

Sayyed Faramarz Tayyari

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/354856/publications.pdf>

Version: 2024-02-01

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	Vibrational assignment of acetylacetone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 2679-2691.	3.9	156
2	Spectroscopic study of hydrogen bonding in the enol form of β^2 -diketones ^{II} . Symmetry of the hydrogen bond. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1979, 35, 1289-1295.	0.1	97
3	Spectroscopic study of hydrogen bonding in the enol form of β^1 -diketones ^I . Vibrational assignment and strength of the bond. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1979, 35, 1265-1276.	0.1	92
4	Fischer-Tropsch synthesis by nano-structured iron catalyst. <i>Journal of Natural Gas Chemistry</i> , 2010, 19, 284-292.	1.8	62
5	On the reassignment of vibrational frequencies of malonaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 54, 255-263.	3.9	61
6	Vibrational assignment and structure of dibenzoylmethane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 394-404.	3.9	57
7	Structure and vibrational assignment of the enol form of 1,1,1-trifluoro-2,4-pentanedione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 387-396.	3.9	56
8	Studies of carbonaceous species in alkali promoted iron catalysts during Fischer-Tropsch synthesis. <i>Journal of Industrial and Engineering Chemistry</i> , 2010, 16, 1025-1032.	5.8	56
9	Structure and vibrational assignment of magnesium acetylacetonate: A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2009, 938, 76-81.	3.6	47
10	Structure and vibrational spectra of the enol form of hexafluoro-acetylacetone. A density functional theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 1669-1679.	3.9	46
11	Deactivation studies of Fischer-Tropsch synthesis on nano-structured iron catalyst. <i>Journal of Molecular Catalysis A</i> , 2010, 330, 112-120.	4.8	43
12	Structure and vibrational assignment of 3,4-diacetyl-2,5-hexanedione. A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2007, 827, 176-187.	3.6	39
13	Effect of nano-particle size on product distribution and kinetic parameters of Fe/Cu/La catalyst in Fischer-Tropsch synthesis. <i>Journal of Natural Gas Chemistry</i> , 2010, 19, 107-116.	1.8	36
14	Vibrational assignment and structure of trifluorobenzoylacetone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 626-636.	3.9	34
15	Vibrational assignment and structure of benzoylacetone: A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2006, 794, 204-214.	3.6	33
16	Vibrational assignment of β^1 -cyanoacetylacetone. <i>Vibrational Spectroscopy</i> , 2001, 26, 187-199.	2.2	32
17	A two-dimensional double minimum potential function for bent hydrogen bonded systems. l-malonaldehyde. <i>Computational and Theoretical Chemistry</i> , 2003, 637, 171-181.	1.5	31
18	Conformation and vibrational spectra and assignment of 2-thenoyltrifluoroacetone. <i>Journal of Molecular Structure</i> , 2009, 932, 112-122.	3.6	31

#	ARTICLE	IF	CITATIONS
19	Influence of temperature, pressure, nanotube's diameter and intertube distance on methane adsorption in homogeneous armchair open-ended SWCNT triangular arrays. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 231-240.	1.4	31
20	Deactivation studies of nano-structured iron catalyst in Fischer-Tropsch synthesis. <i>Journal of Natural Gas Chemistry</i> , 2010, 19, 333-340.	1.8	29
21	Structure and vibrational assignment of bis(benzoylacetato)copper(II). <i>Journal of Molecular Structure</i> , 2014, 1058, 308-317.	3.6	28
22	Fourier transform infrared and Raman spectra, vibrational assignment and density functional theory calculations of naphthazarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 111-120.	3.9	27
23	Water-gas-shift kinetics over a Fe/Cu/La/Si catalyst in Fischer-Tropsch synthesis. <i>Chemical Engineering Research and Design</i> , 2011, 89, 262-269.	5.6	26
24	Vibrational assignment of 4-amino-3-penten-2-one. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 1681-1695.	3.9	24
25	Intramolecular hydrogen bonding in 2-nitromalonaldehyde: Infrared spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2006, 782, 191-199.	3.6	24
26	Investigation of simple and water assisted tautomerism in a derivative of 1,3,4-oxadiazole: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 120-128.	2.4	24
27	Study of interaction of spironolactone with hydroxypropyl- β -cyclodextrin in aqueous solution and in solid state. <i>Journal of Molecular Structure</i> , 2008, 878, 78-83.	3.6	23
28	Theoretical study of intramolecular hydrogen bonding in the halo derivatives of 1-amino-3-imino-prop-1-ene. <i>Journal of Chemical Sciences</i> , 2013, 125, 939-948.	1.5	23
29	Tautomerism in pyridazin-3(2H)-one: A theoretical study using implicit/explicit solvation models. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 49, 47-54.	2.4	23
30	Molecular conformation and intramolecular hydrogen bonding in 4-amino-3-penten-2-one. <i>Computational and Theoretical Chemistry</i> , 2001, 541, 11-15.	1.5	22
31	Vibrational assignment of aluminum(III) Tris-acetylacetonate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 2669-2682.	3.9	22
32	Molecular structure and vibrational assignments of bis(4-aminopent-3-en-2-onato)copper(II): A detailed density functional theoretical study. <i>Journal of Molecular Structure</i> , 2011, 985, 139-147.	3.6	22
33	Theoretical study, and infrared and Raman spectra of copper(II) chelated complex with dibenzoylmethane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 272-279.	3.9	21
34	Molecular structure and vibrational assignment of dimethyl oxaloacetate. <i>Journal of Molecular Structure</i> , 2004, 694, 91-104.	3.6	20
35	Validation of potential energy distribution by VEDA in vibrational assignment some of β -diketones; comparison of theoretical predictions and experimental vibration shifts upon deuteration. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107976.	2.4	20
36	Structure and vibrational assignment of the enol form of 3-chloro-pentane-2,4-dione. <i>Journal of Molecular Structure</i> , 2008, 873, 79-88.	3.6	19

#	ARTICLE	IF	CITATIONS
37	Structure, intramolecular hydrogen bonding, and vibrational spectra of 2,2,6,6-tetramethyl-3,5-heptanedione. <i>Journal of Molecular Structure</i> , 2010, 970, 160-170.	3.6	19
38	Structure and vibrational analysis of methyl 3-amino-2-butenate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 102, 350-357.	3.9	18
39	Water-gas-shift kinetic over nano-structured iron catalyst in Fischerâ€™Tropsch synthesis. <i>Journal of Natural Gas Science and Engineering</i> , 2010, 2, 79-85.	4.4	17
40	Conformational stability, molecular structure, intramolecular hydrogen bonding, and vibrational spectra of 5,5-dimethylhexane-2,4-dione. <i>Journal of Molecular Structure</i> , 2011, 998, 99-109.	3.6	17
41	Conformation, molecular structure, and intramolecular hydrogen bonding of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. <i>Journal of Molecular Structure</i> , 2012, 1021, 102-111.	3.6	17
42	Conformational analysis, intramolecular hydrogen bonding, and vibrational assignment of 4,4-dimethyl-1-phenylpentane-1,3-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 284-298.	3.9	17
43	Intramolecular hydrogen bonding and vibrational assignment of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. <i>Journal of Molecular Structure</i> , 2014, 1076, 262-271.	3.6	17
44	Structure and vibrational assignment of 3-nitro-2,4-pentanedione: A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2008, 892, 32-38.	3.6	15
45	Structure and vibrational assignment of beryllium acetylacetonate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 342-347.	3.9	14
46	Water-gas-shift reaction over nickel catalysts: DFT studies and kinetic modeling. <i>Structural Chemistry</i> , 2019, 30, 1843-1852.	2.0	14
47	A two-dimensional potential function for bent hydrogen bonded systems. II-6-hydroxy-2-formylfulvene. <i>Computational and Theoretical Chemistry</i> , 2005, 730, 17-21.	1.5	13
48	The nature of intramolecular hydrogen bond in 2-nitromalonaldehyde. <i>Chemical Physics</i> , 2010, 368, 62-65.	1.9	13
49	Conformation, structure, intramolecular hydrogen bonding, and vibrational assignment of 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione. <i>Journal of Molecular Structure</i> , 2008, 882, 153-167.	3.6	12
50	Conformational analysis, tautomerization, IR, Raman, and NMR studies of 3-phenylazo-2,4-pentanedione. <i>Journal of Molecular Structure</i> , 2009, 920, 301-309.	3.6	12
51	Molecular structure and intramolecular hydrogen bonding in 2-hydroxybenzophenones: A theoretical study. <i>Journal of Chemical Sciences</i> , 2014, 126, 919-929.	1.5	12
52	CONFORMATIONAL STABILITY, MOLECULAR STRUCTURE, AND INTRAMOLECULAR HYDROGEN BONDING OF THENOYLTRIFLUOROACETONE. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 647-664.	1.8	11
53	Vibrational spectra of tris(acetylacetonato)chromium(III). <i>Journal of Molecular Structure</i> , 2015, 1099, 340-347.	3.6	11
54	Conformation, molecular structure, and vibrational assignment of bis(2,2,6,6-tetramethylheptane-3,5-dionato)copper(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1827-1833.	3.9	11

#	ARTICLE	IF	CITATIONS
55	Proton transfer in acetylacetone and its $\hat{\pm}$ -halo derivatives. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 344-350.	2.8	11
56	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. <i>Journal of Molecular Structure</i> , 2019, 1184, 233-245.	3.6	11
57	Hydrogen bond strength and vibrational assignment of the enol form of 3-(methylthio)pentane-2,4-dione. <i>Computational and Theoretical Chemistry</i> , 2008, 854, 54-62.	1.5	10
58	Hydrogen bond strength and vibrational assignment of the enol form of 3-(phenylthio)pentane-2,4-dione. <i>Journal of Molecular Structure</i> , 2008, 889, 165-176.	3.6	10
59	Conformational analysis, tautomerization, IR, Raman, and NMR studies of benzyl acetoacetate. <i>Journal of Molecular Structure</i> , 2011, 987, 241-254.	3.6	10
60	Conformational analysis, tautomerization, IR, Raman, and NMR studies of ethyl benzoylacetate. <i>Journal of Molecular Structure</i> , 2012, 1015, 74-85.	3.6	10
61	Tautomerism, conformational analysis, and spectroscopy studies of 3-bromo-pentane-2,4-dione. <i>Journal of Molecular Structure</i> , 2015, 1094, 264-273.	3.6	10
62	Conformational analysis, structure, and normal coordinate analysis of vibrational spectra of hexafluoroacetone. A density functional theory study. <i>Journal of Fluorine Chemistry</i> , 2016, 184, 65-71.	1.7	10
63	Molecular structure, spectroscopic studies, and copper oxygen bond strength of $\hat{\pm}$ -methyl and $\hat{\pm}$ -ethyl derivatives of copper (II) acetylacetonate; Experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2018, 1160, 107-116.	3.6	10
64	Vibrational assignment and proton tunneling in pyridine $\hat{\pm}$ pyridinium complexes. <i>Journal of Molecular Structure</i> , 2010, 971, 39-46.	3.6	9
65	Vibrational assignment and crystal structure of 3-amino-1-phenyl-2-buten-1-one. <i>Journal of Molecular Structure</i> , 2013, 1045, 20-28.	3.6	9
66	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. <i>Journal of Molecular Structure</i> , 2017, 1150, 427-437.	3.6	9
67	Vibrational assignment and structure of 4-amino-3-cyano-3-penten-2-one. <i>Journal of Molecular Structure</i> , 2002, 613, 195-208.	3.6	8
68	Structure and vibrational assignment of the enol form of 1-chloro-1,1-difluoro-pentane-2,4-dione. <i>Journal of Molecular Structure</i> , 2008, 878, 10-21.	3.6	8
69	Low frequency vibrational spectra and the nature of metal-oxygen bond of alkaline earth metal acetylacetonates. <i>Journal of Molecular Structure</i> , 2017, 1150, 340-348.	3.6	8
70	Electronic transport behavior of 1-(Phenyldiazenyl)naphthalen-2-ol and its derivatives as optical molecular switches: A first-principles approach. <i>Optik</i> , 2021, 236, 166475.	2.9	8
71	Structure, vibrational assignment, and NMR spectroscopy of 1,2-bis (dichloroacetyl) cyclopentadiene. <i>Journal of Molecular Structure</i> , 2013, 1036, 151-160.	3.6	7
72	Conformational analysis and vibrational assignment of bis-gem-diol of hexafluoroacetylacetone. <i>Journal of Molecular Structure</i> , 2013, 1041, 190-199.	3.6	7

#	ARTICLE	IF	CITATIONS
73	Vibrational spectra, normal coordinate analysis, and hydrogen bond investigation of pyridinium perchlorate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 558-565.	3.9	7
74	o-Phenylenediamine as a New Catalyst in the Highly Regioselective Conversion of Epoxides to Halohydrins with Elemental Halogens. <i>Monatshefte für Chemie</i> , 2004, 135, 1101.	1.8	6
75	Structure and vibrational assignment of bis(4-amino-3-penten-2-onato)nickel(II). A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2011, 997, 117-125.	3.6	6
76	Methane storage in homogeneous armchair open-ended single-walled boron nitride nanotube triangular arrays: a grand canonical Monte Carlo simulation study. <i>Journal of Molecular Modeling</i> , 2012, 18, 2699-2708.	1.8	6
77	X-ray diffraction and vibrational spectroscopic study of trans-bis(acetylacetonato)-bis(4-methylpyridine)cobalt(III). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 94-101.	3.9	6
78	Intramolecular hydrogen bonding in 5-nitrosalicylaldehyde: IR spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2016, 1111, 185-192.	3.6	6
79	Vibrational spectra of $\hat{I}\pm$ -bromo and $\hat{I}\pm$ -chloro derivatives of tris(acetylacetonato)chromium(III). <i>Journal of Molecular Structure</i> , 2016, 1103, 1-8.	3.6	6
80	Vibrational assignments, conformational analysis, and molecular structures of $\$left[\{ext{C}_{ext{n}}\} ext{mim} \} ight]left[\{ext{NTF}_{ext{2}}\} \} ight] \$\$ C n mim NTF 2 (n\hat{A}=\hat{A}2, 4, 6,) Tj ETQq0 0 0 rgBT, /Overlock 10 Tf 50$. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 1281-1300.	2.2	6
81	Structure, isomerism, and vibrational assignment of aluminumtrifluoroacetylacetonate. An experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 15-22.	3.9	6
82	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. <i>Journal of Molecular Liquids</i> , 2021, 334, 116035.	4.9	6
83	Structural, Potential Surface and Vibrational Spectroscopy Studies of Hypophosphorous Acid in the Gas Phase and Chain Conformation. A Theoretical Study. <i>Journal of the Korean Chemical Society</i> , 2005, 49, 129-137.	0.2	6
84	Theoretical and spectroscopic studies on molecular structure and hydrogen bonding of 1,2-bis (monochloroacetyl) cyclopentadiene. <i>Journal of Molecular Structure</i> , 2013, 1038, 177-187.	3.6	5
85	Vibrational assignment and structure of trinuclear oxo-centered of basic formate iron(III) and chromium(III) complexes: A density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 130, 287-294.	3.9	5
86	Hydrogen bond strength and vibrational assignment of the enol form of 3-(ortho-methoxyphenylthio) and 3-(para-methoxyphenylthio)pentane-2,4-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 731-742.	3.9	5
87	Conformational stability, barriers to internal rotations, and normal coordinate analysis of acetone and its $2H$ -isotopomers. <i>Canadian Journal of Chemistry</i> , 2016, 94, 818-826.	1.1	5
88	Vibrational assignments and structure of bis(3-amino-1-phenyl-2-buten-1-onato)copper(II) complex. <i>Journal of Molecular Structure</i> , 2016, 1111, 25-32.	3.6	5
89	Normal coordinate analysis, hydrogen bonding, and conformation analysis of heptane-3,5-dione. <i>Journal of Molecular Structure</i> , 2016, 1103, 35-44.	3.6	5
90	Conformations, molecular structure, and $N\hat{e}^{\hat{H}\hat{a}^{\hat{O}}}$ hydrogen bond strength in 4-Alkylamino-3-penten-2-ones. <i>Journal of Molecular Structure</i> , 2020, 1203, 127440.	3.6	5

#	ARTICLE	IF	CITATIONS
91	Theoretical investigation of solvent effect on the keto-enol tautomerization of pentane-2,4-dione and a comparison between experimental data and theoretical calculations. <i>Canadian Journal of Chemistry</i> , 2021, 99, 411-424.	1.1	5
92	Theoretical Study Intramolecular Hydrogen Bond in Acetylacetone 3- substituted Derivatives: NMR, NBO analysis and Thermo-chemical Investigation. <i>Oriental Journal of Chemistry</i> , 2013, 29, 1121-1128.	0.3	4
93	Very strong intramolecular hydrogen bonding of 1,2-dithenoylcyclopentadiene; DFT and spectroscopic studies. <i>Journal of Molecular Structure</i> , 2014, 1075, 85-95.	3.6	4
94	Theoretical and spectroscopic studies on molecular structure and hydrogen bonding of 2-trifluoroacetylphenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 820-827.	3.9	4
95	Normal coordinate analysis of pyridine and its C 2v 2 H-isotopomers. A new approach. <i>Journal of Molecular Structure</i> , 2018, 1151, 236-244.	3.6	4
96	Conformation, molecular structure, and vibrational assignment of bis(3,5-heptanedionato)copper(II). <i>Journal of Molecular Structure</i> , 2019, 1197, 443-449.	3.6	4
97	The nature of intramolecular hydrogen bond in Naphthazarin. <i>Chemical Physics</i> , 2020, 538, 110907.	1.9	4
98	Voltage-current behavior of 4-phenylamino-3-penten-2-one and its derivatives molecular switch: a first-principles study. <i>Molecular Simulation</i> , 2021, 47, 730-737.	2.0	4
99	Optimized molecular geometry, vibrational analysis, and Fe-O bond strength of Tris(β-cyanoacetylacetonate)iron(III):An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2022, 1248, 131444.	3.6	4
100	Vibrational spectra, normal coordinate analysis, and conformation of bis(β-cyanoacetylacetonato)Cu(II). <i>Journal of Molecular Structure</i> , 2016, 1118, 68-74.	3.6	3
101	Correlation Between Parameters Related to Intramolecular Hydrogen Bond Strength and Hammett Constant in Para Substituted Benzoylacetone (A Theoretical and Experimental Study). <i>Oriental Journal of Chemistry</i> , 2017, 33, 2579-2590.	0.3	3
102	Isomerism, molecular structure, and vibrational assignment of tris(trifluoroacetylacetonato)iron(III): An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2022, 1248, 131347.	3.6	3
103	Application of Hammett equation to intramolecular hydrogen bond strength in para-substituted phenyl ring of trifluorobenzoylacetone and 1-aryl-1,3-diketone malonates. <i>European Journal of Chemistry</i> , 2018, 9, 213-221.	0.6	3
104	Spectroscopic study of 2,3-Bis(p-methoxybenzoyl)cyclopentadiene as potential iron(III)-chelating agent. <i>Russian Journal of General Chemistry</i> , 2006, 76, 753-756.	0.8	0
105	Quantum chemical study of the mechanism of the palladium-catalysed C-H acetoxylation of benzene. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019, 44, 55-66.	2.1	0
106	Conformational analysis, tautomerization, and vibrational spectra of methyl acetoacetate. <i>Journal of the Iranian Chemical Society</i> , 0, , 1.	2.2	0