Anna Komasa

List of Publications by Year
in descending order

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59 papers	1,004 citations	759233 12 h-index	454955 30 g-index
59 all docs	59 docs citations	59 times ranked	898 citing authors

#	Article	IF	Citations
1	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
2	Interactions of pyridoxine (Vitamin B6) with squaric acid and water. Experimental and theoretical studies. Journal of Molecular Structure, 2022, 1251, 131773.	3.6	4
3	A new diastereomeric type of N-morpholino-spiro derivative. Structural, spectroscopic and computational studies. Journal of Molecular Structure, 2021, 1232, 130018.	3.6	0
4	Salts of purine alkaloids caffeine and theobromine with 2,6-dihydroxybenzoic acid as coformer: structural, theoretical, thermal and spectroscopic studies. Acta Crystallographica Section C, Structural Chemistry, 2021, 77, 713-724.	0.5	3
5	Hydrogen-bonding aggregation of N-methylpyrrolidine betaine with p-hydroxybenzoic acid. Journal of Molecular Structure, 2020, 1206, 127695.	3.6	4
6	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
7	Cooperative hydrogen bond between piperidine-ethanol and 2,6-dichloro-4- nitrophenol. Journal of Molecular Structure, 2019, 1184, 468-478.	3.6	7
8	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
9	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
10	Spectroscopic, structural and theoretical investigation of 1,3-bis(3-hydroxymethylpyridinium)propane dibromide, tetrabromozincate and tetrabromocuprate. Journal of Molecular Structure, 2018, 1163, 345-356.	3.6	2
11	Spectroscopic and DFT studies of bis-3-hydroxypyridinium and bis-3-hydroxymethylpyridinium dibromides with tetramethylene linker. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 456-468.	3.9	3
12	Synthesis, spectroscopic, theoretical and antifungal activity study of gemini 3-hydroxy- and 3-hydroxymethylpyridinium dibromides. Journal of Molecular Structure, 2018, 1171, 888-897.	3.6	0
13	Molecular structure and spectral properties of 4-(1-pyridinium)-butyrate dihydrate and its hydrobromide. Vibrational Spectroscopy, 2017, 88, 40-48.	2.2	4
14	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
15	Conformational flexibility and pseudosymmetric aggregation in a betainium salt hydrate. Structural Chemistry, 2017, 28, 859-865.	2.0	4
16	Structural, vibrational and DFT studies of di-(pipecolinium acid) squarate. Vibrational Spectroscopy, 2017, 88, 106-116.	2.2	10
17	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
18	Structure and hydrogen bonding in 5-(dimethylphenylammonium)-valeric acid bromide hydrate. Vibrational Spectroscopy, 2017, 92, 188-193.	2.2	2

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19	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
20	Structure, spectroscopy and DFT calculations of 1,2-di(3-hydroxymethylpyridinium)ethane dibromide. Journal of Molecular Structure, 2016, 1120, 341-350.	3.6	4
21	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
22	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
23	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
24	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
25	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
26	Rare stoichiometry of carboxylâ€“carboxylate benzbetaine complexes: in vitro versus in silico. CrystEngComm, 2015, 17, 4143-4149.	2.6	2
27	Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. Vibrational Spectroscopy, 2015, 79, 16-23.	2.2	8
28	Structural and spectroscopic properties of piperidinium-4-carboxylic acid hydrogen squarate. Vibrational Spectroscopy, 2015, 81, 13-21.	2.2	8
29	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
30	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
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	Spectroscopic and structural investigation of 2,5-dicarboxy-1-methylpyridinium inner salt. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 586-595.	3.9	1
33	Structure and conformation of 2,3-diethoxycarbonyl-1-methylpyridinium iodide studied by NMR, FTIR, Raman, X-ray diffraction and DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 208-218.	3.9	4
34	Supramolecular structure of the 1:2 complex of 1,4-dimethylpiperazine mono-betaine with squaric acid. Supramolecular Chemistry, 2013, 25, 432-440.	1.2	12
35	Structure of methyl 3-(trimethylammonium)benzoate iodide studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra. Journal of Molecular Structure, 2012, 1017, 115-122.	3.6	6
36	Structure of methyl 4-(trimethylammonium)benzoate iodide studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra. Journal of Molecular Structure, 2011, 1006, 330-336.	3.6	6

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37	Structure of 3,4-dicarboxy-1-methylpyridinium inner salt studied by X-ray diffraction, DFT calculations, FTIR, Raman and NMR spectra. Journal of Molecular Structure, 2011, 994, 216-222.	3.6	10
38	Structure and spectroscopic properties of bis(1-carboxyethyl-3-aminopyridinium) hydrobromide monohydrate. Journal of Molecular Structure, 2011, 994, 13-20.	3.6	7
39	Structure of 6-hydroxy-1-methylquinolinium chloride hydrate studied by X-ray, DFT calculations, FTIR and NMR spectroscopes. Journal of Molecular Structure, 2010, 984, 359-370.	3.6	7
40	Structural, spectroscopic and theoretical studies of short OHO hydrogen bonds in 2:1 complexes of 1-methyl-6-oxyquinolinium betaine with mineral acids. Journal of Molecular Structure, 2010, 984, 326-331.	3.6	0
41	Electronic structure and spectral properties of selected trimethyl-alloxazines: Combined experimental and DFT study. Chemical Physics, 2009, 361, 83-93.	1.9	9
42	Molecular structure of 1,3-bis(carboxymethyl)imidazolium bromide and its betaine form in crystal. Journal of Molecular Structure, 2008, 876, 170-176.	3.6	19
43	DFT, FTIR, Raman and NMR study of 1-methyl-8-oxyquinolinium betaine. Journal of Molecular Structure, 2008, 887, 20-33.	3.6	7
44	Molecular structure, hydrogen bonding and spectroscopic properties of the complex of piperidine-4-carboxylic acid with chloroacetic acid. Journal of Molecular Structure, 2008, 889, 112-118.	3.6	9
45	Crystal and molecular structure of 4-carboxypiperidinium chloride (4-piperidinecarboxylic acid) Tj ETQq1 1 0.784314 rgBT /Overlock 10	3.6	419
46	Molecular structure, hydrogen bonding, basicity and spectroscopic properties of 3-hydroxypyridine betaine hydrochloride monohydrate. Journal of Molecular Structure, 2007, 832, 63-72.	3.6	5
47	New photochemically stable riboflavin analogueâ€"3-Methyl-riboflavin tetraacetate. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 186, 14-23.	3.9	20
48	Spectroscopy and photophysics of flavin-related compounds: 5-deaza-riboflavin. Journal of Molecular Structure, 2006, 783, 184-190.	3.6	29
49	Molecular structure of 8-hydroxy-1-methylquinolinium iodide hydrate in crystal and solution. Journal of Molecular Structure, 2006, 791, 106-110.	3.6	12
50	X-ray and spectroscopic studies of the molecular structure of bis(8-oxy-1-methylquinolinium) hydroiodide. Journal of Molecular Structure, 2006, 800, 135-139.	3.6	9
51	Spectroscopy and photophysics of flavin-related compounds: 3-ethyl-lumiflavin. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 170, 267-272.	3.9	14
52	Spectroscopy and photophysics of flavin related compounds: Riboflavin and iso-(6,7)-riboflavin. Chemical Physics, 2005, 314, 239-247.	1.9	72
53	Spectroscopy and photophysics of flavin-related compounds: 3-benzyl-lumiflavin. Photochemical and Photobiological Sciences, 2005, 4, 463.	2.9	25
54	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

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55	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
56	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, Oî—¸Hâ‹¯Oî—»Cî—¸Oî—¸Hâ‹¯Oâ˜’. Journal of Molecular Structure, 1997, 416, 145-160.	3.6	30
57	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
58	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
59	UV, 1H and 13C NMR spectra, and AM1 studies of protonation of aminopyridines. Journal of Molecular Structure, 1994, 322, 223-232.	3.6	55