

Absolute hardness: companion parameter to absolute e

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Citation Report

#	ARTICLE	IF	CITATIONS
12	Polyphenols from dipterocarp species. Copalliferol A and stemonoporol. Journal of the Chemical Society Perkin Transactions 1, 1983, , 699.	0.9	22
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14	Simulated transition state for the hartree-fock and hartree-fock-slater methods. Chemical Physics Letters, 1984, 109, 394-397.	1.2	1
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25	Absolute hardness of ground and hybridised states of atoms. Journal of Physics B: Atomic and Molecular Physics, 1985, 18, L35-L38.	1.6	1
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28	Fukui function: Spin-density and chemical reactivity. Journal of Chemical Physics, 1986, 85, 2337-2338.	1.2	25
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1862	Applications of Density Functional Theory to Chemical Reactivity. <i>Structure and Bonding</i> , 2012, , .	1.0	10
1863	A theoretical study of the mechanism and stereoselectivity of the Diels-Alder cycloaddition between difluoro-2-methylcyclopropane and furan. <i>Tetrahedron Letters</i> , 2012, 53, 5784-5786.	0.7	14
1864	Theoretical Investigations toward the [4 + 2] Cycloaddition of Ketenes with <i>N</i> -Benzoyldiazenes Catalyzed by <i>N</i> -Heterocyclic Carbenes: Mechanism and Enantioselectivity. <i>Journal of Organic Chemistry</i> , 2012, 77, 10729-10737.	1.7	57

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1866	A Model Study on the Possible Effects of an External Electrical Field on Enzymes Having Dinuclear Iron Cluster [2Fe-2S]. Scientific World Journal, The, 2012, 2012, 1-9.	0.8	0
1867	Quantum Information-Theoretical Analyses of Systems and Processes of Chemical and Nanotechnological Interest. , 2012, , .		0
1868	Toward analyzing some neutral and cationic boron-lithium clusters (B_xLi_y ; $x = 2-6$; $y = 1, 2$) as effective hydrogen storage materials: A conceptual density functional study. International Journal of Quantum Chemistry, 2012, 112, 695-702.	1.0	22
1869	Heterocyclic silylenes: a survey of stability with density functional theory. Journal of Physical Organic Chemistry, 2012, 25, 50-57.	0.9	7
1870	A Diels-Alder reaction between cyclopentadiene and protonated N-phenylethyliminoacetates of 8-phenylmenthol and 8-phenylneomenthol: a density functional theory study. Journal of Physical Organic Chemistry, 2012, 25, 515-522.	0.9	4
1871	Degradation of dichloromethane by bispidine. Journal of Physical Organic Chemistry, 2012, 25, 814-827.	0.9	18
1872	How hydrogen-bonded MnO_4^- can influence oxidation of olefins in both gas phase and solution?. Journal of Physical Organic Chemistry, 2012, 25, 1198-1209.	0.9	4
1873	Iodine catalyzed Mukaiyama-Michael reaction: experimental evaluation of catalytic effect in conjunction with computational study of the reaction mechanism. Journal of Physical Organic Chemistry, 2012, 25, 1228-1235.	0.9	11
1874	Density functional computational studies on 2-[(2,4-dimethylphenyl)iminomethyl]-5-dimethoxyphenol. International Journal of Quantum Chemistry, 2012, 112, 2392-2402.	1.0	39
1875	Understanding the inactivation process of organophosphorus herbicides: A DFT study of glyphosate metallic complexes with Zn^{2+} , Ca^{2+} , Mg^{2+} , Cu^{2+} , Co^{3+} , Fe^{3+} , Cr^{3+} , and Al^{3+} . International Journal of Quantum Chemistry, 2012, 112, 2752-2762.	1.0	67
1876	Receptor binding affinity based comparative QSAR study of testosterone derivatives. International Journal of Quantum Chemistry, 2012, 112, 2371-2377.	1.0	0
1877	Density functional theory study of the regio- and stereoselectivity of diels-alder reactions of 5-aryl-2-pyrones. International Journal of Quantum Chemistry, 2012, 112, 2294-2300.	1.0	16
1878	Theoretical study of the chemical reactivity and molecular quantum similarity in a series of derivatives of 2-adamantylthiazolidine-one using density functional theory and the topogeometrical superposition approach. International Journal of Quantum Chemistry, 2012, 112, 2681-2687.	1.0	17
1879	Possible DNA damage by oxidation products of guanine: A density functional and electron propagator theoretical study. International Journal of Quantum Chemistry, 2012, 112, 2840-2847.	1.0	8
1880	Density functional study on electronic structures and reactivity in carbazoloxadiazole dyads used in organic light emitting diodes. International Journal of Quantum Chemistry, 2012, 112, 2808-2815.	1.0	4
1881	Relationship between local reactivity indices and the hammett constant for isatoic anhydride and its derivatives. International Journal of Quantum Chemistry, 2012, 112, 3570-3577.	1.0	5
1882	Soft-Soft interactions in the protein-protein recognition process: The K^+ channel-charybdotoxin case. International Journal of Quantum Chemistry, 2012, 112, 3618-3623.	1.0	3

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1884	Understanding the origin of the asynchronicity in bond-formation in polar cycloaddition reactions. A DFT study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-benzoquinones. <i>RSC Advances</i> , 2012, 2, 1334-1342.	1.7	53
1885	Challenges for Density Functional Theory. <i>Chemical Reviews</i> , 2012, 112, 289-320.	23.0	1,869
1886	Simultaneous production of hydrogen with the degradation of organic pollutants using TiO ₂ photocatalyst modified with dual surface components. <i>Energy and Environmental Science</i> , 2012, 5, 7647.	15.6	236
1887	Elucidation of the reaction mechanisms and diastereoselectivities of phosphine-catalyzed [4 + 2] annulations between allenolates and ketones or aldimines. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7689.	1.5	45
1888	A structural-feature-based computational approach for toxicity prediction of water-soluble arsenicals. <i>Physics and Chemistry of Liquids</i> , 2012, 50, 173-186.	0.4	1
1889	Evaluation of the Electrophilicities and Band Gaps of Conductive Polymers: A New Model. <i>Macromolecular Theory and Simulations</i> , 2012, 21, 529-534.	0.6	0
1890	Structure and reactivity of thiosulfonic acids and their anions: A theoretical study. <i>Heteroatom Chemistry</i> , 2012, 23, 329-339.	0.4	1
1891	Complexation behavior of trivalent actinides and lanthanides with 1,10-phenanthroline-2,9-dicarboxylic acid based ligands: insight from density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11060.	1.3	57
1892	On the Electrophilic Character of Molecules Through Its Relation with Electronegativity and Chemical Hardness. <i>International Journal of Molecular Sciences</i> , 2012, 13, 2160-2175.	1.8	36
1893	The Woodward-Hoffmann Rules Reinterpreted by Conceptual Density Functional Theory. <i>Accounts of Chemical Research</i> , 2012, 45, 683-695.	7.6	156
1894	Polarizability, Ionization Potential, and Softness of Water and Methanol Clusters: An Interrelation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6831-6836.	1.1	21
1895	Effect of Metal Ions on Photoluminescence, Charge Transport, Magnetic and Catalytic Properties of All-Inorganic Colloidal Nanocrystals and Nanocrystal Solids. <i>Journal of the American Chemical Society</i> , 2012, 134, 13604-13615.	6.6	156
1896	A New Piece in the Puzzle of Lithium/Air Batteries: Computational Study on the Chemical Stability of Propylene Carbonate in the Presence of Lithium Peroxide. <i>Chemistry - A European Journal</i> , 2012, 18, 3510-3520.	1.7	51
1897	Viability of M ⁿ -Porphyrin Topologies in [26]- and [28]Hexaphyrins. <i>Chemistry - A European Journal</i> , 2012, 18, 10916-10928.	1.7	48
1898	Theoretical Study of Energetic Complexes (III): Bis(5-nitro-2H-tetrazolato) ²⁻ tetraammine Cobalt(III) Perchlorate (BNCP) and Its Transition Metal (Ni/Fe/Cu/Zn) Perchlorate Analogues. <i>Chinese Journal of Chemistry</i> , 2012, 30, 1624-1630.	2.6	2
1899	Scandium-Catalyzed Preparation of Cytotoxic 3-Functionalized Quinolin-2-ones: Regioselective Ring Enlargement of Isatins or Imino Isatins. <i>ChemPlusChem</i> , 2012, 77, 563-569.	1.3	24
1900	Correlating the site selectivity of protonation in some ambidentate molecules in terms of the dual descriptor. <i>European Physical Journal D</i> , 2012, 66, 1.	0.6	6

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1901	Metal Interactions with Nucleobases, Base Pairs, and Oligomer Sequences; Computational Approach. , 2012, , 1277-1308.		3
1902	Theoretical study of the infrared spectrum of 5-phenyl-1,3,4-oxadiazole-2-thiol by using DFT calculations. <i>Molecular Simulation</i> , 2012, 38, 561-566.	0.9	20
1903	Density functional study of substituted (â€“SH, â€“S, â€“OH, â€“Cl) hydrated ions of Hg ²⁺ . <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	12
1904	Hard and Soft Acids and Bases: Structure and Process. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7147-7153.	1.1	13
1905	Natural orbital Fukui function and application in understanding cycloaddition reaction mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9890.	1.3	26
1906	Symmetries and fuzzy symmetries of graphene molecules. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 1309-1332.	0.7	2
1907	Physical and chemical properties of Co nâ”m Cu m nanoclusters with n=6 atoms via ab-initio calculations. <i>Journal of Nanoparticle Research</i> , 2012, 14, 1.	0.8	10
1908	The adsorptions of silver-doped small gold clusters toward carbon monoxide molecule. <i>Structural Chemistry</i> , 2012, 23, 671-679.	1.0	4
1909	Fitness landscapes in natural rocks system evolution: A conceptual DFT treatment#. <i>Journal of Chemical Sciences</i> , 2012, 124, 29-34.	0.7	7
1910	Comparison of the mechanism of deamination of 5,6-dihydro-5-methylcytosine with other cytosine derivatives. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	5
1911	Radical electrophilicities in solvent. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	23
1912	Metal ion sorption properties of water-insoluble resins based on sodium styrene sulfonate and different comonomers. <i>Polymer Bulletin</i> , 2012, 68, 1537-1549.	1.7	11
1913	UV-spectroscopy, electronic structure and ozonolytic reactivity of sesquiterpenes: a theoretical study. <i>Journal of Molecular Modeling</i> , 2012, 18, 1455-1462.	0.8	1
1914	Theoretical study of the local reactivity of electrophiles of the type MPR 3 + (M=Cu, Ag, Au ;R=H, -Me, ETQ)	0.8	11
1915	Studies on molecular structure and tautomerism of a vitamin B6 analog with density functional theory. <i>Journal of Molecular Modeling</i> , 2012, 18, 1993-2001.	0.8	13
1916	A QSAR study of radical scavenging antioxidant activity of a series of flavonoids using DFT based quantum chemical descriptors â€“ the importance of group frontier electron density. <i>Journal of Molecular Modeling</i> , 2012, 18, 2621-2631.	0.8	69
1917	First-principles study of energetic complexes (II): (5-cyanotetrazolato-N2) pentaammine cobalt (III) perchlorate (CP) and Ni, Fe and Zn analogues. <i>Journal of Molecular Modeling</i> , 2012, 18, 2855-2860.	0.8	1
1918	The electronic properties of trimethylnaphthalenes as properties for the prediction of biodegradation rates: Ab initio and DFT study. <i>Chemosphere</i> , 2012, 88, 91-97.	4.2	11

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1919	On the HSAB based estimate of charge transfer between adsorbates and metal surfaces. <i>Chemical Physics</i> , 2012, 393, 1-12.	0.9	283
1920	On the complementarity of comprehensive decomposition analysis of stabilization energy (CDASE) â€“ Scheme and supermolecular approach. <i>Chemical Physics</i> , 2012, 394, 29-35.	0.9	46
1921	Pd(II)â€“N-heterocyclic carbene complexes of 2,6-bis{N-methyl-(imidazolium/benzimidazolium)}pyrazinechloride: Synthesis, structure, catalysis and theoretical studies. <i>Inorganica Chimica Acta</i> , 2012, 383, 83-90.	1.2	24

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1937	Dual super-electrophilic and Diels-Alder reactivity of neutral 10- π heteroaromatic substrates. <i>Tetrahedron</i> , 2012, 68, 1829-1843.	1.0	30
1938	Induction of photoluminescence and columnar mesomorphism in hemi-disc salphen type Schiff bases via nickel(II) coordination. <i>Polyhedron</i> , 2012, 33, 417-424.	1.0	20
1939	New oxidovanadium(V) complexes of the cation [VO] ₃ ⁺ : Synthesis, structural characterization and DFT studies. <i>Polyhedron</i> , 2012, 36, 21-29.	1.0	13
1940	Structural, calorimetric and vibrational investigations of 2, 3 and 4-hydroxyanilinium perchlorate: A theoretical and experimental study. <i>Vibrational Spectroscopy</i> , 2012, 58, 169-180.	1.2	5
1941	Structure-functional organization of eukaryotic high-affinity copper importer CTR1 determines its ability to transport copper, silver, and cisplatin. <i>Molecular Biology</i> , 2012, 46, 304-315.	0.4	12
1942	Some Schiff base compounds as inhibitors for corrosion of carbon steel in acidic media. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2012, 48, 477-486.	0.3	22
1943	The chemical hardness of molecules and the band gap of solids within charge equilibration formalisms. <i>European Physical Journal B</i> , 2012, 85, 1.	0.6	11
1944	A computational study on the hydrogen adsorption capacity of various lithium-doped boron hydrides. <i>Journal of Computational Chemistry</i> , 2012, 33, 425-434.	1.5	34
1945	Mechanisms of the cascade synthesis of substituted 4-amino-1,2,4-triazol-3-one from huisgen zwitterion and aldehyde hydrazone: A DFT study. <i>Journal of Computational Chemistry</i> , 2012, 33, 715-722.	1.5	22
1946	Nanostructure-Driven Analyte-Interface Electron Transduction: A General Approach to Sensor and Microreactor Design. <i>ChemPhysChem</i> , 2012, 13, 549-561.	1.0	23
1947	Highly Efficient, Irreversible and Selective Ion Exchange Property of Layered Titanate Nanostructures. <i>Advanced Functional Materials</i> , 2012, 22, 835-841.	7.8	220
1948	Theoretical characterization of single-electron iodine-bond weak interactions in CH ₃ -I-Y (Y = BH ₂ , H). <i>J. Phys. Chem. B</i> , 2012, 116, 10784-10793.	1.7	3
1949	Structure-stability diagrams and stability-reactivity landscapes: a conceptual DFT study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
1950	A comparative study of the hydrogen-bonding patterns and prototropism in solid 2-thiocytosine (potential antileukemic agent) and cytosine, as studied by 1H-14N NQDR and QTAIM/ DFT. <i>Journal of Molecular Modeling</i> , 2012, 18, 11-26.	0.8	12
1951	Charge-based DFT descriptors for Diels-Alder reactions. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 187-193.	0.9	12
1952	Theoretical Study of Phenol Adsorption on Pristine, Ga-Doped, and Pd-Decorated (6,0) Zigzag Single-Walled Boron Phosphide Nanotubes. <i>Journal of Cluster Science</i> , 2013, 24, 49-60.	1.7	19
1953	Contact Ion Pair Formation between Hard Acids and Soft Bases in Aqueous Solutions Observed with 2DIR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15306-15312.	1.2	34
1954	New insights in the bonding regime and ligand field in Wernerian complexes. A density functional study. <i>Polyhedron</i> , 2013, 52, 183-195.	1.0	5

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1955	Experimental, quantum chemical calculations, and molecular dynamic simulations insight into the corrosion inhibition properties of 2-(6-methylpyridin-2-yl)oxazolo[5,4-f][1,10]phenanthroline on mild steel. <i>Research on Chemical Intermediates</i> , 2013, 39, 1927-1948.	1.3	97
1956	Quantum chemical studies on some thiadiazolines as corrosion inhibitors for mild steel in acidic medium. <i>Research on Chemical Intermediates</i> , 2013, 39, 895-906.	1.3	12
1957	Aza-Diels-Alder addition of cyclopentadiene to propynyliminoglyoxylates. <i>Computational and Theoretical Chemistry</i> , 2013, 1012, 54-59.	1.1	4
1958	Comparative vibrational spectroscopic studies, HOMO-LUMO and NBO analysis of N-(phenyl)-2,2-dichloroacetamide, N-(2-chloro phenyl)-2,2-dichloroacetamide and N-(4-chloro phenyl)-2,2-dichloroacetamide. <i>Journal of Molecular Structure</i> , 2013, 1016, 8-21.	1.1	116
1959	Alkylation of DNA by nitrogen mustards: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 19-25.	1.1	5
1960	Why Mercury Prefers Soft Ligands. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2317-2322.	2.1	54
1961	Theoretical investigation of ytterbium trichelates compounds. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1447-1452.	1.0	0
1962	Metronidazole as environmentally safe corrosion inhibitor for mild steel in 0.5M HCl: Experimental and theoretical investigation. <i>Journal of Environmental Chemical Engineering</i> , 2013, 1, 431-439.	3.3	158
1963	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	12
1964	Synthesis, spectroscopic and structural evaluation of ethyl 2-cyano-3-[(4-nitro-benzoyl)-hydrazonomethyl]-1H-pyrrol-2-yl-acrylate using experimental and theoretical approaches. <i>Journal of Molecular Structure</i> , 2013, 1049, 419-428.	1.8	17
1965	Breathing viability into cyclonona-3,5,7-trienylidenes \pm -dimethyl and \pm -moieties at DFT. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 540-550.	0.9	26
1966	FT-IR, Micro-Raman and UV-vis spectroscopic and quantum chemical investigations of free 2,2'-dithiodipyridine and its metal (Co, Cu and Zn) halide complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 114, 61-73.	2.0	50
1967	Recent Developments in Colloidal Synthesis of CuInSe ₂ Nanoparticles. <i>Chemistry - A European Journal</i> , 2013, 19, 9746-9753.	1.7	39
1968	Selective depression of pyrite with chitosan in Pb-Fe sulfide flotation. <i>Minerals Engineering</i> , 2013, 46-47, 45-51.	1.8	50
1969	Computation of polarizability, hyper-polarizability and hardness as descriptor for enol-keto tautomerizations of 2-hydroxy pyridines. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 200-207.	1.1	12
1970	Experimental and theoretical studies on polar Diels-Alder reactions of 1-nitronaphthalene developed in ionic liquids. <i>RSC Advances</i> , 2013, 3, 13825.	1.7	10
1971	Reactivity of the ZnS(101 $\bar{1}$ 0) Surface to Small Organic Ligands by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16034-16041.	1.5	6
1972	Spectroscopic (FTIR, FT-Raman, NMR and UV) and molecular structure investigations of 1,5-diphenylpenta-2,4-dien-1-one: a combined experimental and theoretical approach. <i>Molecular Simulation</i> , 2013, 39, 330-349.	0.9	6

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1973	Spectroscopic studies (FTIR, FT-Raman and UV), potential energy surface scan, normal coordinate analysis and NBO analysis of (2R,3R,4R,5S)-1-(2-hydroxyethyl)-2-(hydroxymethyl) piperidine-3,4,5-triol by DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 108, 38-49.	2.0	62
1974	Molecular structure analysis and spectroscopic characterization of 5-ethyl-5-phenyl-1,3-diazinane-4,6-dione with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 106, 310-320.	2.0	14
1975	Modeling the mechanism of glycosylation reactions between ethanol, 1,2-ethanediol and methoxymethanol. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14026.	1.3	6
1976	Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT studies of 1-ethyl-1,4-dihydro-7-methyl-4oxo-1,8 naphthyridine-3-carboxylic acids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 220-235.	2.0	7
1977	A proposal for an extended dual descriptor: a possible solution when Frontier Molecular Orbital Theory fails. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14465.	1.3	67
1978	Cytotoxicity and QSAR study of (thio)ureas derived from phenylalkylamines and pyridylalkylamines. <i>Medicinal Chemistry Research</i> , 2013, 22, 4016-4029.	1.1	17
1979	Experimental and theoretical (HOMO, LUMO, NBO analysis and NLO properties) study of 7-hydroxy-4-phenylcoumarin and 5,7-dihydroxy-4-phenylcoumarin. <i>Journal of Molecular Structure</i> , 2013, 1047, 216-228.	1.8	10
1980	Hydrogen adsorption and dissociation on small Al _n Au clusters: an electronic structure density functional study. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	6
1981	Towards time-dependent, non-equilibrium charge-transfer force fields. <i>European Physical Journal B</i> , 2013, 86, 1.	0.6	18
1982	DFT study of the effect of carbitol on the mechanism of aminolysis of 6-methyl-2-(methylsulfanyl)pyrimidin-4(3H)-one. <i>Russian Journal of Organic Chemistry</i> , 2013, 49, 1042-1046.	0.3	3
1983	Copper(II) ions capturing from water using ligand modified a new type mesoporous adsorbent. <i>Chemical Engineering Journal</i> , 2013, 221, 322-330.	6.6	304
1984	Synthesis, characterization, molecular modeling and biological activity of mixed ligand complexes of Cu(II), Ni(II) and Co(II) based on 1,10-phenanthroline and novel thiosemicarbazone. <i>Inorganica Chimica Acta</i> , 2013, 407, 58-68.	1.2	81
1985	Reactivity of Dicoordinated Stannylones (Sn 0) versus Stannylenes (Sn II): An Investigation Using DFT-Based Reactivity Indices. <i>ChemPhysChem</i> , 2013, 14, 3233-3247.	1.0	6
1986	How reliable is the hard-soft acid-base principle? An assessment from numerical simulations of electron transfer energies. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13959.	1.3	44
1987	Variational principles for mechanistic quantitative structure-activity relationship (QSAR) studies: application on uracil derivatives-anti-HIV action. <i>Structural Chemistry</i> , 2013, 24, 1873-1893.	1.0	26
1988	Effect of axial strain on structural and electronic properties of zig-zag type of boron nitride nanotube (BNNT): a quantum chemical study. <i>Structural Chemistry</i> , 2013, 24, 409-420.	1.0	12
1989	A combined experimental and theoretical approach for radical-scavenging activity of edaravone and its related derivatives. <i>Structural Chemistry</i> , 2013, 24, 349-355.	1.0	9
1990	Adsorption and electronic structure study of thiazole on the (6,0) zigzag single-walled boron phosphide nanotube. <i>Journal of Sulfur Chemistry</i> , 2013, 34, 407-420.	1.0	11

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1991	Computational Redox Biology: Methods and Applications. , 2013, , 187-211.		3
1992	Mechanistic Studies on the Pd-Catalyzed Vinylation of Aryl Halides with Vinylalkoxysilanes in Water: The Effect of the Solvent and NaOH Promoter. <i>Journal of the American Chemical Society</i> , 2013, 135, 13749-13763.	6.6	46
1993	A comparative study on the antioxidant properties of bractein and cernuoside by the DFT method. <i>Monatshefte für Chemie</i> , 2013, 144, 1513-1524.	0.9	5
1994	Thermal and Sc(OTf) ₃ catalyzed 1,3-dipolar cycloaddition of open-chain nitrones to $\hat{1},\hat{2}$ -unsaturated lactones: combined experimental and computational studies. <i>Tetrahedron: Asymmetry</i> , 2013, 24, 89-103.	1.8	12
1995	Protophilicity index and protofelicity equalization principle: new measures of Brønsted-Lowry-Lewis acid-base interactions. <i>Journal of Molecular Modeling</i> , 2013, 19, 3961-3967.	0.8	2
1996	Density functional study of structural and electronic properties of small binary Be n Cu m (n+m=2 ^{1/4}) ₄ clusters. <i>Journal of Molecular Modeling</i> , 2013, 19, 3065-3075.	0.8	4
1997	On the exponential model for energy with respect to number of electrons. <i>Journal of Molecular Modeling</i> , 2013, 19, 2849-2853.	0.8	29
1998	Influence of the monoclinic and tetragonal zirconia phases on the water gas shift reaction. A theoretical study. <i>Journal of Molecular Modeling</i> , 2013, 19, 2885-2891.	0.8	7
1999	Is hyper-hardness more chemically relevant than expected?. <i>Journal of Molecular Modeling</i> , 2013, 19, 2893-2900.	0.8	60
2000	Synthesis and characterization of novel series of Fe(II)-mixed ligand complexes involving 2,2'-bipyridyl ligand. <i>Dyes and Pigments</i> , 2013, 99, 1056-1064.	2.0	17
2001	Koopmans' multiconfigurational self-consistent field (MCSCF) Fukui functions and MCSCF perturbation theory. <i>Canadian Journal of Chemistry</i> , 2013, 91, 886-893.	0.6	2
2002	Synthesis, multiple interactions and spectroscopy analysis of ethyl-4-[(benzoyl)-hydrazonomethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate: Through experimental and quantum chemical approaches. <i>Journal of Molecular Structure</i> , 2013, 1035, 295-306.	1.8	11
2003	An efficient fluctuating charge model for transition metal complexes. <i>Journal of Computational Chemistry</i> , 2013, 34, 1598-1608.	1.5	13
2004	QSAR study of amidino bis-benzimidazole derivatives as potent anti-malarial agents against Plasmodium falciparum. <i>Chemical Papers</i> , 2013, 67, .	1.0	22
2005	Computational investigation of the electronic and structural properties of CN radical on the pristine and Al-doped (6, 0) BN nanotubes. <i>Physica B: Condensed Matter</i> , 2013, 430, 20-26.	1.3	17
2006	Steric Maps to Evaluate the Role of Steric Hindrance on the IPr NHC Ligand. <i>Procedia Computer Science</i> , 2013, 18, 845-854.	1.2	5
2007	NBO, NMR, UV, FT-IR, FT-Raman spectra and molecular structure (monomeric and dimeric structures) investigation of 4-Chloro-3,5-Xylenol: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 170-182.	2.0	7
2008	Experimental and theoretical studies of a new donor-acceptor Re(I) complexes using nitropolypyridil ligand. Analysis of the NLO potential response. <i>Polyhedron</i> , 2013, 57, 94-104.	1.0	19

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2009	Coordination of diorganotellurides to cobalt(III) in cobaloximes. <i>Polyhedron</i> , 2013, 58, 39-46.	1.0	1
2010	A density functional theory study of the regio- and stereoselectivity of the 1,3-dipolar cycloaddition of C-methyl substituted pyrazinium-3-olates with methyl acrylate and methyl methacrylate. <i>Computational and Theoretical Chemistry</i> , 2013, 1025, 58-66.	1.1	5
2011	Understanding the Interaction of Nucleobases with Chiral Semiconducting Single-Walled Carbon Nanotubes: An Alternative Theoretical Approach Based on Density Functional Reactivity Theory. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21539-21550.	1.5	50
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2057	Quantitative structure-mobility relationship analysis of imidazoline receptor ligands in CD-mediated CE. <i>Electrophoresis</i> , 2013, 34, 471-482.	1.3	13
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2059	Synthesis, molecular structure, hydrogen-bonding, NBO and chemical reactivity analysis of a novel 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(4-hydroxyphenyl)-dipyrromethane: A combined experimental and theoretical (DFT and QTAIM) approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 378-385.	2.0	20
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2106	A combined experimental and theoretical (DFT and AIM) studies on synthesis, molecular structure, spectroscopic properties and multiple interactions analysis in a novel Ethyl-4-[2-(thiocarbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 182-190.	2.0	62
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2119	Hardness potential derivatives and their relation to Fukui indices. <i>Journal of Computational Chemistry</i> , 2013, 34, 662-672.	1.5	18
2120	Density dynamics in some quantum systems. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1747-1771.	1.0	7
2121	Effects and Mechanism of Metal Chloride Salts on Pretreatment and Enzymatic Digestibility of Corn Stover. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 1775-1782.	1.8	152
2122	Quantum mechanical study of the structure and spectroscopic, first order hyperpolarizability, Fukui function, NBO, normal coordinate analysis of Phenyl-N-(4-Methyl Phenyl) Nitron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 62-77.	2.0	15
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2124	Conformational stability, vibrational spectra, HOMOâ€“LUMO and NBO analysis of 1,3,4-thiadiazolidine-2,5-dithione with experimental (FT-IR and FT-Raman) techniques and scaled quantum mechanical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 171-181.	2.0	17
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2132	Oxazol-2-ylidenes. A new class of stable carbenes?. <i>RSC Advances</i> , 2013, 3, 7970.	1.7	32
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2137	Fukui function and response function for nonlocal and fractional systems. <i>Journal of Chemical Physics</i> , 2013, 138, 184108.	1.2	18
2138	Kinetic and Thermodynamic Hysteresis Imposed by Intercalation of Proflavine in Ferrocene-Modified Double-Stranded DNA. <i>ChemPhysChem</i> , 2013, 14, 2208-2216.	1.0	8
2139	Synthesis, molecular structure, hydrogen-bonding and chemical reactivity analysis of 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(2-chlorophenyl)-dipyrromethane: A combined experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2013, 1047, 169-178.	1.8	6
2140	Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, TD-DFT and thermodynamic analysis of 4-amino-3-hydroxy-1-naphthalenesulfonic acid by DFT approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 107, 167-178.	2.0	32
2141	Syntheses of phenoxyalkyl esters of 3,3'-bis(indolyl)methanes and studies on their molecular properties from single crystal XRD and DFT techniques. <i>Journal of Molecular Structure</i> , 2013, 1047, 109-120.	1.8	20
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2413	Molecular structure, FT-IR, first order hyperpolarizability, NBO analysis, HOMO and LUMO, MEP analysis of (E)-3-(4-chlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one by HF and density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 526-533.	2.0	13
2414	DFT Study on the Mechanisms and Diastereoselectivities of Lewis Acid-Promoted Ketene–Alkene [2 + 2] Cycloadditions: What is the Role of Lewis Acid in the Ketene and C = X (X = O, CH ₂ , and NH) [2 + 2] Cycloaddition Reactions?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4288-4300.	1.1	46
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2426	Force-Field Representation of Biomolecular Systems. , 2015, , 45-77.		3

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2447	Structural and Electronic Properties of Folic Acid Adsorption on the Carbon Nanotubes: A Density Functional Theory Study. <i>Oriental Journal of Chemistry</i> , 2015, 31, 345-351.	0.1	4
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2449	Applicability of optimal functional tuning in density functional calculations of ionization potentials and electron affinities of adenine-thymine nucleobase pairs and clusters. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4337-4345.	1.3	32
2450	Optical and theoretical studies on Fe ₃ O ₄ -imidazole nanocomposite and clusters. <i>New Journal of Chemistry</i> , 2015, 39, 3801-3812.	1.4	15
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2468	Addition-fragmentation reaction of thionoesters compounds in free-radical polymerisation (methyl, Tj ETQq1 1 0.784314 rgBT /Over	0.8	6
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2474	DFT investigation on A ₄ B ₄ (A=Cu, Ag; B=As, Sn) metal-semiconductor alloy clusters for potential nanomaterials. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 68, 224-231.	1.3	9
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2497	A new equation for calculation of chemical hardness of groups and molecules. <i>Molecular Physics</i> , 2015, 113, 1311-1319.	0.8	132
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2505	Theoretical study of adsorption of CO gas on pristine and AsGa-doped (4, 4) armchair models of BPNTs. <i>Computational Condensed Matter</i> , 2015, 3, 21-29.	0.9	15
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2512	FT-IR, NBO, HOMO-LUMO, MEP analysis and molecular docking study of Methyl N-([2-(2-methoxyacetamido)-4-(phenylsulfanyl)phenyl]amino)[(methoxycarbonyl)] Tj ETQq1 1 0.784314 rgBT / Overlock 10 Tf 50 30 1	2.0	17
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2526	Green chemical functionalization of single-wall carbon nanotube with methylimidazolium dicyanamid ionic liquid: A first principle computational exploration. <i>Journal of Molecular Liquids</i> , 2015, 211, 498-505.	2.3	13
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2532	Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranil-9-acrylic]anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 350-359.	2.0	14
2533	Molecular structure, FT-IR, FT-Raman, NBO, HOMO and LUMO, MEP, NLO and molecular docking study of 2-[(E)-2-(2-bromophenyl)ethenyl]quinoline-6-carboxylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 184-197.	2.0	33
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2535	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. <i>RSC Advances</i> , 2015, 5, 58464-58477.	1.7	53
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2539	Spectroscopic and theoretical characterization of 2-(4-methoxyphenyl)-4,5-dimethyl-1H-imidazole 3-oxide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 965-979.	2.0	36
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2578	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. <i>Journal of Molecular Structure</i> , 2015, 1095, 100-111.	1.8	5
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3252	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2017, 7, 50496-50507.	1.7	33
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3368	Combinatorial experimental and DFT theoretical evaluation of a nano novel thio-dicarboxaldehyde based Schiff base supported on a thin polymer film as a chemosensor for Pb ²⁺ detection. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 360, 152-165.	2.0	23
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3373	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14211-14222.	1.3	8
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3500	Synthesis, structural configuration and DFT molecular orbital studies of [Mn-2[benzo[b]oxazole] acetonitrile] complexes encapsulated in ZSM-5: Direct synthesis of phenol by benzene hydroxylation. <i>Microporous and Mesoporous Materials</i> , 2018, 262, 35-48.	2.2	8
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4757	Probing and comparison of graphene, boron nitride and boron carbide nanosheets for Flutamide adsorption: A DFT computational study. <i>Journal of Molecular Liquids</i> , 2021, 343, 117487.	2.3	7
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4769	Experimental and quantum investigations of novel corrosion inhibitors based triazene derivatives for mild steel. <i>Journal of Molecular Structure</i> , 2021, 1242, 130831.	1.8	5
4770	Synthesis, structural investigation, computational study, antimicrobial activity and molecular docking studies of novel synthesized (E)-4-((pyridine-4-ylmethylene)amino)-N-(pyrimidin-2-yl)benzenesulfonamide from pyridine-4-carboxaldehyde and sulfadiazine. <i>Journal of Molecular Structure</i> , 2021, 1241, 130544.	1.8	55
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4804	A facile synthesis and structural elucidation for furfural based chromophores: Prediction of linear and nonlinear optical properties. <i>Journal of Molecular Structure</i> , 2022, 1249, 131543.	1.8	5
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