018, 96, 67-73.	1.2	2
60	Spectroscopic studies of the 1:1 adduct of N-methylmorpholinium-acetate with hydrobromic acid in the crystalline and gaseous state. <i>Vibrational Spectroscopy</i> , 2015, 80, 36-41.	1.2	1
61	Effect of alkyl chain length in 2-(quinuclidinium)-alkanocarboxylates on structures of their complexes with 2,6-dichloro-4-nitrophenol. <i>Journal of Molecular Structure</i> , 2019, 1180, 812-825.	1.8	0
62	Centrosymmetric and asymmetric dimers of 5-(quinolinium)-valeric acid bromide monohydrate in crystal field and in silico. <i>Journal of Molecular Structure</i> , 2020, 1222, 128912.	1.8	0
63	A new diastereomeric type of N-morpholino-spiro derivative. Structural, spectroscopic and computational studies. <i>Journal of Molecular Structure</i> , 2021, 1232, 130018.	1.8	0