

Zofia Dega-Szafran

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Electrostatic Interactions and Conformations of Zwitterionic Pyridinium Alkanoates. <i>Journal of Organic Chemistry</i> , 1998, 63, 2898-2908.	1.7	61
2	Strong hydrogen bonds in 1:1 and 2:1 complexes of pyridine betaine with strong acids. <i>Journal of Molecular Structure</i> , 1994, 322, 297-308.	1.8	48
3	Chlorine-35 nuclear quadrupole resonance and infrared spectroscopic studies of hydrogen bonding in complexes of dichloroacetic acid with nitrogen and oxygen bases: correlation of spectroscopic properties with proton affinity and aqueous pKa. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1279-1285.	2.9	45
4	X-ray, Fourier-transform infrared, ¹ H and ¹³ C nuclear magnetic resonance, and PM3 studies of (N ⁺ H ⁻) ⁺ and (O ⁻ H ⁻) ⁻ intramolecular hydrogen bonds in a complex of 1,8-bis(dimethylamino)naphthalene with maleic acid. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 2085-2094.	1.7	42
5	X-ray, FT-IR and PM3 studies of hydrogen bonds in complexes of some pyridines with trifluoroacetic acid. <i>Journal of Molecular Structure</i> , 1992, 270, 99-124.	1.8	33
6	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. <i>Journal of Molecular Structure</i> , 1996, 381, 107-125.	1.8	33
7	Integrated intensity of continuous absorption in infrared spectra of complexes with medium-strong and strong hydrogen bonds. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1987, 43, 1553-1559.	0.1	31
8	Molecular structures and hydrogen bonding in the 1 : 1 and 1 : 2 complexes of pyridine betaine with 2,6-dichloro-4-nitrophenol; an example of strongly coupled hydrogen bonds, O ⁻ -H ⁻ -O ⁻ → C ⁻ -O ⁻ -H ⁻ -O ⁻ . <i>Journal of Molecular Structure</i> , 1997, 416, 145-160.	1.8	30
9	Molecular structures and hydrogen bonding of 1:1 and 2:1 complexes of quinoline betaine with perchloric acid. <i>Journal of Molecular Structure</i> , 2002, 609, 19-28.	1.8	30
10	¹ H and ¹³ C NMR spectra of betaines, >N ⁺ (CH ₂) _n COO ⁻ , and their hydrogen halides. Additivity rules for carbon-13 chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2000, 38, 43-50.	1.1	29
11	Conformational analysis of N-methylpiperidine betaine studied by X-ray diffraction, FTIR spectroscopy and ab initio calculations. <i>Journal of Molecular Structure</i> , 1999, 478, 49-55.	1.8	28
12	Hydrogen bonding and proton localization in complexes of carboxybetaines with phenols and carboxylic acids. <i>Journal of Molecular Structure</i> , 1997, 404, 13-23.	1.8	25
13	Complexes of Carboxylic Acids with Pyridines and Pyridine N-Oxides. <i>Heterocycles</i> , 1994, 37, 627.	0.4	24
14	X-ray, phase transition, IR and Raman studies of the solid complex of bis(pyridine betaine)-sulphuric acid. <i>Journal of Molecular Structure</i> , 1997, 406, 127-135.	1.8	24
15	Crystal structure and vibrational spectrum of N-methylpiperidine betaine hexafluorosilicate. <i>Journal of Molecular Structure</i> , 2001, 598, 267-276.	1.8	24
16	Crystal and molecular structure of N-methylpiperidine betaine hydrobromide. <i>Journal of Molecular Structure</i> , 2002, 605, 319-324.	1.8	24
17	A critical review of the isotope effect in IR spectra. <i>Journal of Molecular Structure</i> , 1994, 321, 57-77.	1.8	23
18	Hydrogen bonds in 1:2 complexes of substituted pyridine N-oxides with pentachlorophenol. <i>Journal of Molecular Structure</i> , 1997, 404, 25-32.	1.8	21

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19	Bis(N-methylpiperidine betaine) hydrobromide: crystal structure and hydrogen bonding. <i>Journal of Molecular Structure</i> , 2002, 615, 33-43.	1.8	20
20	NH ⁻ O and OH ⁻ O interactions of glycine derivatives with squaric acid. <i>New Journal of Chemistry</i> , 2014, 38, 3556-3568.	1.4	19
21	X-ray, FTIR, 1H and 13C NMR, PM3 and AM1 studies of (N ⁺ H ⁻ N) ⁺ and (O ⁻ H ⁻ O) ⁻ hydrogen bonds in a complex of 1,8-diaminonaphthalene with maleic acid: proton cavity and basicity of proton sponges. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 87-92.	1.7	16
22	Synthesis, IR and NMR studies of zwitterionic N-(1-pyrrolidine)alkanocarboxylic acids and their N-methyl derivatives. <i>Journal of Molecular Structure</i> , 1997, 436-437, 107-121.	1.8	16
23	Molecular structure and vibrational spectrum of N-methylpyrrolidine betaine hydrogen chloride: experimental and DFT study. <i>Vibrational Spectroscopy</i> , 2000, 23, 1-11.	1.2	16
24	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
25	Collisionally activated dissociation of some pyridinium cations: Novel fragmentation pathways. <i>Organic Mass Spectrometry</i> , 1989, 24, 1017-1021.	1.3	14
26	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
27	Deprotonation of 1-(carbethoxyalkyl)pyridinium halides with strong N-bases. <i>Journal of Physical Organic Chemistry</i> , 1999, 12, 39-46.	0.9	14
28	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
29	Proton and carbon-13 NMR studies of 1-substituted pyridinium salts. <i>Magnetic Resonance in Chemistry</i> , 1989, 27, 1090-1093.	1.1	13
30	Evidence for a single minimum potential for hydrogen bonds of pyridine N-oxide complexes with dichloroacetic acid in dichloromethane. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1991, 47, 125-131.	0.1	13
31	FTIR studies of complexes of N-methylmorpholine betaine with phenols. <i>Journal of Molecular Structure</i> , 2002, 614, 189-194.	1.8	13
32	Calorimetric and molecular modeling studies of N-alkoxycarbonylmethyl-N-alkyl-piperidinium chlorides. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008, 318, 301-306.	2.3	12
33	Supramolecular structure of the 1:2 complex of 1,4-dimethylpiperazine mono-betaine with squaric acid. <i>Supramolecular Chemistry</i> , 2013, 25, 432-440.	1.5	12
34	Synthesis and Antimicrobial Activities of some Quaternary Morpholinium Chlorides. <i>Polish Journal of Microbiology</i> , 2010, 59, 49-53.	0.6	12
35	FT-IR, UV-visible 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
36	Conformational richness and multiple hydrogen bonds in salt co-crystal of N-methylpiperidine betaine with N-methylpiperidine betaine hexafluorosilicate. <i>Acta Crystallographica Section B: Structural Science</i> , 2008, 64, 483-490.	1.8	11

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37	Localization of the proton in complexes of trifluoroacetic acid with pyridine N-oxides in dichloromethane by second-derivative infrared spectroscopy. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1991, 87, 3825.	1.7	10
38	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
39	Stable Molecular Complex of Squaric Acid with 2-(Quinuclidinium)propionate. <i>Australian Journal of Chemistry</i> , 2013, 66, 836.	0.5	10
40	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
41	Structural, vibrational and DFT studies of di-(pipercolinium acid) squarate. <i>Vibrational Spectroscopy</i> , 2017, 88, 106-116.	1.2	10
42	Nitrogen-15 NMR studies of hydrogen bonding and proton transfer in complexes of pyridine N-oxides with dichloroacetic acid in CDCl ₃ . <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 746-750.	0.9	9
43	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
44	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
45	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
46	Ion cyclotron resonance mass spectrometric study of ion-molecule reactions in toluene-pyridine mixtures. <i>Organic Mass Spectrometry</i> , 1994, 29, 96-101.	1.3	8
47	X-Ray, FTIR and quantum chemical studies of short and asymmetric hydrogen bonds in bis(2,6-dimethylpyridine-N-oxide) sulphate [2,6-(CH ₃) ₂ C ₅ H ₃ N ₂ -OH] ₂ [SO ₄]. <i>Journal of Molecular Structure</i> , 1997, 416, 81-90.	1.8	8
48	Antimicrobial Activity of N-Alkoxy carbonylmethyl-N-alkyl-piperidinium Chlorides. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2004, 59, 782-786.	0.6	8
49	Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. <i>Vibrational Spectroscopy</i> , 2015, 79, 16-23.	1.2	8
50	Structural and spectroscopic properties of piperidinium-4-carboxylic acid hydrogen squarate. <i>Vibrational Spectroscopy</i> , 2015, 81, 13-21.	1.2	8
51	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
52	Collisionally activated dissociation of 2,4,6-triphenylpyridinium cations. <i>Organic Mass Spectrometry</i> , 1992, 27, 1317-1321.	1.3	7
53	Structure, conformation and hydrogen bonding of some pyridiniumpropionate complexes. <i>Journal of Molecular Structure</i> , 1998, 448, 77-89.	1.8	7
54	Mass Spectra of Iso-Cinchona- and Halogenated Cinchona Alkaloids. <i>European Journal of Mass Spectrometry</i> , 2000, 6, 347-355.	0.5	7

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55	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
56	Experimental and theoretical studies of 4-hydroxy-1-methylpiperidinium perchlorate. <i>Journal of Molecular Structure</i> , 2008, 889, 344-351.	1.8	7
57	Systematics in NH⁺â€“N-Bonded Monosalts of 4,4â€“Bipyridine (44â€“biPy) with Mineral Acids. <i>Crystal Growth and Design</i> , 2013, 13, 4378-4384.	1.4	7
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	Synthesis and characterization of 1-carbalkoxymethyl-4-hydroxy-1-methylpiperidinium chlorides. <i>Arkivoc</i> , 2007, 2007, 90-102.	0.3	5
67	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
68	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
69	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
70	Conformational flexibility and pseudosymmetric aggregation in a betainium salt hydrate. <i>Structural Chemistry</i> , 2017, 28, 859-865.	1.0	4
71	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
72	Hydrogen-bonding aggregation of N-methylpyrrolidine betaine with p-hydroxybenzoic acid. <i>Journal of Molecular Structure</i> , 2020, 1206, 127695.	1.8	4

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73	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
74	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
75	Spectroscopic studies of 1-piperidineacetic acid complexes with phenols. <i>Journal of Molecular Structure</i> , 2005, 744-747, 801-807.	1.8	3
76	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. <i>Journal of Molecular Structure</i> , 2006, 792-793, 36-49.	1.8	3
77	Rare stoichiometry of carboxylate-carboxylate benzbetaine complexes: in vitro versus in silico. <i>CrystEngComm</i> , 2015, 17, 4143-4149.	1.3	2
78	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
79	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
80	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
81	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