Sayyed Faramarz Tayyari

List of Publications by Year
in descending order

106 papers	2,032 citations	257450 24 h-index	302126 39 g-index
111 all docs	111 docs citations	111 times ranked	1422 citing authors

#	Article	IF	Citations
1	Isomerism, molecular structure, and vibrational assignment of tris(triflouroacetylacetonato)iron(III): An experimental and theoretical study. Journal of Molecular Structure, 2022, 1248, 131347.	3.6	3
2	Optimized molecular geometry, vibrational analysis, and Fe-O bond strength of Tris(Î±-cyanoacetylacetonate)iron(III):An experimental and theoretical study. Journal of Molecular Structure, 2022, 1248, 131444.	3.6	4
3	Voltageâ€“current behavior of 4-phenylamino-3-penten-2-one and its derivatives molecular switch: a first-principles study. Molecular Simulation, 2021, 47, 730-737.	2.0	4
4	Theoretical investigation of solvent effect on the ketoâ€“enol tautomerization of pentane-2,4-dione and a comparison between experimental data and theoretical calculations. Canadian Journal of Chemistry, 2021, 99, 411-424.	1.1	5
5	Electronic transport behavior of 1-(Phenyldiazenyl)naphthalen-2-ol and its derivatives as optical molecular switches: A first-principles approach. Optik, 2021, 236, 166475.	2.9	8
6	Molecular structure, intramolecular hydrogen bond strength, vibrational assignment, and spectroscopic insight of 4-phenylamino-3-penten-2-one and its derivatives: A theoretical and experimental study. Journal of Molecular Liquids, 2021, 334, 116035.	4.9	6
7	Validation of potential energy distribution by VEDA in vibrational assignment some of Î²-diketones; comparison of theoretical predictions and experimental vibration shifts upon deutration. Journal of Molecular Graphics and Modelling, 2021, 107, 107976.	2.4	20
8	Conformations, molecular structure, and Nâ€“Hâ‹¯O hydrogen bond strength in 4-Alkylamino-3-penten-2-ones. Journal of Molecular Structure, 2020, 1203, 127440.	3.6	5
9	The nature of intramolecular hydrogen bond in Naphthazarin. Chemical Physics, 2020, 538, 110907.	1.9	4
10	Conformation, molecular structure, and vibrational assignment of bis(3,5-heptanedionato)copper(II). Journal of Molecular Structure, 2019, 1197, 443-449.	3.6	4
11	Quantum chemical study of the mechanism of the palladium-catalysed Câˆ’H acetoxylation of benzene. Progress in Reaction Kinetics and Mechanism, 2019, 44, 55-66.	2.1	0
12	Water-gas-shift reaction over nickel catalysts: DFT studies and kinetic modeling. Structural Chemistry, 2019, 30, 1843-1852.	2.0	14
13	Molecular structure and intramolecular hydrogen bond strength of 3-methyl-4-amino-3-penten-2-one and its N Me and N-Ph substitutions by experimental and theoretical methods. Journal of Molecular Structure, 2019, 1184, 233-245.	3.6	11
14	Molecular structure, spectroscopic studies, and copper oxygen bond strength of Î±-methyl and Î±-ethyl derivatives of copper (II) acetylacetonate; Experimental and theoretical approach. Journal of Molecular Structure, 2018, 1160, 107-116.	3.6	10
15	Normal coordinate analysis of pyridine and its C 2v 2 H-isotopomers. A new approach. Journal of Molecular Structure, 2018, 1151, 236-244.	3.6	4
16	Structure, isomerism, and vibrational assignment of aluminumtrifluoroacetylacetonate. An experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 15-22.	3.9	6
17	Vibrational spectra, normal coordinate analysis, and hydrogen bond investigation of pyridinium perchlorate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 558-565.	3.9	7
18	Application of Hammett equation to intramolecular hydrogen bond strength in para-substituted phenyl ring of trifluorobenzoylacetone and 1-aryl-1,3-diketone malonates. European Journal of Chemistry, 2018, 9, 213-221.	0.6	3

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19	Vibrational assignments, conformational analysis, and molecular structures of $$left[{ext{C}_{ext{n}} ext{mim}} ight]left[{ext{NTF}_{ext{2}} } ight]$$ C n mim NTF 2 (nÂ=Â2, 4, 6,) Tj ETQq1 1 0.784314 rgBT /Overlock Journal of the Iranian Chemical Society, 2017, 14, 1281-1300.	2.2	6
20	Low frequency vibrational spectra and the nature of metal-oxygen bond of alkaline earth metal acetylacetonates. Journal of Molecular Structure, 2017, 1150, 340-348.	3.6	8
21	Tautomerism, molecular structure, intramolecular hydrogen bond, and enol-enol equilibrium of para halo substituted 4,4,4-trifluoro-1-phenyl-1,3-butanedione; Experimental and theoretical studies. Journal of Molecular Structure, 2017, 1150, 427-437.	3.6	9
22	Correlation Between Parameters Related to Intramolecular Hydrogen Bond Strength and Hammett Constant in Para Substituted Benzoylacetone (A Theoretical and Experimental Study). Oriental Journal of Chemistry, 2017, 33, 2579-2590.	0.3	3
23	Vibrational spectra, normal coordinate analysis, and conformation of bis(É‘-cyanoacetylacetonato)Cu(II). Journal of Molecular Structure, 2016, 1118, 68-74.	3.6	3
24	Conformational stability, barriers to internal rotations, and normal coordinate analysis of acetone and its2H-isotopomers. Canadian Journal of Chemistry, 2016, 94, 818-826.	1.1	5
25	Intramolecular hydrogen bonding in 5-nitrosalicylaldehyde: IR spectrum and quantum chemical calculations. Journal of Molecular Structure, 2016, 1111, 185-192.	3.6	6
26	Vibrational assignments and structure of bis(3-amino-1- phenyl-2-buten-1-onato)copper(II) complex. Journal of Molecular Structure, 2016, 1111, 25-32.	3.6	5
27	Conformational analysis, structure, and normal coordinate analysis of vibrational spectra of hexafluoroacetone. A density functional theory study. Journal of Fluorine Chemistry, 2016, 184, 65-71.	1.7	10
28	Proton transfer in acetylacetone and its Î±-halo derivatives. Physical Chemistry Chemical Physics, 2016, 18, 344-350.	2.8	11
29	Normal coordinate analysis, hydrogen bonding, and conformation analysis of heptane-3,5-dione. Journal of Molecular Structure, 2016, 1103, 35-44.	3.6	5
30	Vibrational spectra of Î±-bromo and Î±-chloro derivatives of tris(acetylacetonato)chromium(III). Journal of Molecular Structure, 2016, 1103, 1-8.	3.6	6
31	X-ray diffraction and vibrational spectroscopic study of trans-bis(acetylacetonato)-bis(4-methylpyridine)cobalt(III). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 94-101.	3.9	6
32	Vibrational spectra of tris(acetylacetonato)chromium(III). Journal of Molecular Structure, 2015, 1099, 340-347.	3.6	11
33	Tautomerism, conformational analysis, and spectroscopy studies of 3-bromo-pentane-2,4-dione. Journal of Molecular Structure, 2015, 1094, 264-273.	3.6	10
34	Conformation, molecular structure, and vibrational assignment of bis(2,2,6,6-tetramethylheptane-3,5-dionato)copper(II). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1827-1833.	3.9	11
35	Theoretical and spectroscopic studies on molecular structure and hydrogen bonding of 2-trifluoroacetylphenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 820-827.	3.9	4
36	Hydrogen bond strength and vibrational assignment of the enol form of 3-(ortho-methoxyphenylthio) and 3-(para-methoxyphenylthio)pentane-2,4-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 731-742.	3.9	5

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37	Conformational analysis, intramolecular hydrogen bonding, and vibrational assignment of 4,4-dimethyl-1-phenylpentane-1,3-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 284-298.	3.9	17
38	Tautomerism in pyridazin-3(2H)-one: A theoretical study using implicit/explicit solvation models. Journal of Molecular Graphics and Modelling, 2014, 49, 47-54.	2.4	23
39	Theoretical study, and infrared and Raman spectra of copper(II) chelated complex with dibenzoylmethane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 272-279.	3.9	21
40	Structure and vibrational assignment of bis(benzoylacetonato)copper(II). Journal of Molecular Structure, 2014, 1058, 308-317.	3.6	28
41	Intramolecular hydrogen bonding and vibrational assignment of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. Journal of Molecular Structure, 2014, 1076, 262-271.	3.6	17
42	Molecular structure and intramolecular hydrogen bonding in 2-hydroxybenzophenones: A theoretical study. Journal of Chemical Sciences, 2014, 126, 919-929.	1.5	12
43	Very strong intramolecular hydrogen bonding of 1,2-dithenoylcyclopentadiene; DFT and spectroscopic studies. Journal of Molecular Structure, 2014, 1075, 85-95.	3.6	4
44	Vibrational assignment and structure of trinuclear oxo-centered of basic formate iron(III) and chromium(III) complexes: A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 287-294.	3.9	5
45	Investigation of simple and water assisted tautomerism in a derivative of 1,3,4-oxadiazole: A DFT study. Journal of Molecular Graphics and Modelling, 2013, 44, 120-128.	2.4	24
46	Theoretical and spectroscopic studies on molecular structure and hydrogen bonding of 1,2-bis (monochloroacetyl) cyclopentadiene. Journal of Molecular Structure, 2013, 1038, 177-187.	3.6	5
47	Structure, vibrational assignment, and NMR spectroscopy of 1,2-bis (dichloroacetyl) cyclopentadiene. Journal of Molecular Structure, 2013, 1036, 151-160.	3.6	7
48	Conformational analysis and vibrational assignment of bis-gem-diol of hexafluoroacetylacetone. Journal of Molecular Structure, 2013, 1041, 190-199.	3.6	7
49	Vibrational assignment and crystal structure of 3-amino-1-phenyl-2-buten-1-one. Journal of Molecular Structure, 2013, 1045, 20-28.	3.6	9
50	Structure and vibrational analysis of methyl 3-amino-2-butenoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 350-357.	3.9	18
51	Theoretical study of intramolecular hydrogen bonding in the halo derivatives of 1-amino-3-imino-prop-1-ene. Journal of Chemical Sciences, 2013, 125, 939-948.	1.5	23
52	Theoretical Study Intramolecular Hydrogen Bond in Acetylacetone 3- substituted Derivatives: NMR, NBO analysis and Thermo-chemical Investigation. Oriental Journal of Chemistry, 2013, 29, 1121-1128.	0.3	4
53	Conformation, molecular structure, and intramolecular hydrogen bonding of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. Journal of Molecular Structure, 2012, 1021, 102-111.	3.6	17
54	Methane storage in homogeneous armchair open-ended single-walled boron nitride nanotube triangular arrays: a grand canonical Monte Carlo simulation study. Journal of Molecular Modeling, 2012, 18, 2699-2708.	1.8	6

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55	Conformational analysis, tautomerization, IR, Raman, and NMR studies of ethyl benzoylacetate. Journal of Molecular Structure, 2012, 1015, 74-85.	3.6	10
56	Influence of temperature, pressure, nanotubeâ€™s diameter and intertube distance on methane adsorption in homogeneous armchair open-ended SWCNT triangular arrays. Theoretical Chemistry Accounts, 2011, 128, 231-240.	1.4	31
57	Water-gas-shift kinetics over a Fe/Cu/La/Si catalyst in Fischerâ€“Tropsch synthesis. Chemical Engineering Research and Design, 2011, 89, 262-269.	5.6	26
58	Molecular structure and vibrational assignments of bis(4-aminopent-3-en-2-onato)copper(II): A detailed density functional theoretical study. Journal of Molecular Structure, 2011, 985, 139-147.	3.6	22
59	Conformational analysis, tautomerization, IR, Raman, and NMR studies of benzyl acetoacetate. Journal of Molecular Structure, 2011, 987, 241-254.	3.6	10
60	Conformational stability, molecular structure, intramolecular hydrogen bonding, and vibrational spectra of 5,5-dimethylhexane-2,4-dione. Journal of Molecular Structure, 2011, 998, 99-109.	3.6	17
61	Structure and vibrational assignment of bis(4-amino-3-penten-2-onato)nickel(II). A density functional theoretical study. Journal of Molecular Structure, 2011, 997, 117-125.	3.6	6
62	Structure, intramolecular hydrogen bonding, and vibrational spectra of 2,2,6,6-tetramethyl-3,5-heptanedione. Journal of Molecular Structure, 2010, 970, 160-170.	3.6	19
63	Effect of nano-particle size on product distribution and kinetic parameters of Fe/Cu/La catalyst in Fischer-Tropsch synthesis. Journal of Natural Gas Chemistry, 2010, 19, 107-116.	1.8	36
64	Fischer-Tropsch synthesis by nano-structured iron catalyst. Journal of Natural Gas Chemistry, 2010, 19, 284-292.	1.8	62
65	Deactivation studies of nano-structured iron catalyst in Fischer-Tropsch synthesis. Journal of Natural Gas Chemistry, 2010, 19, 333-340.	1.8	29
66	Studies of carbonaceous species in alkali promoted iron catalysts during Fischerâ€“Tropsch synthesis. Journal of Industrial and Engineering Chemistry, 2010, 16, 1025-1032.	5.8	56
67	Deactivation studies of Fischerâ€“Tropsch synthesis on nano-structured iron catalyst. Journal of Molecular Catalysis A, 2010, 330, 112-120.	4.8	43
68	Water-gas-shift kinetic over nano-structured iron catalyst in Fischerâ€“Tropsch synthesis. Journal of Natural Gas Science and Engineering, 2010, 2, 79-85.	4.4	17
69	Vibrational assignment and proton tunneling in pyridineâ€“pyridinium complexes. Journal of Molecular Structure, 2010, 971, 39-46.	3.6	9
70	The nature of intramolecular hydrogen bond in 2-nitromalonaldehyde. Chemical Physics, 2010, 368, 62-65.	1.9	13
71	Conformational analysis, tautomerization, IR, Raman, and NMR studies of 3-phenylazo-2,4-pentanedione. Journal of Molecular Structure, 2009, 920, 301-309.	3.6	12
72	Conformation and vibrational spectra and assignment of 2-thenoyltrifluoroacetone. Journal of Molecular Structure, 2009, 932, 112-122.	3.6	31

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73	Structure and vibrational assignment of magnesium acetylacetonate: A density functional theoretical study. Journal of Molecular Structure, 2009, 938, 76-81.	3.6	47
74	Structure and vibrational assignment of beryllium acetylacetonate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 342-347.	3.9	14
75	Structure and vibrational assignment of 3-nitro-2,4-pentanedione: A density functional theoretical study. Journal of Molecular Structure, 2008, 892, 32-38.	3.6	15
76	Hydrogen bond strength and vibrational assignment of the enol form of 3-(methylthio)pentane-2,4-dione. Computational and Theoretical Chemistry, 2008, 854, 54-62.	1.5	10
77	Structure and vibrational assignment of the enol form of 3-chloro-pentane-2,4-dione. Journal of Molecular Structure, 2008, 873, 79-88.	3.6	19
78	Structure and vibrational assignment of the enol form of 1-chloro-1,1-difluoro-pentane-2,4-dione. Journal of Molecular Structure, 2008, 878, 10-21.	3.6	8
79	Study of interaction of spironolactone with hydroxypropyl-Î²-cyclodextrin in aqueous solution and in solid state. Journal of Molecular Structure, 2008, 878, 78-83.	3.6	23
80	Conformation, structure, intramolecular hydrogen bonding, and vibrational assignment of 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione. Journal of Molecular Structure, 2008, 882, 153-167.	3.6	12
81	Hydrogen bond strength and vibrational assignment of the enol form of 3-(phenylthio)pentane-2,4-dione. Journal of Molecular Structure, 2008, 889, 165-176.	3.6	10
82	Structure and vibrational assignment of 3,4-diacetyl-2,5-hexanedione. A density functional theoretical study. Journal of Molecular Structure, 2007, 827, 176-187.	3.6	39
83	Vibrational assignment and structure of dibenzoylmethane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 394-404.	3.9	57
84	Vibrational assignment and structure of trifluorobenzoylacetone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 626-636.	3.9	34
85	Intramolecular hydrogen bonding in 2-nitromalonaldehyde: Infrared spectrum and quantum chemical calculations. Journal of Molecular Structure, 2006, 782, 191-199.	3.6	24
86	Vibrational assignment and structure of benzoylacetone: A density functional theoretical study. Journal of Molecular Structure, 2006, 794, 204-214.	3.6	33
87	Structure and vibrational assignment of the enol form of 1,1,1-trifluoro-2,4-pentanedione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 387-396.	3.9	56
88	Spectroscopic study of 2,3-Bis(p-methoxybenzoyl)cyclopentadiene as potential iron(III)-chelating agent. Russian Journal of General Chemistry, 2006, 76, 753-756.	0.8	0
89	CONFORMATIONAL STABILITY, MOLECULAR STRUCTURE, AND INTRAMOLECULAR HYDROGEN BONDING OF THENOYLTRIFLUOROACETONE. Journal of Theoretical and Computational Chemistry, 2006, 05, 647-664.	1.8	11
90	A two-dimensional potential function for bent hydrogen bonded systems. II-6-hydroxy-2-formylfulvene. Computational and Theoretical Chemistry, 2005, 730, 17-21.	1.5	13

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91	Structural, Potential Surface and Vibrational Spectroscopy Studies of Hypophosphorous Acid in the Gas Phase and Chain Conformation. A Theoretical Study. Journal of the Korean Chemical Society, 2005, 49, 129-137.	0.2	6
92	o-Phenylenediamine as a New Catalyst in the Highly Regioselective Conversion of Epoxides to Halohydrins with Elemental Halogens. Monatshefte FÃ¼r Chemie, 2004, 135, 1101.	1.8	6
93	Fourier transform infrared and Raman spectra, vibrational assignment and density functional theory calculations of naphthazarin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 111-120.	3.9	27
94	Molecular structure and vibrational assignment of dimethyl oxaloacetate. Journal of Molecular Structure, 2004, 694, 91-104.	3.6	20
95	A two-dimensional double minimum potential function for bent hydrogen bonded systems. I-malonaldehyde. Computational and Theoretical Chemistry, 2003, 637, 171-181.	1.5	31
96	Structure and vibrational spectra of the enol form of hexafluoro-acetylacetone. A density functional theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1669-1679.	3.9	46
97	Vibrational assignment of 4-amino-3-penten-2-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1681-1695.	3.9	24
98	Vibrational assignment of aluminum(III) Trisâ€“acetylacetone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 2669-2682.	3.9	22
99	Vibrational assignment and structure of 4-amino-3-cyano-3-penten-2-one. Journal of Molecular Structure, 2002, 613, 195-208.	3.6	8
100	Vibrational assignment of Î±-cyanoacetylacetone. Vibrational Spectroscopy, 2001, 26, 187-199.	2.2	32
101	Molecular conformation and intramolecular hydrogen bonding in 4-amino-3-penten-2-one. Computational and Theoretical Chemistry, 2001, 541, 11-15.	1.5	22
102	Vibrational assignment of acetylacetone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2000, 56, 2679-2691.	3.9	156
103	On the reassignment of vibrational frequencies of malonaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 255-263.	3.9	61
104	Spectroscopic study of hydrogen bonding in the enol form of Î²-diketonesâ€”II. Symmetry of the hydrogen bond. Spectrochimica Acta Part A: Molecular Spectroscopy, 1979, 35, 1289-1295.	0.1	97
105	Spectroscopic study of hydrogen bonding in the enol form of Î²-diketonesâ€”I. Vibrational assignment and strength of the bond. Spectrochimica Acta Part A: Molecular Spectroscopy, 1979, 35, 1265-1276.	0.1	92
106	Conformational analysis, tautomerization, and vibrational spectra of methyl acetoacetate. Journal of the Iranian Chemical Society, 0, , 1.	2.2	0