

Aida Ben Altabef

List of Publications by Year in descending order

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72

papers

891

citations

471509

17

h-index

580821

25

g-index

72

all docs

72

docs citations

72

times ranked

709

citing authors

#	ARTICLE	IF	CITATIONS
1	Ab-initio and DFT calculations on molecular structure, NBO, HOMOâ€“LUMO study and a new vibrational analysis of 4-(Dimethylamino) Benzaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 635-643.	3.9	63
2	Synthesis and vibrational analysis of Nâ€“(2â€“furyl)imidazole. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 1004-1010.	2.5	40
3	The force constants in the isoelectronic series CF 3 SO 2 X (X=F, OH, NH 2 , CH 3): a study based on DFT calculations and experimental data. <i>Journal of Molecular Structure</i> , 2002, 612, 1-11.	3.6	37
4	Exploring weak intermolecular interactions in thiocyanate-bonded Zn(<i><scp>ii</scp></i>) and Cd(<i><scp>ii</scp></i>) complexes with methylimidazole: crystal structures, Hirshfeld surface analysis and luminescence properties. <i>RSC Advances</i> , 2018, 8, 23891-23902.	3.6	36
5	Structural and vibrational study of 2â€“(2â€“furyl)â€“H <i>< /i></i> imidazole. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 1086-1097.	1.9	34
6	Theoretical and experimental study of the vibrational spectra of 1,5-dimethylcytosine. <i>Vibrational Spectroscopy</i> , 2008, 46, 89-99.	2.2	29
7	Gas Phase Structure of Methyl Trifluoromethanesulfonate, CH3OSO2CF3, and Conformational Properties of Covalent Sulfonates. <i>Inorganic Chemistry</i> , 1999, 38, 3051-3055.	4.0	26
8	New coordination polymers based on 2-methylimidazole and transition metal nitroprusside containing building blocks: synthesis, structure and magnetic properties. <i>New Journal of Chemistry</i> , 2018, 42, 1347-1355.	2.8	26
9	Structural and vibrational study of 2â€“(2â€“furyl)â€“4,5â€“H <i>< /i></i> dihydroimidazole. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 1166-1177.	1.9	25
10	Biofilm inhibition by a new Mn(II) complex with sulfamethoxazole: Synthesis, spectroscopic characterization and crystal structure. <i>Inorganica Chimica Acta</i> , 2015, 436, 16-22.	2.4	25
11	Supramolecular architectures in luminescent Zn(II) and Cd(II) complexes containing imidazole derivatives: Crystal structures, vibrational and thermal properties, Hirshfeld surface analysis and electrostatic potentials. <i>Journal of Molecular Structure</i> , 2017, 1134, 492-503.	3.6	25
12	Infrared and Raman spectra of ethyl trifluoromethanesulfonate, CF3SO2OCH2CH3. An experimental and theoretical study. <i>Journal of Raman Spectroscopy</i> , 2005, 36, 427-434.	2.5	24
13	Structural and vibrational study of 4-(2â€“furyl)-1-methylimidazole. <i>Journal of Molecular Structure</i> , 2009, 924-926, 322-331.	3.6	23
14	Gas-Phase Structure and Vibrational Properties of Trifluoromethyl Trifluoromethanesulfonate, CF3SO2OCF3. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1381-1389.	2.0	22
15	Experimental and theoretical structure and vibrational analysis of ethyl trifluoroacetate, CF ₃ CO ₂ CH ₂ CH ₂ CH ₃ . <i>Journal of Raman Spectroscopy</i> , 2010, 41, 1357-1368.	2.5	21
16	Experimental and theoretical vibrational study of 2,2,2-trifluoroethyl trifluoromethanesulfonate, CF3SO2OCH2CF3. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 611-619.	3.9	19
17	Molecular view of the interaction of S-methyl methanethiosulfonate with DPPC bilayer. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 38-46.	2.6	18
18	FTIR and Raman analysis of <i><scp>l</scp></i> -cysteine ethyl ester HCl interaction with dipalmitoylphosphatidylcholine in anhydrous and hydrated states. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 369-376.	2.5	17

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19	Theoretical study of the structure and vibrational spectra of VO ₂ X ₂ ⁺ (X=F, Cl, Br, I) anions. Computational and Theoretical Chemistry, 2003, 626, 101-111.	1.5	15
20	Structural, vibrational spectra and normal coordinate analysis for two tautomers of 4(5)-furylimidazole. Journal of Raman Spectroscopy, 2010, 41, 587-597.	2.5	15
21	Experimental and theoretical studies of the vibrations and structure of 2,2,2-trifluoroethyl trifluoroacetate, CF ₃ CO ₂ CH ₂ CF ₃ . Journal of Molecular Structure, 2009, 917, 183-192.	3.6	15
22	A conformational and vibrational study of CF ₃ COSCH ₂ CH ₃ . Journal of Chemical Physics, 2009, 131, 214303.	3.0	15
23	Reorganization of Hydration Water of DPPC Multilamellar Vesicles Induced by l-Cysteine Interaction. Journal of Physical Chemistry B, 2018, 122, 5193-5204.	2.6	15
24	Structural and vibrational theoretical analysis of the vanadium oxotrihalides, VO _X 3 (X=F, Cl, Br, I). Computational and Theoretical Chemistry, 2004, 672, 45-50.	1.5	14
25	Gas-Phase Structure, Rotational Barrier, and Vibrational Properties of Methyl Methanethiosulfonate, CH ₃ SO ₂ SCH ₃ : An Experimental and Computational Study. Journal of Physical Chemistry A, 2007, 111, 9952-9960.	2.5	14
26	DFT calculation of the chromyl nitrate, CrO ₂ (NO ₃) ₂ . Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 1027-1043.	3.9	13
27	Vibrational and electronic spectra of vanadyl nitrate, VO(NO ₃) ₃ . Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 669-675.	3.9	12
28	Theoretical Structure and Vibrational Analysis of Ethyl Methanesulfonate, CH ₃ SO ₂ OCH ₂ CH ₃ . Journal of Physical Chemistry A, 2005, 109, 7946-7956.	2.5	12
29	Electronic and Fourier transform infrared and Raman spectra of chromyl nitrate, CrO ₂ (NO ₃) ₂ . Vibrational Spectroscopy, 1993, 5, 219-225.	2.2	11
30	A new vibrational study of chromyl fluorosulfate, CrO ₂ (SO ₃ F) ₂ by DFT calculations. Journal of Molecular Structure, 2010, 981, 146-152.	3.6	11
31	A detailed exploration of intermolecular interactions in 4-(4-dimethylaminobenzylideneamino)-N-(5-methyl-3-isoxazolyl)benzenesulfonamide and related Schiff bases: Crystal structure, spectral studies, DFT methods, Pixel energies and Hirshfeld surface analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 286-297.	3.9	11
32	Experimental and Theoretical Vibrational Study of the Oxotetrachlorochromate(V) Anion in [AsPh ₄][CrOCl ₄]. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2495-2499.	1.2	10
33	Gas-phase structure and new vibrational study of methyl trifluoroacetate (CF ₃ C(O)OCH ₃). Journal of Raman Spectroscopy, 2009, 40, 2053-2062.	2.5	10
34	Synthesis, crystal structure, conformational and vibrational properties of 6-acetyl-2,2-dimethyl-chromane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 74-84.	3.9	10
35	Interaction of N-acetylcysteine with DPPC liposomes at different pH: a physicochemical study. New Journal of Chemistry, 2020, 44, 14837-14848.	2.8	10
36	Theoretical structural and experimental vibrational study of niobyl nitrate. Journal of Molecular Structure, 2011, 994, 202-208.	3.6	9

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37	Molecular view of the structural reorganization of water in DPPC multilamellar membranes induced by l-cysteine methyl ester. <i>Journal of Molecular Structure</i> , 2018, 1156, 360-368.	3.6	9
38	Infrared and Raman spectra and quantum chemistry calculations for 2,2,2-trifluoroethyl trichloromethanesulfonate, $\text{CCl}_3\text{SO}_2\text{OCH}_2\text{CF}_3$. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 1011-1019.	3.9	8
39	Layered crystal structure, conformational and vibrational properties of 2,2,2-trichloroethoxysulfonamide: An experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 122-131.	3.9	8
40	DFT calculations of structure and vibrational properties of 2,2,2-trichloroethylacetate, $\text{CH}_3\text{CO}_2\text{CH}_2\text{CCl}_3$. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 123, 290-297.	3.9	8
41	Theoretical study on the molecular structure and vibrational properties, NBO and HOMO-LUMO analysis of the POX3 ($X=\text{F, Cl, Br, I}$) series of molecules. <i>Journal of Molecular Structure</i> , 2015, 1081, 536-542.	3.6	8
42	Interaction of cysteine and its derivatives with monolayers of dipalmitoylphosphatidylcholine. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019, 184, 110548.	5.0	8
43	DFT Calculations of the Molecular Force Field of Vanadyl Nitrate, $\text{VO}(\text{NO}_3)_3$. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2009, 635, 582-592.	1.2	7
44	Interaction of S-methyl methanethiosulfonate with DPPC bilayer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 479-489.	3.9	7
45	Synthesis and vibrational properties of trifluoromethyl trifluoromethanethiosulfonate and comparison with covalent sulfonates. <i>Vibrational Spectroscopy</i> , 2012, 59, 40-46.	2.2	7
46	Vibrational and Structural Behavior of $\text{l-Cysteine Ethyl Ester Hydrochloride}$ in the Solid State and in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14243-14252.	2.5	7
47	Synthesis, characterization and crystal structure of 2-chloroethyl(methylsulfonyl)methanesulfonate. <i>New Journal of Chemistry</i> , 2018, 42, 11073-11084.	2.8	7
48	A quantum chemical guided interpretation of the infrared and Raman spectra of trimethylsilyl trifluoromethanesulfonate, $\text{CF}_3\text{SO}_2\text{OSi}(\text{CH}_3)_3$. <i>Journal of Molecular Structure</i> , 2000, 553, 255-266.	3.6	6
49	Conformational and Vibrational Analysis of Methyl Methanesulfonate, $\text{CH}_3\text{SO}_2\text{OCH}_3$. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8401-8408.	2.5	6
50	Bis (trifluoromethyl) sulfone, $\text{CF}_3\text{SO}_2\text{CF}_3$: Synthesis, vibrational and conformational properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 332-339.	3.9	6
51	Vibrational spectroscopy and conformation of S-ethyl thioacetate: $\text{CH}_3\text{COSCH}_2\text{CH}_3$ and comparison with C(O)S and C(O)O compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 907-914.	3.9	6
52	Synthesis, spectroscopic and structural properties of $\text{CF}_3\text{SO}_2\text{OCCl}_3$. <i>Vibrational Spectroscopy</i> , 2011, 55, 153-159.	2.2	5
53	Trimethylsilyl trichloroacetate vibrational, structural and electronic properties and their comparison with related acetates. <i>Vibrational Spectroscopy</i> , 2013, 65, 124-131.	2.2	5
54	Gas-phase structure of 2,2,2-trichloroethyl chloroformate studied by electron diffraction and quantum-chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 393-402.	2.8	5

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55	Layered Crystal Structure and Vibrational Spectra of Sodium Trichloromethanesulfonate “ An Experimental and Theoretical Study. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 1501-1507.	1.2	4
56	Vibrational studies (FTIR and Raman), conformational analysis, NBO, HOMO-LUMO and reactivity descriptors of S-methyl thiobutanoate, $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{SCH}_3$. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 408-418.	3.9	4
57	Theoretical and experimental study of a new thiosulfonate derivative: Methyl trifluoromethanethiosulfonate, $\text{CF}_3\text{SO}_2\text{SCH}_3$. Conformational transferability in $\text{CX}_3\text{SO}_2\text{S-R}$ compounds. Inorganica Chimica Acta, 2017, 455, 254-261.	2.4	4
58	Experimental study of the vibrational spectra of $(\text{CH}_{3\text{sub}}3)_{3\text{sub}}\text{GeBr}$ supported by DFT calculations. Journal of Raman Spectroscopy, 2009, 40, 289-296.	2.5	3
59	Characterization of interactions of eggPC lipid structures with different biomolecules. Chemistry and Physics of Lipids, 2018, 210, 60-69.	3.2	3
60	A Raman, SERS and UV-circular dichroism spectroscopic study of N-acetyl-l-cysteine in aqueous solutions. New Journal of Chemistry, 2019, 43, 15201-15212.	2.8	3
61	A first exploration of isostructurality in transition metal nitroprussides: X-ray analysis, magnetic properties and DFT calculations. CrystEngComm, 2021, 23, 1158-1171.	2.6	3
62	Scaled Quantum Mechanical Force Fields for the CF_3SX Molecules (X = H, F, Cl, Br, I). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2007, 633, 1500-1505.	1.2	2
63	Study of the vibrational spectra of $(\text{CH}_{3\text{sub}}3)_{3\text{sub}}\text{GeCl}$ from experimental and DFT calculations. Journal of Raman Spectroscopy, 2009, 40, 1591-1598.	2.5	2
64	Gas-phase structure, rotational barrier and vibrational properties of trimethylsilyl trifluoroacetate $\text{CF}_3\text{C}(\text{O})\text{OSi}(\text{CH}_3)_3$: An experimental and computational study. Journal of Molecular Structure, 2010, 978, 114-123.	3.6	2
65	Interactions of valproic acid with lipid membranes of 1,2-dimyristoyl-sn-glycero-3-phosphocholine. Chemistry and Physics of Lipids, 2019, 218, 125-135.	3.2	2
66	Investigation of the gas-phase structure and rotational barrier of trimethylsilyl trifluoromethanesulfonate and comparison with covalent sulfonates. Journal of Molecular Structure, 2010, 984, 376-382.	3.6	1
67	Structure and bonding of 2,2,2-trichloroethylacetate: An experimental gas phase and computational study. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 1253-1260.	0.7	1
68	Experimental and quantum chemical studies on the molecular structure of 3,3,3-trifluoropropene-1-sulfonyl chloride: $\text{CF}_3\text{CH}_2\text{CH}_2\text{SO}_2\text{Cl}$. Journal of Molecular Structure, 2017, 1127, 377-385.	3.6	1
69	Novel “main-part” isostructuralism in metal complexes with 1-methylimidazole: crystal structures, energy calculations and magnetic properties. Dalton Transactions, 2021, 50, 17029-17040.	3.3	1
70	Structural and Vibrational Study of Chromyl Nitrate. Springer Briefs in Molecular Science, 2013, , 45-83.	0.1	0
71	Structural and Vibrational Study of Chromyl Fluorosulfate. Springer Briefs in Molecular Science, 2013, , 21-44.	0.1	0
72	Structural, spectroscopic and biological study of trifluoroethyl methansulfonate (methylsulfonyl), TFMSMS. Journal of Molecular Structure, 2022, , 133000.	3.6	0