MirosÅ‚aw Szafran

List of Publications by Year
in descending order

Version: 2024-02-01

63 papers	823 citations	516710 16 h-index	580821 25 g-index
63 all docs	63 docs citations	63 times ranked	451 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.	3.6	63
2	Electrostatic Interactions and Conformations of Zwitterionic Pyridinium Alkanoates. Journal of Organic Chemistry, 1998, 63, 2898-2908.	3.2	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.	3.6	48
4	Differences between the NÂ·HÂ·O and OÂ·HÂ·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.	3.6	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.	3.6	30
6	1H and13C NMR spectra of betaines, >N+(CH2)nCOOâ¯, and their hydrogen halides. Additivity rules for carbon-13 chemical shifts. Magnetic Resonance in Chemistry, 2000, 38, 43-50.	1.9	29
7	Structure and vibrational spectra of pyridine betaine hydrochloride. Journal of Molecular Structure, 1997, 436-437, 123-142.	3.6	28
8	Influence of Electrostatic Interactions on Complexes with Short OÂ·Â·Â·O Hydrogen Bonds in Basic Salts of Pyridine Betaines and Acid Salts of Ï‰â€Phenyloalkanocarboxylic Acids. Israel Journal of Chemistry, 1999, 39, 253-260.	2.3	26
9	Hydrogen bonding and proton localization in complexes of carboxybetaines with phenols and carboxylic acids. Journal of Molecular Structure, 1997, 404, 13-23.	3.6	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.	3.6	24
11	Crystal structure and vibrational spectrum of N-methylpiperidine betaine hexafluorosilicate. Journal of Molecular Structure, 2001, 598, 267-276.	3.6	24
12	Crystal and molecular structure of N -methylpiperidine betaine hydrobromide. Journal of Molecular Structure, 2002, 605, 319-324.	3.6	24
13	Calculation of the vibrational spectra of pyridine betaine. Journal of Molecular Structure, 1996, 381, 157-167.	3.6	21
14	Bis(N-methylpiperidine betaine) hydrobromide: crystal structure and hydrogen bonding. Journal of Molecular Structure, 2002, 615, 33-43.	3.6	20
15	NHâ‹¯O and OHâ‹¯O interactions of glycine derivatives with squaric acid. New Journal of Chemistry, 2014, 38, 3556-3568.	2.8	19
16	X-ray, FTIR,1H and13C NMR, PM3 and AM1 studies of (Nâ€”Hâ‹¯N)+and (Oâ€”Hâ‹¯O)â€“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.	2.2	16
18	Crystal and molecular structure of 3-(2-amino-pyridinium)-propionate monohydrate. Journal of Molecular Structure, 2006, 786, 25-32.	3.6	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. Vibrational Spectroscopy, 2016, 84, 92-100.	2.2	15
20	Crystal structure and vibrational spectra of the 1:1 and 1:2 complexes of pyridine betaine with pentachlorophenol. Journal of Molecular Structure, 1997, 436-437, 143-151.	3.6	14
21	Deprotonation of 1-(carbethoxyalkyl)pyridinium halides with strong N-bases. Journal of Physical Organic Chemistry, 1999, 12, 39-46.	1.9	14
22	Hydrogen bonds in 1:1 complex of piperidine-3-carboxylic acid with salicylic acid. Journal of Molecular Structure, 2009, 920, 68-74.	3.6	14
23	Comparison of low-barrier hydrogen bonds in acid salts of carboxylic acids and basic salts of betaines â€“ FTIR study. Journal of Molecular Structure, 1999, 484, 117-124.	3.6	13
24	FTIR studies of complexes of N-methylmorpholine betaine with phenols. Journal of Molecular Structure, 2002, 614, 189-194.	3.6	13
25	FT-IR, UVâ€”visible and X-ray studies of complexes of pyridine N-oxides with pentachlorophenol. Journal of Molecular Structure, 1995, 356, 169-182.	3.6	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. Journal of Molecular Structure, 2001, 598, 251-260.	3.6	10
27	Structural, spectroscopic and theoretical studies of dimethylphenyl betaine complex with two molecules of 2,6-dichloro-4-nitro-phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1216-1226.	3.9	10
28	Structural, vibrational and DFT studies of di-(pipecolinium acid) squarate. Vibrational Spectroscopy, 2017, 88, 106-116.	2.2	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. Journal of Molecular Structure, 1999, 484, 125-138.	3.6	9
30	Structural, spectroscopic, and theoretical studies of a very short OHO hydrogen bond in bis(4â€(Nâ€methylpiperidinium)â€butyrate) hydrobromide. Journal of Physical Organic Chemistry, 2009, 22, 356-361.	1.9	9
31	Structural, spectroscopic and computational studies of the 2:1 complex of nipecotic acid with squaric acid. Chemical Physics, 2014, 444, 7-14.	1.9	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-(CH3)2C5H3N+î—¸OH]2[SO2â^'4]. Journal of Molecular Structure, 1997, 416, 81-90.	3.6	8
33	Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. Vibrational Spectroscopy, 2015, 79, 16-23.	2.2	8
34	Structural and spectroscopic properties of piperidinium-4-carboxylic acid hydrogen squarate. Vibrational Spectroscopy, 2015, 81, 13-21.	2.2	8
35	Spectroscopic studies of the 1:1 complex of piperidine-4-carboxylic acid (isonipecotic acid) with 2,6-dichloro-4-nitrophenol. Vibrational Spectroscopy, 2016, 85, 35-42.	2.2	8
36	Structure, conformation and hydrogen bonding of some pyridiniumpropionate complexes. Journal of Molecular Structure, 1998, 448, 77-89.	3.6	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. Journal of Molecular Structure, 2001, 563-564, 555-564.	3.6	7
38	Experimental and theoretical studies of 4-hydroxy-1-methylpiperidinium perchlorate. Journal of Molecular Structure, 2008, 889, 344-351.	3.6	7
39	Cooperative hydrogen bond between piperidine-ethanol and 2,6-dichloro-4- nitrophenol. Journal of Molecular Structure, 2019, 1184, 468-478.	3.6	7
40	Formation of the homoconjugated cation (Nî—¸Oâ‹¯Hâ‹¯Oî—¸N)+ of N-dodecyl-N,N-dimethylamine oxide in carbon tetrachloride. Journal of Molecular Structure, 1990, 239, 1-11.	3.6	6
41	Conformational Analysis of N-Methylpyrrolidine Betaine Hydrochloride by X-Ray Diffraction and Ab Initio Calculations. Journal of Chemical Research Synopses, 1998, , 296-297.	0.3	6
42	Conformations of, and NHO hydrogen bond in, piperidine-1-valeric acid and its dihydrate. Journal of the Chemical Society Perkin Transactions II, 1999, , 1967-1971.	0.9	6
43	Disproportional proton tautomers of pipecolic acid and 2,6-dichloro-4-nitrophenol in a 2:3 complex. Chemical Physics, 2016, 477, 88-95.	1.9	6
44	Synthesis, spectroscopic and theoretical studies of (R/S)-piperidinium-3-carboxylic acid 2,6-dichloro-4-nitrophenolate. Vibrational Spectroscopy, 2016, 83, 46-56.	2.2	6
45	Three-component complex of piperidine-ethanol, p-hydroxybenzoic acid and water studied by X-ray, Raman, FTIR and DFT. Vibrational Spectroscopy, 2017, 92, 194-199.	2.2	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. Journal of Molecular Structure, 1996, 375, 197-206.	3.6	5
47	Spectroscopic, structural and theoretical investigation of bis(4-trimethylammoniumbenzoate) hydroiodide hydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1149-1156.	3.9	5
48	Structures and hydrogen bonding in the 1:1 and 1:2 complexes of trimethylamine Nâ€“oxide with pentachlorophenol. Journal of Molecular Structure, 1999, 477, 49-60.	3.6	4
49	Structure, spectroscopy and DFT calculations of 1,2-di(3-hydroxymethylpyridinium)ethane dibromide. Journal of Molecular Structure, 2016, 1120, 341-350.	3.6	4
50	Tautomers of N -ethyl-3-oxopyridinium and its adduct with squaric acid studied by X-ray, Raman, FTIR, NMR and DFT methods. Vibrational Spectroscopy, 2017, 89, 102-112.	2.2	4
51	Conformational flexibility and pseudosymmetric aggregation in a betainium salt hydrate. Structural Chemistry, 2017, 28, 859-865.	2.0	4
52	Spectroscopic and theoretical studies of the H-bonded complex of quinuclidine with 2,6-dichloro-4-nitrophenol. Vibrational Spectroscopy, 2017, 93, 29-35.	2.2	4
53	Hydrogen-bonding aggregation of N-methylpyrrolidine betaine with p-hydroxybenzoic acid. Journal of Molecular Structure, 2020, 1206, 127695.	3.6	4
54	Crystal and molecular structure of 8-hydroxyquinoline betaine monohydrate studied by X-ray, FTIR, NMR and DFT. Journal of Molecular Structure, 2022, 1248, 131421.	3.6	4

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55	Interactions of pyridoxine (Vitamin B6) with squaric acid and water. Experimental and theoretical studies. Journal of Molecular Structure, 2022, 1251, 131773.	3.6	4
56	Structure of 3-hydroxy-3-phenyl-pyrido[2,1-c][1,4]dihydrooxazinium bromide studied by X-ray, FTIR, 1H, 13C and 15N NMR, and DFT methods. Journal of Molecular Structure, 2006, 792-793, 36-49.	3.6	3
57	THEORETICAL AND EXPERIMENTAL 1H AND 13C NMR SPECTRA OF 3-HYDROXYPYRIDINE, 3-METHOXYPYRIDINE, AND N-ETHYL-3-OXYPYRIDINIUM BETAINE*. Computational Methods in Science and Technology, 2004, 10, 47-56.	0.3	3
58	Rare stoichiometry of carboxylâ€“carboxylate benzbetaine complexes: in vitro versus in silico. CrystEngComm, 2015, 17, 4143-4149.	2.6	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. Vibrational Spectroscopy, 2018, 96, 67-73.	2.2	2
60	Spectroscopic studies of the 1:1 adduct of N-methylmorpholinium-acetate with hydrobromic acid in the crystalline and gaseous state. Vibrational Spectroscopy, 2015, 80, 36-41.	2.2	1
61	Effect of alkyl chain length in 2-(quinuclidinium)-alkanocarboxylates on structures of their complexes with 2,6-dichloro-4-nitrophenol. Journal of Molecular Structure, 2019, 1180, 812-825.	3.6	0
62	Centrosymmetric and asymmetric dimers of 5-(quinolinium)-valeric acid bromide monohydrate in crystal field and in silico. Journal of Molecular Structure, 2020, 1222, 128912.	3.6	0
63	A new diastereomeric type of N-morpholino-spiro derivative. Structural, spectroscopic and computational studies. Journal of Molecular Structure, 2021, 1232, 130018.	3.6	0