

Hasan Tanak

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Experimental (XRD, FT-IR and UV-Vis) and theoretical modeling studies of Schiff base (E)-N ² -((5-nitrothiophen-2-yl)methylene)-2-phenoxyaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 672-682.	3.9	87
2	Crystal Structure, Spectroscopy, and Quantum Chemical Studies of (E)-2-[(2-Chlorophenyl)iminomethyl]-4-trifluoromethoxyphenol. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13865-13876.	2.5	78
3	Experimental and quantum chemical calculational studies on 2-[(4-Fluorophenylimino)methyl]-3,5-dimethoxyphenol. <i>Journal of Molecular Modeling</i> , 2010, 16, 577-587.	1.8	76
4	Experimental and Computational Approaches to the Molecular Structure of 3-(2-Mercaptopyridine)phthalonitrile. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 673-680.	1.9	64
5	Quantum chemical computational studies on 2-methyl-6-[2-(trifluoromethyl)phenyliminomethyl]phenol. <i>Computational and Theoretical Chemistry</i> , 2010, 950, 5-12.	1.5	61
6	Density functional computational studies on (E)-2-[(2-Hydroxy-5-nitrophenyl)iminomethyl]-4-nitrophenolate. <i>Journal of Molecular Modeling</i> , 2010, 16, 235-241.	1.8	54
7	Experimental (XRD, IR and NMR) and theoretical investigations on 1-(2-nitrobenzoyl)-3,5-bis(4-methoxyphenyl)-4,5-dihydro-1H-pyrazole. <i>Journal of Molecular Structure</i> , 2016, 1126, 117-126.	3.6	46
8	An experimental and DFT computational study on 4-(3-(1H-imidazol-1-yl)propyl)-5-methyl-2H-1,2,4-triazol-3(4H)-one monohydrate. <i>Molecular Physics</i> , 2010, 108, 127-139.	1.7	44
9	Theoretical modeling and experimental studies on N-n-Decyl-2-oxo-5-nitro-1-benzylidene-methylamine. <i>Journal of Molecular Modeling</i> , 2009, 15, 1281-1290.	1.8	43
10	Density functional modelling studies on N-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidenemethylamine. <i>Computational and Theoretical Chemistry</i> , 2010, 961, 9-16.	1.5	41
11	DFT computational modeling studies on 4-(2,3-Dihydroxybenzylideneamino)-3-methyl-1H-1,2,4-triazol-5(4H)-one. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 93-101.	2.5	41
12	Quantum-chemical, spectroscopic and X-ray diffraction studies of (E)-2-[(2-Bromophenyl)iminomethyl]-4-trifluoromethoxyphenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 87, 15-24.	3.9	40
13	Combined experimental and DFT computational studies on (E)-1-(5-nitrothiophen-2-yl)-N-[4-(trifluoromethyl)phenyl]methanimine. <i>Journal of Molecular Structure</i> , 2013, 1048, 41-50.	3.6	40
14	Density functional computational studies on 2-[(2,4-Dimethylphenyl)iminomethyl]-3,5-dimethoxyphenol. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2392-2402.	2.0	39
15	Experimental and quantum chemical calculational studies on 2-[(4-propylphenylimino)methyl]-4-nitrophenol. <i>Molecular Physics</i> , 2010, 108, 1759-1772.	1.7	37
16	Molecular structure, spectroscopic and quantum chemical studies on 2-chloro-4-dimethylamino azobenzene. <i>Journal of Molecular Structure</i> , 2014, 1068, 189-197.	3.6	35
17	FT-IR, FT-Raman, and DFT computational studies of melaminium nitrate molecular ionic crystal. <i>Journal of Molecular Structure</i> , 2013, 1034, 363-373.	3.6	32
18	Crystal structure, spectroscopic investigations and density functional studies of 4-(4-methoxyphenethyl)-5-benzyl-2H-1,2,4-triazol-3(4H)-one monohydrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 106-115.	3.9	31

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19	Structural, vibrational and theoretical studies of anilinium trichloroacetate: New hydrogen bonded molecular crystal with nonlinear optical properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 82-93.	3.9	29
20	Combined experimental and computational modeling studies on 4-((2-hydroxy-3-methylbenzylidene)amino)-1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2123-2136.	2.0	20
21	Molecular structure, spectroscopic (FT-IR and UV-Vis) and DFT quantum-chemical studies on 2-[(2,4-Dimethylphenyl)iminomethyl]-6-methylphenol. <i>Molecular Physics</i> , 2014, 112, 1553-1565.	1.7	25
22	Experimental and theoretical studies of the molecular structure of 4-(3-(1H-imidazol-1-yl)propyl)-5-p-tolyl-2H-1,2,4-triazol-3(4H)-one. <i>Journal of Molecular Structure</i> , 2010, 984, 137-145.	3.6	21
23	5-Benzyl-4-[3-(1H-imidazol-1-yl)propyl]-2H-1,2,4-triazol-3(4H)-ones: Synthesis, spectroscopic characterization, crystal structure and a comparison of theoretical and experimental IR results by DFT calculations. <i>Journal of Molecular Structure</i> , 2009, 936, 46-55.	3.6	20
24	DFT QUANTUM CHEMICAL STUDIES ON 1-[N-(2-PYRIDYL)AMINO]METHYL-2-(1H)-NAPHTALENONE. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 745-762.	1.8	20
25	Molecular structure and vibrational and chemical shift assignments of 3-chloro-4-dimethylamino azobenzene by DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 152, 530-536.	3.9	20
26	Experimental and DFT computational studies on 5-benzyl-4-(3,4-dimethoxyphenethyl)-2H-1,2,4-triazol-3(4H)-one. <i>Journal of Molecular Modeling</i> , 2010, 16, 447-457.	1.8	19
27	Identification of structural and spectral properties of synthesized 3-(p-isopropylphenyl)-5-(o,m,p-nitrophenyl)-1-phenylformazans: A combined experimental and DFT study. <i>Dyes and Pigments</i> , 2015, 113, 510-521.	3.7	18
28	Quantum chemical studies on the molecular structure, spectroscopic and electronic properties of (6-Methoxy-2-oxo-2H-chromen-4-yl)-methyl pyrrolidine-1-carbodithioate. <i>Materials Science-Poland</i> , 2016, 34, 886-904.	1.0	18
29	Molecular structure, vibrational spectra, NLO and MEP analysis of bis[2-hydroxy- δ° O-N-(2-pyridyl)-1-naphthaldiminato- δ° N]zinc(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 145-153.	3.9	17
30	2-[(2,4-Dimethylphenyl)iminomethyl]-6-methylphenol. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2009, 65, o2291-o2291.	0.2	17
31	Experimental and DFT studies of ethyl N-3-(1H-imidazol-1-yl) propylcarbamoyl benzohydrionate monohydrate. <i>Structural Chemistry</i> , 2009, 20, 409-416.	2.0	15
32	The synthesis of some new imidazole and triazole derivatives: crystal Structure and DFT-TDDFT investigation on electronic structure. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2010, 67, 325-334.	1.6	15
33	2-Ethyl-N-[(5-nitrothiophen-2-yl)methylidene]aniline. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o2004-o2004.	0.2	15
34	A combined experimental (XRD, FT-IR, and UV-Vis) and DFT computational studies on (E)-N-[4-bromo-2-(trifluoromethoxy)phenyl]-1-(5-nitrothiophen-2-yl) methanimine. <i>Molecular Physics</i> , 2016, 114, 197-212.	1.7	15
35	Molecular structure and vibrational spectra of Bis(melaminium) terephthalate dihydrate: A DFT computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 156-164.	3.9	14
36	Synthesis, crystal structure, spectral analysis and DFT computational studies on a novel isoindoline derivative. <i>Journal of Molecular Structure</i> , 2016, 1118, 1-9.	3.6	14

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37	Molecular structure, vibrational spectra and DFT computational studies of melaminium N-acetylglycinate dihydrate. <i>Journal of Molecular Structure</i> , 2016, 1121, 142-155.	3.6	13
38	4-(2,3-Dihydroxybenzylideneamino)-3-methyl-1H-1,2,4-triazol-5(4H)-one. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2009, 65, o3039-o3039.	0.2	12
39	Structural, spectroscopic and electronic properties of 4-bromo-5-fluoro-2-((3-nitrophenylimino)methyl)phenol Schiff-base molecule: Experimental and theoretical investigations. <i>Journal of Molecular Structure</i> , 2019, 1197, 9-18.	3.6	11
40	Molecular structure, spectroscopic and DFT computational studies on 4,5-bis(tert-butylsulfanyl)phthalonitrile. <i>Journal of Molecular Structure</i> , 2015, 1090, 86-92.	3.6	10
41	Martensitic Transformation and Magnetic Properties of the CuAl, CuAlMn, and CuAlMnZn Alloys. <i>Journal of Superconductivity and Novel Magnetism</i> , 2018, 31, 3919-3923.	1.8	9
42	DFT Quantum Chemical Studies on Structural, Nonlinear Optical, Reactivity and Thermodynamic Properties of 4-(4-methoxy-2-((E)-(thiophen-2-yl)ethylimino)methyl)phenol. <i>ChemistrySelect</i> , 2019, 4, 10876-10883.	1.5	9
43	Ethyl 4-(3-ethyl-5-oxo-4,5-dihydro-1H-1,2,4-triazol-4-yl)benzoate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, o1294-o1294.	0.2	8
44	Investigation of antimicrobial activities, DNA interaction, structural and spectroscopic properties of 2-chloro-6-(trifluoromethyl)pyridine. <i>Journal of Molecular Structure</i> , 2017, 1137, 206-215.	3.6	8
45	Experimental and DFT computational studies of novel 3-(p-cyanophenyl)-5-(o,m,p-nitrophenyl)-5-phenylformazans. <i>Journal of Molecular Structure</i> , 2020, 1213, 128178.	3.6	8
46	Experimental and computational studies on zwitterionic (E)-2-(1-(2-(4-methylphenylsulfonamido)ethyliminio)ethyl) phenolate. <i>Structural Chemistry</i> , 2010, 21, 1027-1036.	2.0	7
47	Molecular structure and vibrational assignment of 1-[N-(2-pyridyl)aminomethylidene]-2(1H)-Naphthalenone by density functional theory (DFT) and ab initio Hartree-Fock (HF) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 152, 525-529.	3.9	7
48	DFT quantum chemical studies of (E)-4-Bromo-N-(2-chlorobenzylidene)-aniline. <i>Applied Physics A: Materials Science and Processing</i> , 2017, 123, 1.	2.3	7
49	Molecular structure, spectroscopic, and density functional theory studies of <i>o</i> -Dianisidine. <i>Molecular Crystals and Liquid Crystals</i> , 2017, 648, 183-201.	0.9	7
50	Crystal Structure of N-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidene-methylamine. <i>Analytical Sciences: X-ray Structure Analysis Online</i> , 2008, 24, X237-X238.	0.1	6
51	Crystal structure of 4-[benzylideneamino]-3-thiophen-2-yl-methyl-4,5-dihydro-1H-[1,2,4]triazole-5-one. <i>Crystallography Reports</i> , 2013, 58, 1103-1106.	0.6	6
52	Synthesis, crystal structure, spectroscopic characterization and DFT studies of bis[(1Z,2E)-N-(2,6-diethylphenyl)-N-(2-hydroxy-2-(hydroxyimino)acetimidamido)]nickel(II). <i>Inorganica Chimica Acta</i> , 2017, 459, 36-44.	2.4	6
53	Comparative structural, spectroscopic and nonlinear optical analysis of a Schiff base compound with experimental and theoretical methods (HF, B3LYP and WB97X-D). <i>Optik</i> , 2021, 228, 166133.	2.9	6
54	2-((E)-[(2-Methyl-3-nitrophenyl)imino]methyl)-4-nitrophenol. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013, 69, o1085-o1085.	0.2	5

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55	Crystal structure of (E)-3-fluoro-N-((5-nitrothiophen-2-yl)methylene)aniline. <i>Crystallography Reports</i> , 2016, 61, 410-413.	0.6	5
56	2-[(2,4-Dimethylphenyl)iminomethyl]-3,5-dimethoxyphenol. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2009, 65, o1572-o1572.	0.2	5
57	Crystal Structure of 4-Amino-3-(thiophen-2-ylmethyl)-1H-1,2,4-triazole-5(4H)one Monohydrate. <i>Crystallography Reports</i> , 2018, 63, 585-588.	0.6	4
58	Molecular and Crystal Structure of 2-[(E)-[(5-Chloro-2-methoxyphenyl)imino]methyl]-4-nitrophenol. <i>Crystallography Reports</i> , 2018, 63, 372-374.	0.6	4
59	Synthesis, Molecular Structure and Quantum Chemical Studies of N-(2-Fluorophenyl)-1-(5-Nitrothiophen-2-yl)methanimine. <i>Crystallography Reports</i> , 2020, 65, 1212-1216.	0.6	4
60	Crystal structure of 2-[[5-nitrothiophen-2-yl)methylidene]amino]phenol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, o418-o418.	0.5	3
61	Experimental and theoretical studies of bis[(E)-1-(3-chloro-4-methylphenylimino)methyl)naphthalen-2-olate-N,O]copper(II). <i>Journal of Molecular Structure</i> , 2018, 1174, 184-191.	3.6	3
62	Synthesis and Structural and Biochemical Activity Studies of Dioxime Ligand and its Mononuclear Cu(II), Ni(II), and Co(II) Complexes. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2011, 41, 1249-1256.	0.6	2
63	Molecular and crystal structure of 3-benzyl-4-(4-carboxyphenyl)-4,5-dihydro-1H-1,2,4-triazol-5-one. <i>Crystallography Reports</i> , 2014, 59, 974-978.	0.6	2
64	Molecular and crystal structure of 2-[(E)-[(4-Methylphenyl)imino]methyl]-4-nitrophenol: A redetermination. <i>Crystallography Reports</i> , 2016, 61, 239-242.	0.6	2
65	Analysis on molecular, spectroscopic and electronic behavior of 4,4'-(butane-1,4-diyl)bis(1-((1-(4-chlorobenzyl)-1H-1,2,3-triazol-5-yl)methyl)-3-methyl-1H-1,2,4-triazol-5(4H)-one): A theoretical approach. <i>Journal of Molecular Structure</i> , 2018, 1174, 60-66.	3.6	2
66	Crystal and Molecular Structure of N-(Phenylthio)phthalimide. <i>Crystallography Reports</i> , 2018, 63, 379-381.	0.6	2
67	Congo red filtration by polyacrylonitrile-based copolymer membranes. <i>Canadian Journal of Chemistry</i> , 2020, 98, 421-426.	1.1	2
68	1-Benzoylmethyl-3-(2-thienylmethyl)-4-(2-thienylmethyleneamino)-1H-1,2,4-triazol-5(4H)-one. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, o301-o301.	0.2	2
69	Crystal Structure, Spectroscopic and DFT Computational Studies of N-(4-Fluorophenyl)-1-(5-Nitrothiophen-2-yl)methanimine. <i>Crystallography Reports</i> , 2020, 65, 1221-1225.	0.6	2
70	Crystal structure of 4-[(Benzylidene-amino)]-2-(2-oxo-2-phenylethyl)-5-thiophen-2-ylmethyl-2,4-dihydro-[1,2,4]triazol-3-one. <i>Crystallography Reports</i> , 2014, 59, 969-973.	0.6	1
71	Crystal and Molecular Structure of 3,5-Diphenyl-4,5-dihydro-2-phenylcarboxamide-1H-pyrazole. <i>Crystallography Reports</i> , 2017, 62, 1078-1082.	0.6	1
72	Crystal Structure of 2-[(E)-(5-Bromo-2-hydroxybenzylidene)hydrazono]-1,2-diphenylethanone. <i>Crystallography Reports</i> , 2018, 63, 375-378.	0.6	1

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73	Molecular structure, spectroscopic and density functional studies on 2-[[5-nitrothiophen-2-yl)methylidene]amino}phenol. Optik, 2019, 195, 163144.	2.9	1
74	Molecular and Electronic Analysis of (7-Chloro-2-oxo-2H-chromen-4-yl)-methyl diethylcarbamo-dithioate by DFT and HF Calculations. Acta Physica Polonica A, 2019, 136, 3-17.	0.5	1
75	Crystal and Molecular Structure of 2-(4-Ethoxyphenyl)isoindoline-1,3-dione. Crystallography Reports, 2018, 63, 1116-1119.	0.6	0
76	Synthesis, Molecular Structure and Spectroscopic Studies of 6,6'-(1E,1'E)-(Ethane-1,2-Diylbis(azan-1-yl-1-ylidene))bis(Phenylmethan-1-yl-1-ylidene)bis(3-(Octyloxy)phenol). Crystallography Reports, 2020, 65, 1217-1220.	0.6	0
77	Crystal structure and DFT computational studies of (<i>E</i>)-2,4-di- <i>tert</i>-butyl-6-[3-(trifluoromethyl)benzyl]iminomethyl}phenol. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 732-735.</i>	0.5	0