Silvia BrandÃ¡n

List of Publications by Year
in descending order

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40	948	361045	476904
papers	citations	20	29
		h-index	g-index

40	40	40	863
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A complete characterization of the vibrational spectra of sucrose. Carbohydrate Research, 2012, 361, 212-218.	1.1	91
2	Structural and spectroscopic study of a pectin isolated from citrus peel by using FTIR and FT-Raman spectra and DFT calculations. Infrared Physics and Technology, 2016, 76, 315-327.	1.3	70
3	Experimental FTIR and FT-Raman and theoretical studies on the molecular structures of monomer and dimer of 3-thiopheneacrylic acid. Journal of Molecular Structure, 2017, 1135, 209-221.	1.8	57
4	Synthesis and characterization of p -xylylenediaminium bis(nitrate). Effects of the coordination modes of nitrate groups on their structural and vibrational properties. Journal of Molecular Structure, 2018, 1151, 152-168.	1.8	52
5	FT-IR, FT-Raman, UVâ€“Vis, NMR and structural studies of carquejyl acetate, a distinctive component of the essential oil from Baccharis trimera (less.) DC. (Asteraceae). Journal of Molecular Structure, 2019, 1177, 499-510.	1.8	52
6	An experimental and theoretical study of l-tryptophan in an aqueous solution, combining two-layered ONIOM and SCRF calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 162-170.	2.0	42
7	Synthesis, crystal structure, spectroscopic studies, NBO, AIM and SQMFF calculations of new pyridazinone derivative. Journal of Molecular Structure, 2021, 1223, 129213.	1.8	42
8	Analysis of the structure and the FT-IR and Raman spectra of 2-(4-nitrophenyl)-4H-3,1-benzoxazin-4-one. Comparisons with the chlorinated and methylated derivatives. Journal of Molecular Structure, 2017, 1140, 2-11.	1.8	35
9	Structural and vibrational characterization of anhydrous and dihydrated species of trehalose based on the FTIR and FTRaman spectra and DFT calculations. Journal of King Saud University - Science, 2018, 30, 229-249.	1.6	34
10	An experimental study of the structural and vibrational properties of sesquiterpene lactone cnicin using FT-IR, FT-Raman, UVâ€“visible and NMR spectroscopies. Journal of Molecular Structure, 2014, 1065-1066, 160-169.	1.8	33
11	Structural, FT-IR, FT-Raman and ECD studies on the free base, cationic and hydrobromide species of scopolamine alkaloid. Journal of Molecular Structure, 2019, 1180, 603-617.	1.8	29
12	Structural and vibrational studies of the potential anticancer agent, 5-difluoromethyl-1,3,4-thiadiazole-2-amino by DFT calculations. Computational and Theoretical Chemistry, 2013, 1011, 57-64.	1.1	27
13	A structural and vibrational investigation on the antiviral deoxyribonucleoside thymidine agent in gas and aqueous solution phases. International Journal of Quantum Chemistry, 2014, 114, 209-221.	1.0	26
14	A structural and spectroscopic study on carquejol, a relevant constituent of the medicinal plant Baccharis trimera (Less.) DC. (Asteraceae). Journal of Molecular Structure, 2017, 1150, 8-20.	1.8	26
15	Spectroscopic and structural investigation on intermediates species structurally associated to the tricyclic bisguanidine compound and to the toxic agent, saxitoxin. Journal of Molecular Structure, 2016, 1119, 25-38.	1.8	24
16	Structural, electronic, topological and vibrational properties of a series of N-benzylamides derived from Maca (Lepidium meyenii) combining spectroscopic studies with ONION calculations. Journal of Molecular Structure, 2016, 1105, 403-414.	1.8	24
17	A complete assignment of the vibrational spectra of sucrose in aqueous medium based on the SQM methodology and SCRF calculations. Carbohydrate Research, 2014, 388, 112-124.	1.1	23
18	Structural and vibrational study on zwitterions of l-threonine in aqueous phase using the FT-Raman and SCRF calculations. Journal of Molecular Structure, 2013, 1045, 171-179.	1.8	22

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19	Bidentate cation-anion coordination in the ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate supported by vibrational spectra and NBO, AIM and SQMFF calculations. Journal of Molecular Structure, 2020, 1212, 128104.	1.8	22
20	Synthesis, NMR, Raman, thermal and nonlinear optical properties of dicationic ionic liquids from experimental and theoretical studies. Journal of Molecular Structure, 2020, 1220, 128713.	1.8	20
21	Spectroscopic and structural studies on lactose species in aqueous solution combining the HATR and Raman spectra with SCRF calculations. Carbohydrate Research, 2015, 407, 34-41.	1.1	17
22	Effect of the side chain on the properties from cidofovir to brincidofovir, an experimental antiviral drug against to Ebola virus disease. Arabian Journal of Chemistry, 2019, 12, 2959-2972.	2.3	17
23	Evaluation of the structural, electronic, topological and vibrational properties of N-(3,4-dimethoxybenzyl)-hexadecanamide isolated from Maca (Lepidium meyenii) using different spectroscopic techniques. Journal of Molecular Structure, 2017, 1128, 653-664.	1.8	16
24	Stabilities of aqueous solutions of sucrose containing ascorbic and citric acids by using FTIR spectroscopy and physicochemical studies. Journal of Molecular Liquids, 2014, 200, 448-459.	2.3	14
25	S(-) and R(+) species derived from antihistaminic promethazine agent: structural and vibrational studies. Heliyon, 2019, 5, e02322.	1.4	13
26	Structural study and vibrational spectra of 3-amino-2-(4-chlorophenyl) quinazolin-4(3H)-one. Computational and Theoretical Chemistry, 2012, 995, 43-48.	1.1	12
27	A complete assignment of the vibrational spectra of 2-furoic acid based on the structures of the more stable monomer and dimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 623-631.	2.0	11
28	Structural and spectroscopic differences among the potassium 5-hydroxypentanoyltrifluoroborate salt and the furoyl and isonicotinoyl salts. Journal of Molecular Structure, 2019, 1176, 718-728.	1.8	11
29	Normal internal coordinates, force fields, and vibrational study of species derived from antiviral adamantadine. International Journal of Quantum Chemistry, 2021, 121, e26425.	1.0	11
30	Molecular structure of 4-hidroxy-3-(3-methyl-2-butenyl) acetophenone, a plant antifungal, by X-ray diffraction, DFT calculation, and NMR and FTIR spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 196-203.	2.0	10
31	FTIR, HATR and FT-Raman studies on the anhydrous and monohydrate species of maltose in aqueous solution. Carbohydrate Research, 2016, 428, 41-56.	1.1	10
32	Evaluating structures, properties and vibrational and electronic spectra of the potassium 2-isonicotinoyltrifluoroborate salt. Journal of Molecular Structure, 2018, 1163, 41-53.	1.8	10
33	Crystal structure, computational study, optical and vibrational properties of a new luminescent material based on bismuth(III): (C10H28N4)[Bi2Cl10]. Journal of Solid State Chemistry, 2021, 303, 122485.	1.4	10
34	Vibrational and structural study of onopordopicrin based on the FTIR spectrum and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 381-389.	2.0	7
35	Experimental and DFT studies on structure, spectroscopic and thermal properties of N-Methyl-N,N,N-trioctylammonium chloride ionic liquid. Journal of Molecular Structure, 2021, 1230, 129625.	1.8	6
36	Structural And Vibrational Studies on Isomers of Antiviral Ribavirin Drug in Gas and Aqueous Environmental by Using The SQM Approach. Journal of Advances in Chemistry, 0, 16, 6325-6353.	0.1	6

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37	Behaviours of antiviral Oseltamivir in different media: DFT and SQMFF calculations. Journal of Molecular Modeling, 2021, 27, 357.	0.8	6
38	Experimental isolation and spectroscopic characterization of squamocin acetogenin combining FT-IR, FT-Raman and UVâ€“Vis spectra with DFT calculations. Journal of Molecular Structure, 2020, 1219, 128610.	1.8	5
39	Structure and absolute configuration of parodiolide, a new dimeric sesquiterpene lactone isolated from Mikania parodii Cabrera possessing an uncommon spiro connexion. Journal of Molecular Structure, 2022, 1253, 132270.	1.8	3
40	Exploring properties of potassium 6-X-2-isonicotinoyltrifluoroborate (X=H, F, Cl, Br) salts and their anions by using ab initio calculations. Journal of Molecular Modeling, 2019, 25, 348.	0.8	2