

Development of the Colle-Salvetti correlation-energy formula for electron density

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Ab initio approach for many-electron systems without invoking orbitals: An integral formulation of density-functional theory. <i>Physical Review A</i> , 1988, 38, 5494-5503.	1.0	16
2	Comparative study of spectroscopic properties of some indium, tin and antimony compounds. <i>Molecular Physics</i> , 1989, 68, 209-223.	0.8	31
3	Core-valence correlation potentials based on density functional theory. Applications to valence-electron-only calculations on Na and K diatomics. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , 1989, 13, 355-361.	1.0	16
4	Results obtained with the correlation energy density functionals of Becke and Lee, Yang and Parr. <i>Chemical Physics Letters</i> , 1989, 157, 200-206.	1.2	6,521
5	Pseudopotential investigations on indium, tin and antimony compounds. <i>Computational and Theoretical Chemistry</i> , 1990, 209, 313-331.	1.5	5
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8	Interpretation of the absorption spectrum of Na ₈ . <i>Chemical Physics Letters</i> , 1990, 170, 26-34.	1.2	65
9	Nonlocal Wigner-like correlation-energy density functional through coordinate scaling. <i>Physical Review B</i> , 1990, 41, 12930-12932.	1.1	142
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14110	HNC(1E) production from the $\langle \text{mml:math altimg="si2.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:cb="http://www.elsevier.com/xml/co$	1.2	11
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14121	$\langle \text{mml:math altimg="si8.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:cb="http://www.elsevier.com/xml/co$	1.2	1
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18863	Synthesis, IR, UV/vis-, ¹ H NMR and DFT study of chelator functionalized 1,3-benzoxazinone spiropyran. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1146-1152.	2.0	14
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30336	A study on interaction of Be ⁺⁺ , Mg ⁺⁺ and Ca ⁺⁺ with phenylalanine: Binding energies, metal ion affinities and IR signature of complex stability. <i>Vibrational Spectroscopy</i> , 2011, 56, 42-50.	1.2	3
30337	Effect of pyridine on zinc phthalocyanine studied by density functional theory calculations and infrared absorption spectroscopy. <i>Vibrational Spectroscopy</i> , 2011, 56, 60-65.	1.2	11
30338	Vibrational study of fluorobenzene and its solvation with methanol via polarized Raman measurements and quantum chemical calculations. <i>Vibrational Spectroscopy</i> , 2011, 56, 26-33.	1.2	22
30339	Vibrational spectroscopic and density functional theory studies of chloranil ⁺ imidazole interaction. <i>Vibrational Spectroscopy</i> , 2011, 56, 66-73.	1.2	15
30340	Vibrational spectra and reinvestigation of the crystal structure of a polymeric copper(II) ⁺ orotate complex, [Cu(1/4-HOr)(H ₂ O) ₂] _n : The performance of new DFT methods, M06 and M05-2X, in theoretical studies. <i>Vibrational Spectroscopy</i> , 2011, 55, 207-215.	1.2	55
30341	Combined study of vibrational spectra of $\hat{L}\pm$ -carboline by theoretical and experimental IR methods. <i>Vibrational Spectroscopy</i> , 2011, 55, 287-294.	1.2	1
30342	Terahertz, infrared and Raman vibrational assignments of [FeFe]-hydrogenase model compounds. <i>Vibrational Spectroscopy</i> , 2011, 56, 219-227.	1.2	11
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30344	A study of the structure of high-energy states of nitrogen trioxide and the (NO) ₂ dimer: DFT calculations within the symmetrized Kohn-Sham formalism. <i>Journal of Structural Chemistry</i> , 2011, 52, 445-453.	0.3	2
30345	Hydrogen-bonding interaction of urea with DNA bases: A density functional theory study. <i>Journal of Structural Chemistry</i> , 2011, 52, 462-470.	0.3	10
30346	Thiacalix[4]arenes: Extraction of palladium and the electronic structure. <i>Journal of Structural Chemistry</i> , 2011, 52, 718-725.	0.3	7
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30348	XES and quantum chemical investigation of the electronic structure of phthalocyanine complexes MPcH16 and MPcF16 with M = Cu, Co. <i>Journal of Structural Chemistry</i> , 2011, 52, 21-35.	0.3	2
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30351	Synthesis of hollow polypyrrole-platinum complex spheres and their successful application as a catalyst for decomposition of hydrogen peroxide. <i>Kinetics and Catalysis</i> , 2011, 52, 716-722.	0.3	1
30352	Role of the surface hydroxyl groups of modified titanium oxide in catalytic ethylene oxide hydration. <i>Kinetics and Catalysis</i> , 2011, 52, 659-671.	0.3	4

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30354	Density Functional Theory Combined with Molecular Mechanics: The Infrared Spectra of Flavin in Solution. <i>Photochemistry and Photobiology</i> , 2011, 87, 511-523.	1.3	19
30355	Metal coordination polymers of 2,3-bis(benzimidazol-1-ylmethyl)quinoxaline: Syntheses, crystal structures and luminescent properties. <i>Solid State Sciences</i> , 2011, 13, 1256-1260.	1.5	6
30356	Experimental (X-Ray Photoelectron Spectroscopy) and theoretical studies of benzene based organics intercalated into layered double hydroxide. <i>Solid State Sciences</i> , 2011, 13, 1676-1686.	1.5	35
30357	Dicyanovinyl substituted oligothiophenes: Thermal stability, mobility measurements, and performance in photovoltaic devices. <i>Solar Energy Materials and Solar Cells</i> , 2011, 95, 3171-3175.	3.0	21
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30359	Twisted molecular geometry and localized electronic structure of the triplet excited gem-diphenyltrimethylenemethane biradical: substituent effects on thermoluminescence and related theoretical calculations. <i>Tetrahedron</i> , 2011, 67, 7431-7439.	1.0	12
30360	Structure and photochemical behaviour of 3-azido-acrylophenones: a matrix isolation infrared spectroscopy study. <i>Tetrahedron</i> , 2011, 67, 7794-7804.	1.0	13
30361	Cyclization of C-phosphorylated (P(III)) arylformamidines to 3H-1,3-benzazaphospholes. <i>Tetrahedron</i> , 2011, 67, 7748-7758.	1.0	44
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30364	Oxazolidinone cross-alkylation during Evans [™] asymmetric alkylation reaction. <i>Tetrahedron</i> , 2011, 67, 9104-9111.	1.0	6
30365	endo-Mode cyclizations of vinylogous N-acyliminium ions as a route to the synthesis of condensed thiazolidines. <i>Tetrahedron</i> , 2011, 67, 9541-9554.	1.0	13
30366	Determination of the absolute configuration of 1,3,5-triphenyl-4,5-dihydropyrazole enantiomers by a combination of VCD, ECD measurements, and theoretical calculations. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 1120-1124.	1.8	11
30367	Curtin [™] Hammett versus non-Curtin [™] Hammett frameworks in optimizing the enantioselective binolam/titanium(IV)-catalyzed cyanobenzoylation of aldehydes: Part 2. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 1292-1305.	1.8	5
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30369	Synthesis and characterization of a new ethynyl-bridged C60 derivative bearing a diketopyrrolopyrrole moiety. <i>Tetrahedron Letters</i> , 2011, 52, 5008-5011.	0.7	18
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30374	Diels-Alder reactions of N-tosylpyrroles developed in protic ionic liquids. Theoretical studies using DFT methods. <i>Tetrahedron Letters</i> , 2011, 52, 6754-6757.	0.7	25
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30376	Promotion effect of tungsten oxide on SCR of NO with NH ₃ for the V ₂ O ₅ -WO ₃ /Ti _{0.5} Sn _{0.5} O ₂ catalyst: Experiments combined with DFT calculations. <i>Journal of Molecular Catalysis A</i> , 2011, 346, 29-38.	4.8	56
30377	Tungsten(II)-catalyzed rearrangements of norbornadiene: Effects of alternative complexation stages. <i>Journal of Molecular Catalysis A</i> , 2011, 351, 143-153.	4.8	6
30378	X-ray structures and computational studies of several cathinones. <i>Journal of Molecular Structure</i> , 2011, 1002, 10-18.	1.8	20
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30386	Comparative vibrational spectroscopic studies, HOMO-LUMO and NBO analysis of 5,7-dibromo-8-hydroxyquinoline and 5,7-dichloro-8-hydroxyquinoline based on Density Functional Theory. <i>Journal of Molecular Structure</i> , 2011, 1004, 51-66.	1.8	28
30387	A new crystal structure and fluorescence property of N-2-fluorobenzoyl-N ² -4-tolylthiourea. <i>Journal of Molecular Structure</i> , 2011, 1004, 74-81.	1.8	19
30388	The structure elucidation of mequindox and 1,4-bisdesoxymequindox: NMR analyses, FT-IR spectra, DFT calculations and thermochemical studies. <i>Journal of Molecular Structure</i> , 2011, 1004, 109-115.	1.8	8

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30406	Synthesis, density functional theory, molecular dynamics and electrochemical studies of 3-thiopheneacetic acid-capped gold nanoparticles. Journal of Molecular Structure, 2011, 1006, 494-501.	1.8	8

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30409	Factors determining tautomeric equilibria in Schiff bases. <i>Journal of Molecular Structure</i> , 2011, 1006, 600-605.	1.8	14
30410	Structures and conformations of acridinium mono- and polymethine cyanine dyes and their UV-Vis absorption spectra in protic solvents: A PCM/TD-DFT study. <i>Journal of Molecular Structure</i> , 2011, 1006, 635-641.	1.8	5
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30422	Water assisted photo-oxidation from hydroquinone to p-benzoquinone in a solid Ne matrix. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 223, 182-188.	2.0	9
30423	New pyran dyes for dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 224, 116-122.	2.0	45
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30426	Electron momentum density and band structure calculations of \hat{I}^{\pm} - and \hat{I}^2 -GeTe. <i>Radiation Physics and Chemistry</i> , 2011, 80, 1316-1322.	1.4	6
30427	Vibrational spectroscopic studies and Natural Bond Orbital analysis of 4,6-dichloro-2-(methylthio)pyrimidine based on density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 1-7.	2.0	20
30428	FT-IR and FT-Raman spectroscopic investigation, computed vibrational frequency analysis and IR intensity and Raman activity peak resemblance analysis on 2-nitroanisoole using HF and DFT (B3LYP and) Tj ETQq1 1,0,784314 rgBT / Oe 83, 8-16.	2.0	19
30429	A characterization study on 2,6-dimethyl-4-nitropyridine N-oxide by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 104-110.	2.0	10
30430	A new Schiff base compound N,N \hat{e} 2-(2,2-dimethylpropane)-bis(dihydroxyacetophenone): Synthesis, experimental and theoretical studies on its crystal structure, FTIR, UV \hat{e} visible, 1H NMR and 13C NMR spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 144-150.	2.0	22
30431	Vibrational and electronic spectra of 9,10-dihydrobenzo(a)pyren-7(8H)-one and 7,8,9,10-tetrahydrobenzo(a)pyrene: An experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 162-171.	2.0	7
30432	Molecular interaction study of the diisopropyl ether \hat{e} propionic acid mixture by spectroscopic and dielectric studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 172-177.	2.0	19
30433	Vibrational spectroscopy investigation and HOMO, LUMO analysis using DFT (B3LYP) on the structure of 1,3-dichloro 5-nitrobenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 242-50.	2.0	4
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30435	An efficient and simple approach for the synthesis of pyranopyrazoles using imidazole (catalytic) in aqueous medium, and the vibrational spectroscopic studies on 6-amino-4-(4 \hat{e} 2-methoxyphenyl)-5-cyano-3-methyl-1-phenyl-1,4-dihydropyrano[2,3-c]pyrazole using density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 431-440.	2.0	106
30436	FTIR and FT-Raman spectra, molecular geometry, vibrational assignments, first-order hyperpolarizability, ab initio and DFT calculations for 3,4-dimethoxybenzoxonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 466-474.	2.0	9
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30438	MP2, DFT and ab initio calculations on thioxanthone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 49-55.	2.0	16
30439	Vibrational spectroscopic, electronic and quantum chemical investigations on 2,3-hexadiene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 620-630.	2.0	20
30440	Spectroscopic properties of neuroleptics: IR and Raman spectra of Risperidone (Risperdal) and of its mono- and di-protonated forms. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 631-639.	2.0	11
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30442	Synthesis, spectroscopy, and characterization of some bis-nicotinamide metal(II) dihalide complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 684-689.	2.0	15

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30444	Molecular spectroscopic analyses of gelatin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 724-729.	2.0	30
30445	2-[(1H-Benzimidazol-2-ylmethyl)-amino]-benzoic acid methyl ester: Crystal structure, DFT calculations and biological activity evaluation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 754-763.	2.0	24
30446	Highly selective fluorescent recognition of Zn ²⁺ based on naphthalene macrocyclic derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 200-204.	2.0	31
30447	Vibrational analysis of 4-amino pyrazolo (3,4-d) pyrimidine A joint FTIR, Laser Raman and scaled quantum mechanical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 228-234.	2.0	32
30448	Molecular structure, vibrational spectra and HOMO, LUMO analysis of yohimbine hydrochloride by density functional theory and ab initio Hartree-Fock calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 270-278.	2.0	19
30449	Molecular structure, vibrational spectroscopic, first hyperpolarizability, NBO and HOMO, LUMO studies of P-Iodobenzene sulfonyl chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 332-339.	2.0	19
30450	Synthesis, spectroscopic characterization, X-ray structure and DFT studies on 4-(2-hydroxyphenyl)-4,5,6,7-tetrahydro-1H-imidazo[4,5-c]pyridin-5-ium chloride hydrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 360-367.	2.0	3
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30452	Synthesis, molecular conformation, vibrational and electronic transition, isometric chemical shift, polarizability and hyperpolarizability analysis of 3-(4-Methoxy-phenyl)-2-(4-nitro-phenyl)-acrylonitrile: A combined experimental and theoretical analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 444-455.	2.0	116
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30454	Experimental and DFT studies on the vibrational and electronic spectra of 4,5-dihydro-6-methyl-4-[(E)-(3-pyridinylmethylene)amino]-1,2,4-triazin-3(2H)-one. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 112-119.	2.0	7
30455	Spectroscopic (NMR, UV, FT-IR and FT-Raman) analysis and theoretical investigation of nicotinamide N-oxide with density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 250-258.	2.0	32
30456	Infrared, ¹ H and ¹³ C NMR spectra, structural characterization and DFT calculations of novel adenine-cyclodiphosphazane derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 304-313.	2.0	5
30457	Vibrational and electronic investigations, thermodynamic parameters, HOMO and LUMO analysis on crotonaldehyde by ab initio and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 411-419.	2.0	44
30458	Enhanced Raman spectrum of lawsone on Ag surface: Vibrational analyses, frequency shifts, and molecular geometry. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 425-431.	2.0	24
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30460	Vibrational spectral analysis and first hyperpolarizability studies of 1-bromonaphthalene based on ab initio and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 553-560.	2.0	11

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30467	Spectroscopic, electronic structure and natural bond orbital analysis of o-fluoronitrobenzene and p-fluoronitrobenzene: A comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 196-209.	2.0	16
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30469	Molecular structure and spectroscopic studies on novel complexes of coumarin-3-carboxylic acid with Ni(II), Co(II), Zn(II) and Mn(II) ions based on density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 275-285.	2.0	26
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31143	Vibrational spectroscopic study on 2-[2-(4-dipropylamino-phenyl)-vinyl]-1,3,3-trimethyl-3H-indolium chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 967-980.	2.0	4
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32064	Synthesis, FTIR, FT-Raman, UV-visible, ab initio and DFT studies on benzohydrazide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 486-496.	2.0	43
32065	Spectroscopic analysis of 2-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-ylimino)-2-(4-nitro-phenyl) acetonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 618-624.	2.0	14

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32070	A combined experimental and theoretical quantum chemical studies on 4-morpholinecarboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1395-1401.	2.0	3
32071	Density functional theory (DFT) investigation of molecular structure and frontier molecular orbitals (FMOs) of P-N,N-dimethylaminobenzylidenemalononitrile (DBM). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1499-1504.	2.0	20
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32073	Vibrational study of tolazoline hydrochloride by using FTIR-Raman and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1710-1714.	2.0	21
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32075	Vibrational spectroscopic (FT-IR and FT-Raman), first-order hyperpolarizability, HOMO, LUMO, NBO, Mulliken charges and structure determination of 2-bromo-4-chlorotoluene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1747-1756.	2.0	22
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33896	What is Wrong with Quantitative Structure–Property Relations Models Based on Three-Dimensional Descriptors?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1984-1993.	2.5	38
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36069	Thermal decomposition mechanism of levoglucosan during cellulose pyrolysis. <i>Journal of Analytical and Applied Pyrolysis</i> , 2012, 96, 110-119.	2.6	91
36070	A periodic hybrid DFT approach (including dispersion) to MgCl ₂ -supported Ziegler-Natta catalysts α -1: TiCl ₄ adsorption on MgCl ₂ crystal surfaces. <i>Journal of Catalysis</i> , 2012, 286, 103-110.	3.1	103
36071	DFT investigation of hydroperoxide decomposition over copper and cobalt sites within metal-organic frameworks. <i>Journal of Catalysis</i> , 2012, 286, 95-102.	3.1	26
36072	Theoretical and experimental investigations on site occupancy for palladium oxidation states in mesoporous Al-MCM-41 materials. <i>Journal of Catalysis</i> , 2012, 289, 227-237.	3.1	21
36073	The interaction of an azo compound with a surfactant and ion pair adsorption to solid phases. <i>Journal of Colloid and Interface Science</i> , 2012, 367, 370-377.	5.0	12
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36075	Novel palladium(II) and platinum(II) complexes with 1H-benzimidazol-2-ylmethyl-N-(4-bromo-phenyl)-amine: Structural studies and anticancer activity. <i>European Journal of Medicinal Chemistry</i> , 2012, 47, 399-411.	2.6	105
36076	Influence of susceptibility to hydrolysis and hydrophobicity of arylsemicarbazones on their anti-nociceptive and anti-inflammatory activities. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 140-148.	2.6	7
36077	2-Acetylpyridine- and 2-benzoylpyridine-derived hydrazones and their gallium(III) complexes are highly cytotoxic to glioma cells. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 163-172.	2.6	58
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36080	Dynamic water networks in cytochrome cbb3 oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2012, 1817, 726-734.	0.5	16
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36082	N-(4-Substituted-benzoyl)-N ² -(¹² -d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 1801-1816.	1.4	13
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36087	A Combined Study Using Ligand-Based Design, Synthesis, and Pharmacological Evaluation of Analogues of the Acetaminophen <i>ortho</i> -Regioisomer with Potent Analgesic Activity. <i>Chemical Biology and Drug Design</i> , 2012, 80, 99-105.	1.5	3
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36089	Ligand- and Structure-Based Drug Design Strategies and PPAR γ Selectivity. <i>Chemical Biology and Drug Design</i> , 2012, 80, 533-544.	1.5	8
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36095	DFT studies on some properties of maleonitriledithiolate complexes [M(mnt) $_2$] $^{2-}$ (M=Ni, Pd, Pt and Zn). <i>ETQq1_1_0.784314 rgBT</i> 2.0 5	2.0	5
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36099	A structural and spectroscopic study on para-aminohippuric acid with experimental and theoretical approaches. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 241-250.	2.0	13
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36101	Determination of structural and vibrational spectroscopic properties of 2-, 3-, 4-nitrobenzenesulfonamide using FT-IR and FT-Raman experimental techniques and DFT quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 261-270.	2.0	24
36102	Theoretical investigations of <i>ortho</i> , <i>meta</i> , <i>para</i> -trifluoro-3-, <i>para</i> - and <i>ortho</i> -nitrotoluene by means of density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 271-282.	2.0	7
36103	A new Schiff base system bearing two naphthalene groups as fluorescent chemodosimeter for Zn $^{2+}$ ion and its logic gate behavior. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 85, 293-297.	2.0	31

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36105	Spectroscopic (FT-IR, FT-Raman and UV-vis) investigation and frontier molecular orbitals analysis on 3-methyl-2-nitrophenol using hybrid computational calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 86, 139-151.	2.0	24
36106	Molecular structure, vibrational spectra, HOMO, LUMO and NMR studies of 1,2-dichloro-4-nitrobenzene and 2,3,5,6-tetrachloro-1-nitrobenzene based on density functional calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 86, 196-204.	2.0	12
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36109	FT-IR, FT-Raman, UV spectra and DFT calculations on monomeric and dimeric structure of 2-amino-5-bromobenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 86, 590-599.	2.0	89
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36111	Concomitant polymorphism of a pyridine-2,6-dicarboxamide derivative in a single space group: Experimental and molecular modeling study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 86, 614-624.	2.0	6
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36114	Theoretical study of the alkoxy groups effect on PPV-ether excited states, a relationship with femtosecond decay. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 23-30.	2.0	21
36115	Molecular structure, spectroscopic (FT-IR, FT-Raman, ¹³ C and ¹ H NMR, UV), polarizability and first-order hyperpolarizability, HOMO and LUMO analysis of 4-methylbiphenyl-2-carbonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 87, 273-285.	2.0	30
36116	FT-IR, FT-Raman and UV spectral investigation: Computed frequency estimation analysis and electronic structure calculations on chlorobenzene using HF and DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 37-48.	2.0	50
36117	Synthesis, molecular structure and spectral analysis of ethyl 4-[(3,5-dinitrobenzoyl)-hydrazonomethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate: A combined experimental and quantum chemical approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 60-71.	2.0	3
36118	The band 12 issue of norbornane: A study of higher shake-up states. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 102-110.	2.0	6
36119	An experimental and theoretical study of l-tryptophan in an aqueous solution, combining two-layered ONIOM and SCRF calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 162-170.	2.0	42
36120	Experimental, quantum chemical and natural bond orbital investigations of N-(2,4-dimethylphenyl)-2,2-dichloroacetamide and N-(3,5-dimethylphenyl)-2,2-dichloroacetamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 192-209.	2.0	6
36121	Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 222-230.	2.0	7

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36122	FTIR, FT-Raman, FT-NMR, UV-vis visible and quantum chemical investigations of 2-amino-4-methylbenzothiazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 220-231.	2.0	35
36123	N-(4-Nitrobenzoyl)-N ² -(1,5-dimethyl-3-oxo-2-phenyl-1H-3(2H)-pyrazolyl)-thiourea hydrate: Synthesis, spectroscopic characterization, X-ray structure and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 30-38.	2.0	19
36124	Chemical, spectroscopic characterization, DFT studies and antibacterial activities in vitro of a new gold(I) complex with rimantadine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 114-118.	2.0	10
36125	IR and Raman spectra of nitroanthracene isomers: Substitutional effects based on density functional theory study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 129-136.	2.0	12
36126	Molecular structure and vibrational spectra of ibuprofen using density function theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 201-209.	2.0	21
36127	Synthesis, characterization and DFT study of methoxybenzylidene containing chromophores for DSSC materials. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 239-243.	2.0	46
36128	Single crystal structure, spectroscopic (FT-IR, FT-Raman, ¹ H NMR, ¹³ C NMR) studies, physico-chemical properties and theoretical calculations of 1-(4-chlorophenyl)-3-(4-nitrophenyl)triazene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 90, 193-201.	2.0	17
36129	Experimental (FT-IR, FT-Raman, NMR) and theoretical spectroscopic properties of intermolecular hydrogen bonded 1-acetyl-2-thiohydantoin polymorphs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 90, 141-151.	2.0	6
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36132	Conformational analysis, vibrational and NMR spectroscopic study of the methanesulfonamide-N ² -1,2-ethanedithiolbis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 39-47.	2.0	25
36133	Structural and spectroscopic characterization of 2-mesityl-1H-benzo[d]imidazol-3-ium chloride: A combined experimental and theoretical analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 51-60.	2.0	11
36134	Molecular structure (monomeric and dimeric structure) and HOMO-LUMO analysis of 2-aminonicotinic acid: A comparison of calculated spectroscopic properties with FT-IR and UV-vis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 83-96.	2.0	42
36135	Theoretical and experimental study on the excited states of the X-, ¹ ± and ² ±-forms of lithium phthalocyanine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 118-125.	2.0	9
36136	DFT/TD-DFT study of the spin transition complex [Fe(pmea)(NCS) ₂]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 205-209.	2.0	3
36137	Molecular structures of 2-arylaminomethyl-1H-benzimidazole: Spectral, electrochemical, DFT and biological studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 272-284.	2.0	45
36138	Vibrational, conformational and electronic structure investigations of ¹ ±, ¹ ±-dibromo-o-xylene, ¹ ±, ¹ ±-dibromo-m-xylene and ¹ ±, ¹ ±-dibromo-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 166-177.	2.0	4
36139	A comparative study on vibrational, conformational and electronic structure of ¹ ±, ¹ ±-diol-o-xylene, ¹ ±, ¹ ±-diol-m-xylene and ¹ ±, ¹ ±-diol-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 1-15.	2.0	2

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36140	Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, ¹³ C, ¹ H, UV) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 4-[(4-aminobenzene) sulfonyl] aniline by ab initio HF and density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 154-163.	2.0	136
36141	The spectroscopic (FT-IR, FT-Raman, UV) and first order hyperpolarizability, HOMO and LUMO analysis of 3-aminobenzophenone by density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 365-376.	2.0	26
36142	Molecular structure, heteronuclear resonance assisted hydrogen bond analysis, chemical reactivity and first hyperpolarizability of a novel ethyl-4-[[[2,4-dinitrophenyl]-hydrazono]-ethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate: A combined DFT and AIM approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 295-304.	2.0	32
36143	Experimental and quantum chemical computational study of (E)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 208-213.	2.0	19
36144	A comparative study on vibrational, conformational and electronic structure of 2-chloro-4-methyl-3-nitropyridine and 2-chloro-6-methylpyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 305-317.	2.0	9
36145	Vibrational spectroscopic investigation on the structure of 2-ethylpyridine-4-carbothioamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 214-222.	2.0	55
36146	Molecular structure, spectroscopic investigations, second-order nonlinear optical properties and intramolecular proton transfer of (E)-5-(diethylamino)-2-[(4-propylphenylimino)methyl]phenol: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 1-9.	2.0	43
36147	A theoretical study on cellular antioxidant activity of selected flavonoids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 235-239.	2.0	18
36148	SERS and DFT investigation of 1-(2-pyridylazo)-2-naphthol and its metal complexes with Al(III), Mn(II), Fe(III), Cu(II), Zn(II) and Pb(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 266-273.	2.0	30
36149	Spectroscopic analysis (FT-IR/FT-Raman) and molecular structure investigation on m-fluoronitrobenzene using hybrid computational calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 318-330.	2.0	5
36150	Molecular structure, spectral studies, intra and intermolecular interactions analyses in a novel ethyl 4-[3-(2-chloro-phenyl)-acryloyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer: A combined DFT and AIM approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 288-301.	2.0	27
36151	Photophysical properties of a hydrazone-based switch: A TDDFT study and comparison. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 222-227.	2.0	3
36152	Vanillin and isovanillin: Comparative vibrational spectroscopic studies, conformational stability and NLO properties by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 354-368.	2.0	54
36153	Spectroscopic (infrared, Raman, UV and NMR) analysis, Gaussian hybrid computational investigation (MEP maps/HOMO and LUMO) on cyclohexanone oxime. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 207-220.	2.0	76
36154	Experimental and theoretical vibrational investigation on the saccharinate ion in aqueous solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 399-406.	2.0	35
36155	3-Amino-1,2,4-triazolium ion in [24(3at)]Cl and [24(3at)] ₂ SnCl ₆ ·H ₂ O. Comparative X-ray, vibrational and theoretical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 204-212.	2.0	16
36156	A novel tridentate Schiff base dioxo-molybdenum(VI) complex: Synthesis, experimental and theoretical studies on its crystal structure, FTIR, UV-Vis, ¹ H NMR and ¹³ C NMR spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 29-36.	2.0	15
36157	Solvent effect on the vibrational spectra of Carvedilol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 148-164.	2.0	11

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36159	Vibrational spectra of silatranes and germatranes XM(OCH ₂ CH ₂) ₃ N (X=F,Cl,H; M=Si,Ge). The problem of the theoretical prediction of condensed phase spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 37-45.	2.0	16
36161	Ab initio Hartree-Fock and density functional theory investigations on the conformational stability, molecular structure and vibrational spectra of 5-chloro-3-(2-(4-methylpiperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one drug molecule. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 282-299.	2.0	18
36162	DFT calculation of vibrational frequencies of clusters in GaAs and the Raman spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 172-176.	2.0	4
36163	A study of molecular structure and vibrational spectra of copper(II) halide complex of 2-(2-thienyl)pyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 139-147.	2.0	20
36164	Structural characteristics and harmonic vibrational analysis of the stable conformer of 2,3-epoxypropanol by quantum chemical methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 24-34.	2.0	6
36165	Spectroscopic, electronic structure and natural bond analysis of 2-aminopyrimidine and 4-aminopyrazolo[3,4-d]pyrimidine: A comparative study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 226-241.	2.0	19
36166	Bis (trifluoromethyl) sulfone, CF ₃ SO ₂ CF ₃ : Synthesis, vibrational and conformational properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 332-339.	2.0	6
36167	Tautomeric purine forms of 2-amino-6-chloropurine (N ⁹ H ¹⁰ and N ⁷ H ¹⁰): Structures, vibrational assignments, NBO analysis, hyperpolarizability, HOMO-LUMO study using B3 based density functional calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 340-351.	2.0	48
36168	Experimental and theoretical quantum chemical investigations of 8-hydroxy-5-nitroquinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 506-516.	2.0	32
36169	Conformational analysis of the chemical shifts for molecules containing diastereotopic methylene protons. <i>Journal of Magnetic Resonance</i> , 2012, 214, 1-9.	1.2	13
36170	Vibronic fine-structure in the S ₀ →S ₁ absorption spectrum of zinc porphyrin: A Franck-Condon simulation incorporating Herzberg-Teller theory and the Duschinsky effect. <i>Journal of Molecular Spectroscopy</i> , 2012, 275, 61-70.	0.4	13
36171	Hyperfine structure in the electronic spectrum of TaS. <i>Journal of Molecular Spectroscopy</i> , 2012, 276-277, 14-18.	0.4	3
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36173	A density functional theory and laser flash photolysis investigation of carbofuran photodegradation in aqueous medium. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 235, 1-6.	2.0	8
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36304	Formal [3+3] cyclocondensations of 1,3-bis(silyloxy)-1,3-butadienes with 1-chloro-1,1-difluoro-4,4-dimethoxybut-3-en-2-one and 1,1-difluoro-4,4-dimethoxybut-3-en-2-one. Regioselective synthesis of fluorinated salicylates and pyran-4-ones. <i>Journal of Fluorine Chemistry</i> , 2012, 139, 28-45.	0.9	7
36305	Synthesis and structure of a bis-trifluoromethylthiolate complex of nickel. <i>Journal of Fluorine Chemistry</i> , 2012, 140, 112-115.	0.9	5
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36310	The impact of isomers of hemiaminal-1,2,4-triazole conjugates differently substituted in the phenyl ring and their Cu ²⁺ complexes on the catalytic activity of the antigenomic delta ribozyme. <i>Journal of Inorganic Biochemistry</i> , 2012, 108, 62-68.	1.5	1
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36312	Theoretical investigation of astacin proteolysis. <i>Journal of Inorganic Biochemistry</i> , 2012, 111, 70-79.	1.5	17
36313	Single-crystal structure, photophysical characteristics and electroluminescent properties of bis(2-(4-trifluoromethyl-2-hydroxyphenyl)benzothiazolate)zinc. <i>Journal of Luminescence</i> , 2012, 132, 919-923.	1.5	18
36314	Catalytic effects of Lewis acids on 1,3-DC reaction: A luminescent study. <i>Journal of Luminescence</i> , 2012, 132, 1456-1461.	1.5	3
36315	Synthesis and characterization of two new fluorescent macrocycles: A novel fluorescent chemosensor for zinc ion. <i>Journal of Luminescence</i> , 2012, 132, 1860-1866.	1.5	26
36316	Laser induced multi-component luminescence of [CuNCS(1,10-phen)P(CH ₂ N(CH ₂ CH ₂) ₂ O) ₃] ⁺ the first example of CuNCS complexes with diimines and tris(aminomethyl)phosphanes. <i>Journal of Luminescence</i> , 2012, 132, 1842-1847.	1.5	9
36317	Specific interactions and binding energies between thermolysin and potent inhibitors: Molecular simulations based on ab initio molecular orbital method. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 33, 1-11.	1.3	8
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36325	Microsolvation and hydrogen bond interactions in Glycine Dipeptide: Molecular dynamics and density functional theory studies. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 35, 11-20.	1.3	27
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36331	Quantum chemical computations including intermolecular interactions, natural bond orbital analysis and scaled quantum mechanical force field calculations on bezafibrate-A cholesterol drug for HIV infected. <i>Vibrational Spectroscopy</i> , 2012, 59, 9-17.	1.2	5
36332	Structural and vibrational study of 3- or 5-methyl substituted 2-N-ethylamino-4-nitropyridine N-oxides. <i>Vibrational Spectroscopy</i> , 2012, 59, 59-70.	1.2	12
36333	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. <i>Vibrational Spectroscopy</i> , 2012, 61, 156-166.	1.2	51
36334	Raman spectroscopic characterization of different regioisomers of monoacyl and diacyl chlorogenic acid. <i>Vibrational Spectroscopy</i> , 2012, 61, 10-16.	1.2	26
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36341	Structures of benzoxazine-fused triazoles as potential diuretic agents. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2012, 68, o302-o307.	0.4	3
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36353	Structure of adducts of the intermolecular interaction of dimethylpyrazole and diphenylformamidine with hydrogen halides in the solution. <i>Journal of Structural Chemistry</i> , 2012, 53, 283-289.	0.3	0
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37876	Effect of Pillar Modules and Their Stoichiometry in 3D Porous Frameworks of Zn(II) with [Fe(CN) ₆] ³⁻ : High CO ₂ /N ₂ and CO ₂ /CH ₄ Selectivity. <i>Inorganic Chemistry</i> , 2013, 52, 11385-11397.	1.9	25
37877	Density Functional Theory Assessment of Molecular Structures and Energies of Neutral and Anionic Al _n (n = 2-10) Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9293-9303.	1.1	41
37878	Studies of titanocene and zirconocene pyridine-2,6-bis-thiocarboxylates exhibiting partial desulfurization. <i>Inorganica Chimica Acta</i> , 2013, 395, 230-236.	1.2	6
37879	Structures and electronic properties of neutral (CuS) _n clusters (n=1-6): A DFT approach. <i>Chemical Physics Letters</i> , 2013, 570, 132-135.	1.2	20
37880	Role of Solvent on Charge Transfer in 7-Aminocoumarin Dyes: New Hints from TD-CAM-B3LYP and State Specific PCM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4087-4096.	2.3	133
37881	Molecular and vibrational structure of thiosulfonate S-esters. <i>Journal of Molecular Structure</i> , 2013, 1049, 165-171.	1.8	3
37882	Charged Bis-Cyclometalated Iridium(III) Complexes with Carbene-Based Ancillary Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 10292-10305.	1.9	110
37883	Ab initio Studies of Structural and Electronic Properties. , 2013, , 21-73.		1
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37885	A nonempirical scaling correction approach for density functional methods involving substantial amount of Hartree-Fock exchange. <i>Journal of Chemical Physics</i> , 2013, 138, 174105.	1.2	23
37886	Toward extension of the gas-phase basicity scale by novel pyridine containing guanidines. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 113-122.	0.7	20
37887	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. <i>Journal of Chemical Physics</i> , 2013, 139, 104112.	1.2	51
37888	Surface diffusion and coverage effect of Li atom on graphene as studied by several density functional theory methods. <i>Applied Surface Science</i> , 2013, 285, 846-852.	3.1	11
37889	Photochromic cycle of 2-hydroxyacetophenone azine studied by absorption and emission spectroscopy in different solvents. <i>Journal of Chemical Physics</i> , 2013, 139, 104305.	1.2	1
37890	Binding of modulators to mouse and human multidrug resistance P-glycoprotein. A computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 46, 10-21.	1.3	35
37891	Electronic structure and absorption spectra of 6-picoline Schiff base: A DFT and XRD based approach. <i>Journal of Molecular Structure</i> , 2013, 1050, 10-14.	1.8	14
37892	The nature of the M-NO bond in [M(Imidazole)(PPIX)(L)] _q complexes (M=Fe ²⁺ , Ru ²⁺ ; L=NO ⁺ , NO and) Tj ETQq _{1,2} 0.7843 ₃ 14 rgBT	1.1	1

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37894	Predicting the stability of aprotic solvents in Li-air batteries: pKa calculations of aliphatic C-H acids in dimethyl sulfoxide. <i>Chemical Physics Letters</i> , 2013, 558, 42-47.	1.2	49
37895	Cation-Cation Interactions in [(UO ₂) ₂ (OH) ₄] ⁴⁺ Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 11269-11279.	1.9	8
37896	Ruthenium-Catalyzed Hydrogenation of Oxygen-Functionalized Aromatic Compounds in Water. <i>ChemCatChem</i> , 2013, 5, 3241-3248.	1.8	12
37897	High-efficiency near-infrared organic light-emitting devices based on an iridium complex with negligible efficiency roll-off. <i>Journal of Materials Chemistry C</i> , 2013, 1, 6446.	2.7	87
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37900	5-Fluorolysine as alternative substrate of lysine 5,6-aminomutase: A computational study. <i>Computational and Theoretical Chemistry</i> , 2013, 1022, 1-5.	1.1	5
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37905	Semiconductive and Magnetic One-Dimensional Coordination Polymers of Cu(II) with Modified Nucleobases. <i>Inorganic Chemistry</i> , 2013, 52, 11428-11437.	1.9	38
37906	Synthesis of Solution-Processable Poly(cyclopenta[<i>c</i>]selenylvinylene) and Its Charge Transport Properties: Comparative Study with the Thiophene Analogue. <i>Macromolecules</i> , 2013, 46, 5943-5950.	2.2	16
37907	In Silico Design of Heteroaromatic Half-Sandwich Rh ^I Catalysts for Acetylene [2+2+2] Cyclotrimerization: Evidence of a Reverse Indenyl Effect. <i>Chemistry - A European Journal</i> , 2013, 19, 13337-13347.	1.7	27
37908	The Lewis Base Stabilized Parent Arsanylborane H ₂ AsBH ₂ ...NMe ₃ . <i>Chemistry - A European Journal</i> , 2013, 19, 11887-11891.	1.7	57
37909	The preferred all-gauche conformations in 3-fluoro-1,2-propanediol. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 6766.	1.5	24
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37922	pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3660-3669.	2.3	12
37923	Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in <i>Pseudomonas aeruginosa</i> Azurin. <i>Journal of the American Chemical Society</i> , 2013, 135, 4822-4833.	6.6	26
37924	Theoretical Prediction of Rare Gas Containing Hydride Cations: HRgBF ⁺ (Rg = He, Ar, Kr,) Tj ETQq1 1 0,784314 rgBT /Over	1.1	37
37925	A first principles simulation study of vibrational spectral diffusion in aqueous NaBr solutions: Dynamics of water in ion hydration shells. <i>Chemical Physics</i> , 2013, 412, 13-21.	0.9	18
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37927	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4421-4427.	2.3	28
37928	The first application of water-soluble ruthenium phenanthroline complex for dye sensitized solar cells from aqueous solution using PEDOT:PSS counter electrode versus platinum counter electrode. <i>Inorganica Chimica Acta</i> , 2013, 405, 252-257.	1.2	6

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37946	Structures and optical absorptions of PbSe clusters from <i>ab initio</i> calculations. Journal of Chemical Physics, 2013, 139, 094305.	1.2	16

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37948	Discovery of Most Stable Structures of Neutral and Anionic Phenylalanine through Automated Scanning of Tautomeric and Conformational Spaces. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4374-4381.	2.3	5
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37966	Silver(I) complexes with symmetrical Schiff bases: Synthesis, structural characterization, DFT studies and antimycobacterial assays. <i>Polyhedron</i> , 2013, 62, 104-109.	1.0	22
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37968	Quantitatively Correct UV-vis Spectrum of Ferrocene with TDB3LYP. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4064-4073.	2.3	48
37969	Synthesis and Electronic Structure of Dissymmetrical, Naphthalene-Bridged Sandwich Complexes [Cp ² Fe(1/4-C ₁₀ H ₈)MCP*] ^x (x = 0, +1; M = Fe, Ru; Cp ² = 1,1'-ETQq, 0,0'-rgBT, 1,1'-C ₁₀ H ₈)	1.1	16
37970	Synthesis of a Strained Acetylenic Macrocyclic Incorporating a <i>para</i> -Oligo[2]cruciform Bridge Bent over Nanoscopic Dimensions: Structural, Electronic, Spectroscopic, and Ion-Sensing Properties. <i>Chemistry - A European Journal</i> , 2013, 19, 12336-12349.	1.7	8
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37981	Infrared Spectra of NgBeS (Ng = Ne, Ar, Kr, Xe) and BeS ₂ in Noble-Gas Matrixes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1508-1513.	1.1	56
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38006	Unexpected strong stacking interactions between the homogeneous dimers of C ₆ F ₁₄ (6- <i>x</i>) (x=0, 1, 2, 3, 4) Tj ETQq _{1,1} 0.784314 rgB ₁₂	1.1	12
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38427	An A–D–A small molecule based on the 3,6-dithienylcarbazole electron donor (D) unit and nitrophenyl acrylonitrile electron acceptor (A) units for solution processed organic solar cells. <i>Journal of Materials Chemistry A</i> , 2013, 1, 2297-2306.	5.2	38
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38506	Structural, electronic, thermodynamical and charge transfer properties of Chloramphenicol Palmitate using vibrational spectroscopy and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 101, 335-342.	2.0	22
38507	Conformational stability, vibrational spectra, molecular structure, NBO and HOMO-LUMO analysis of 5-nitro-2-furaldehyde oxime based on DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 104, 14-25.	2.0	22
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38779	Molecular structures of N-ethylpiperidine betaine hydrate and its 1:1 complex with squaric acid. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 170-178.	1.8	8
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38797	Kinetics study on thermal dissociation of levoglucosan during cellulose pyrolysis. <i>Fuel</i> , 2013, 109, 476-483.	3.4	26
38798	A combined experimental and quantum chemical (DFT and AIM) study on molecular structure, spectroscopic properties, NBO and multiple interaction analysis in a novel ethyl 4-[2-(carbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. <i>Journal of Molecular Structure</i> , 2013, 1035, 427-440.	1.8	84
38799	A density functional theory study of the hydrolysis mechanism of phosphodiester catalyzed by a mononuclear Zn(II) complex. <i>Journal of Molecular Catalysis A</i> , 2013, 368-369, 53-60.	4.8	2
38800	Lithium binding in fluorinated phosphazene trimers. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 25-34.	1.1	6
38801	Electronic and magnetic properties of the binuclear $[Mn_2\{(OPPh)_2N\}_4]$ complex, as revealed by magnetometry, EPR and density functional broken-symmetry studies. <i>Polyhedron</i> , 2013, 52, 706-712.	1.0	1
38802	Solvent rearrangements during the transition from hydrophilic to hydrophobic solvation. <i>Chemical Physics</i> , 2013, 410, 25-30.	0.9	10
38803	Redox regulation of protein tyrosine phosphatase 1B (PTP1B): Importance of steric and electronic effects on the unusual cyclization of the sulfenic acid intermediate to a sulfenyl amide. <i>Journal of Molecular Structure</i> , 2013, 1048, 410-419.	1.8	4
38804	Low temperature Raman study of a liquid crystalline system 4-Decyloxy benzoic acid (4DBA). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 377-383.	2.0	13
38805	Interactions in 1-ethyl-3-methyl imidazolium tetracyanoborate ion pair: Spectroscopic and density functional study. <i>Journal of Molecular Structure</i> , 2013, 1038, 12-18.	1.8	31
38806	Wogonin hosted @ β -cyclodextrin: Structural, electronic and nuclear studies. <i>Journal of Molecular Liquids</i> , 2013, 188, 13-21.	2.3	6
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38808	Evolution of the electronic structure and properties of charged titanium doped aluminum nanoclusters. <i>Computational Materials Science</i> , 2013, 79, 599-610.	1.4	2
38809	Thermal decomposition of a diazido ester: Pyrolysis GC-MS and DFT study. <i>Journal of Analytical and Applied Pyrolysis</i> , 2013, 104, 603-608.	2.6	13
38810	Nitric oxide and nitroxyl formation in the reduction of trans-tetraamminenitrosyltriethylphosphiteruthenium(II) ion. <i>Inorganica Chimica Acta</i> , 2013, 394, 765-769.	1.2	9
38811	Initial growth mechanisms of ZrO ₂ and TiO ₂ thin films using cycloheptatrienyl-cyclopentadienyl heteroleptic precursors: A comparative study by density functional theory. <i>Applied Surface Science</i> , 2013, 283, 968-974.	3.1	4
38812	Excited state dynamics of a push-pull stilbene: A femtosecond transient absorption spectroscopic study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 263, 50-60.	2.0	30
38813	Structural and spectral speciation on methyl 2-(3-(furan-2-carbonyl)thioureido)benzoate: A comparative experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2013, 1048, 500-509.	1.8	8
38814	Structures, molecular orbitals and UV-vis spectra investigations on Br ₂ C ₆ H ₄ : A computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 866-875.	2.0	2

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38815	Intra- and inter-molecular hydrogen bonds, conformation and vibrational characteristics of hydrazo-group in 5-nitro-2-(2-phenylhydrazinyl)pyridine and its 3-, 4- or 6-methyl isomers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 263-275.	2.0	12
38816	Structure, stability, and vibrational fundamentals of low-lying isomers of. <i>Computational and Theoretical Chemistry</i> , 2013, 1006, 100-104.	1.1	2
38817	Ferrocene-dipeptide conjugates derived from aminoferrocene and 1-acetyl-1- ϵ^2 -aminoferrocene: synthesis and conformational studies. <i>Tetrahedron</i> , 2013, 69, 10497-10506.	1.0	19
38818	The effect of supercritical water on coal pyrolysis and hydrogen production: A combined ReaxFF and DFT study. <i>Fuel</i> , 2013, 108, 682-690.	3.4	140
38819	Characterization of citrate capped gold nanoparticle-quercetin complex: Experimental and quantum chemical approach. <i>Journal of Molecular Structure</i> , 2013, 1046, 153-163.	1.8	48
38820	Synthesis and characterisation of oxygenated magnesium phthalocyanine. <i>Polyhedron</i> , 2013, 56, 200-210.	1.0	4
38821	^{33}S NMR spectroscopy. 4. Substituent effects on the ^{33}S nuclear quadrupole coupling constants and electric field gradient in 3- and 4-substituted benzenesulphonates studied by DFT calculations in vacuo and in aqueous solution. <i>Journal of Molecular Structure</i> , 2013, 1051, 115-123.	1.8	0
38822	DNA adduct formation of mitomycin C. A test case for DFT calculations on model systems. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 9-15.	1.1	2
38823	Bonding analysis of the neutral electrophilic phosphinidene complexes of vanadium and niobium [($\eta^5\text{-C}_5\text{H}_5$)(CO) $_3\text{M}(\text{PNR}_2)$] (R = Me, iPr, tBu): A DFT study. <i>Journal of Organometallic Chemistry</i> , 2013, 740, 135-140.	0.8	7
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38825	An all cis-polyaniline nanotube film: Facile synthesis and applications. <i>Electrochimica Acta</i> , 2013, 99, 38-45.	2.6	16
38826	Highly selective and sensitive colourimetric detection of Hg $^{2+}$ ions by unsymmetrical squaraine dyes. <i>Dyes and Pigments</i> , 2013, 96, 714-721.	2.0	35
38827	Luminescent copper(II) (pseudo)halide complexes with neocuproine and a novel bulky tris (aminomethyl) phosphine derived from 2-piperazinopyridine. <i>Journal of Luminescence</i> , 2013, 143, 137-144.	1.5	12
38828	Pathways of liquefied petroleum gas pyrolysis in hydrogen plasma: A density functional theory study. <i>Journal of Energy Chemistry</i> , 2013, 22, 484-492.	7.1	4
38829	Cation site preference in zeolite clinoptilolite: A density functional study. <i>Microporous and Mesoporous Materials</i> , 2013, 177, 113-119.	2.2	27
38830	FT-IR spectroscopic analyses of 4-hydroxy-1-methyl-3-[2-nitro-2-oxoacetyl-2(1H)quinolinone (HMNOQ)]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 113, 191-195.	2.0	19
38831	Protonated pyrimidine nucleosides probed by IRMPD spectroscopy. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 54-61.	0.7	39
38832	Intermolecular spin-spin coupling constants between ^{31}P atoms. <i>Comptes Rendus Chimie</i> , 2013, 16, 937-944.	0.2	11

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38833	Investigation of coordination properties of isolated adenine to copper metal: A systematic spectroscopic and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 410-416.	2.0	10
38834	Novel oxorhenium(V) complexes of 8-hydroxyquinoline derivatives – Synthesis, spectroscopic characterization, X-ray crystal structures and DFT calculations. <i>Polyhedron</i> , 2013, 51, 263-274.	1.0	12
38835	Theoretical investigations on the electronic and optical characteristics of fused-ring homopolymers: Comparison of oligomer method and PBC~DFT method. <i>Chemical Physics Letters</i> , 2013, 570, 153-158.	1.2	19
38836	A novel 1D silver(I) coordination polymer constructed from indol-3-butyric acid: Synthesis, crystal structure and natural bond orbital analysis by DFT. <i>Journal of Molecular Structure</i> , 2013, 1037, 109-115.	1.8	9
38837	Conformational landscape of l-threonine in neutral, acid and basic solutions from vibrational circular dichroism spectroscopy and quantum chemical calculations. <i>Tetrahedron: Asymmetry</i> , 2013, 24, 1537-1547.	1.8	17
38838	Structural and computational features of four highly polar quinolin-2(1H)-ylidene derivatives: Equilibrium preference for enaminothione, enamine, and enamino tautomeric structures. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 262-270.	1.8	5
38839	Energetics of H-atom addition to naphthalene: A thermochemical cycle from tetralin to naphthalene. <i>Journal of Chemical Thermodynamics</i> , 2013, 61, 83-89.	1.0	3
38840	Host-guest inclusion complex between β -cyclodextrin and paeonol: A theoretical approach. <i>Comptes Rendus Chimie</i> , 2013, 16, 372-379.	0.2	17
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38842	Non-empirical tuning of CAM-B3LYP functional in time-dependent density functional theory for excitation energies of diarylethene derivatives. <i>Chemical Physics Letters</i> , 2013, 585, 201-206.	1.2	31
38843	The cage fragmentation of doubly ionized norbornane: A Born-Oppenheimer molecular dynamics study. <i>Chemical Physics Letters</i> , 2013, 584, 24-29.	1.2	3
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38845	The doorsill of fullerene. <i>Chemical Physics Letters</i> , 2013, 555, 217-221.	1.2	0
38846	Relativistic time-dependent density functional calculations for the excited states of the cadmium dimer. <i>Chemical Physics</i> , 2013, 415, 112-118.	0.9	2
38847	Controlled synthesis of copper halide-incorporated triiron carbonyl sulfide clusters: Synthesis, electrochemistry, and computational studies. <i>Polyhedron</i> , 2013, 52, 879-889.	1.0	4
38848	Experimental and theoretical insights into the sequential oxidations of 3i~2spiro molecules derived from oligophenylenes: A comparative study of 1,2-b-DiSpiroFluorene-IndenoFluorene versus 1,2-b-DiSpiroFluorene(tert-butyl)4-IndenoFluorene. <i>Electrochimica Acta</i> , 2013, 110, 735-740.	2.6	9
38849	Synthesis and mesomorphic investigation of calamitic liquid crystalline system ethyl-[4-(4~decyloxy)benzoyloxy]-benzoate (4-EDBB): A temperature dependent micro-Raman study and DFT calculations. <i>Vibrational Spectroscopy</i> , 2013, 69, 40-48.	1.2	18
38850	Structural and electronic properties of stable Lin (n=2~10) clusters: A density functional study. <i>Physica B: Condensed Matter</i> , 2013, 430, 74-80.	1.3	9

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38852	Ab initio calculations of the Fe(II) and Fe(III) isotopic effects in citrates, nicotianamine, and phytosiderophore, and new Fe isotopic measurements in higher plants. <i>Comptes Rendus - Geoscience</i> , 2013, 345, 230-240.	0.4	35
38853	Exploring physicochemical aspects of N-alkylimidazolium based ionic liquids. <i>Journal of Molecular Liquids</i> , 2013, 181, 142-151.	2.3	32
38854	2-[(Diphenylphosphino)methyl]-6-methylpyridine (PN) coordination chemistry at trismium clusters: Regiospecific ligand activation and DFT evaluation of the isomeric Os ₃ (CO) ₁₀ (PN) clusters. <i>Journal of Organometallic Chemistry</i> , 2013, 744, 24-34.	0.8	6
38855	Competitive supramolecular interaction of carbachol and berberine with cucurbit[7]uril and its analytical application. <i>Microchemical Journal</i> , 2013, 110, 285-291.	2.3	14
38856	A study of the valence shell electronic structure and photoionisation dynamics of para-dichlorobenzene and para-bromochlorobenzene. <i>Chemical Physics</i> , 2013, 415, 291-308.	0.9	15
38857	Investigation of spectroscopic, structural and non-linear optical properties of ethyl 3,5-dimethyl-4-[(benzenesulfonyl)-hydrazonoethyl]-1H-pyrrol-2-carboxylate. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 123-133.	1.8	18
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38859	Synthesis and structural characterization of asymmetric mononuclear ruthenium (II) complexes derived from 2-(1,2,3-thiadiazol-4-yl)pyridine and azoimine ligands. <i>Inorganica Chimica Acta</i> , 2013, 400, 20-25.	1.2	9
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38861	Fluorinated bis(phenoxy-imine)titanium complexes with methylaluminoxane for the synthesis of ultra high molecular weight polyethylene. <i>Polymer</i> , 2013, 54, 3217-3222.	1.8	6
38862	Stabilization of diketo tautomer of curcumin by pre-micellar anionic surfactants: UV-Visible, fluorescence, tensiometric and TD-DFT evidences. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 104, 150-157.	2.0	41
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38864	Computational study on the mechanism of non-catalyzed and catalyzed bromolactonization. <i>Computational and Theoretical Chemistry</i> , 2013, 1024, 45-51.	1.1	2
38865	ESIPT-inspired benzothiazole fluorescein: Photophysics of microenvironment pH and viscosity. <i>Dyes and Pigments</i> , 2013, 98, 507-517.	2.0	42
38866	Zone centre phonon frequencies for lithium manganese oxides Li _x Mn ₂ O ₄ (x=1, 0.5 and 0.015). <i>Computational Materials Science</i> , 2013, 77, 384-386.	1.4	2
38867	Intramolecular cyclization reaction mechanism and regioselectivities of unsubstituted and benzene-substituted 4-penteniminy radicals: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 75-83.	1.1	10
38868	Pesticide interaction with environmentally important cations: A theoretical study of atrazine in interaction with two Ca ²⁺ cations. <i>Computational and Theoretical Chemistry</i> , 2013, 1022, 6-13.	1.1	11

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38870	Theoretical study on the electronic structures and phosphorescence properties of five osmium(II) complexes with different P [^] P ancillary ligands. <i>Chemical Physics Letters</i> , 2013, 573, 29-34.	1.2	4
38871	Effect of synthesis method on selective adsorption of thiosulfate by calcined MgAl-layered double hydroxides. <i>Chemical Engineering Journal</i> , 2013, 232, 510-518.	6.6	23
38872	Interaction of protonated tyramine with a hexaarylbenzene-based receptor: Extraction and DFT study. <i>Journal of Molecular Structure</i> , 2013, 1047, 277-281.	1.8	7
38873	Dynamical (e,2e) investigations of tetrahydrofuran and tetrahydrofurfuryl alcohol as DNA analogues. <i>Chemical Physics Letters</i> , 2013, 572, 32-37.	1.2	39
38874	Overcoming the existent computational challenges in the ab initio calculations of the two-photon circular dichroism spectra of large molecules using a fragment-recombination approach. <i>Chemical Physics Letters</i> , 2013, 568-569, 176-183.	1.2	6
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38881	A theoretical study of factors affecting corrosion in supercritical water reaction vessels. <i>Journal of Supercritical Fluids</i> , 2013, 79, 261-267.	1.6	10
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38883	Sensitive electron capture decay rate of ⁷ Be encapsulated in carbon nanotubes: A density functional study. <i>Chemical Physics Letters</i> , 2013, 561-562, 137-141.	1.2	5
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38885	The effect of density functional and dispersion interaction on structure and bonding analysis of uranium(VI) nitride complex [NU{N(CH ₂ CH ₂ NSiMe ₃) ₃ }] [^] : A theoretical study. <i>Inorganic Chemistry Communication</i> , 2013, 37, 4-6.	1.8	3
38886	Modeling of multifunctional donor-bridge-acceptor 4,6-di(thiophen-2-yl)pyrimidine derivatives: A first principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 168-176.	1.3	30

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38888	Effects of interfacial structure and polarity on charge transfer between carbonaceous nanomaterials and rutile (110) surface. <i>Computational Materials Science</i> , 2013, 69, 180-185.	1.4	4
38889	Iron-iron bonding versus iron-phosphorus bonding in binuclear diphosphacyclobutadiene iron carbonyl complexes. <i>Polyhedron</i> , 2013, 65, 298-307.	1.0	4
38890	The addition mechanism of TMS-CN into N-acetylpyridinium to give 2-cyanoacetylpyridinium: The roles of TpW(NO)(PMe ₃) and DABCO. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 117-128.	0.8	2
38891	Boronic acid sensors for saccharides: A theoretical study. <i>Chemical Physics Letters</i> , 2013, 586, 111-115.	1.2	14
38892	Experimental and DFT studies on the antioxidant activity of a C-glycoside from <i>Rhynchosia capitata</i> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 103, 442-452.	2.0	50
38893	Theoretical study of hydrogen adsorption on Co clusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 183-190.	1.1	13
38894	Methylborabenzene ligands in binuclear iron carbonyl derivatives: High spin states and iron-iron multiple bonding. <i>Journal of Organometallic Chemistry</i> , 2013, 747, 106-112.	0.8	1
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38899	Benchmark calculations of density functionals for organothiol adsorption on gold surfaces. <i>Computational and Theoretical Chemistry</i> , 2013, 1009, 60-69.	1.1	3
38900	NMR spectroscopic and computational investigations of RuHCl(CO)(PPh ₃) ₃ catalyzed isomerization of 1,4-cyclohexadiene. <i>Journal of Organometallic Chemistry</i> , 2013, 741-742, 15-19.	0.8	6
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38902	Water assisted reaction mechanism of OH [•] with CCl ₄ in aqueous solution - Hybrid quantum mechanical and molecular mechanics investigation. <i>Chemical Physics Letters</i> , 2013, 559, 30-34.	1.2	5
38903	A combined experimental and theoretical study of micronized coal reburning. <i>Frontiers in Energy</i> , 2013, 7, 119-126.	1.2	3
38904	Conjugated push-pull salts derived from linear benzobisthiazole: preparation and optical properties. <i>Chemical Papers</i> , 2013, 67, .	1.0	4

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38906	Experimental and Theoretical Characterization of a Lone Pair π Complex: Water π -Hexafluorobenzene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1336-1350.	1.1	40
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38908	Nanoscale insight into the exfoliation mechanism of graphene with organic dyes: effect of charge, dipole and molecular structure. <i>Nanoscale</i> , 2013, 5, 4205.	2.8	116
38909	Photophysical properties, photostability and laser activity of 2,6-bis [1 ² -(2-benzoxazolyl) vinyl] naphthalene (BBVN). <i>Journal of Molecular Structure</i> , 2013, 1037, 323-331.	1.8	9
38910	Quantum chemical investigation of epoxide and ether groups in graphene oxide and their vibrational spectra. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3725.	1.3	42
38911	Molecular Design of Porphyrins for Dye-Sensitized Solar Cells: A DFT/TDDFT Study. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 524-530.	2.1	123
38912	Density Functional Theory and Molecular Interactions: Dispersion Interactions. <i>Structure and Bonding</i> , 2013, , 65-96.	1.0	8
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38918	Can surface energy be a parameter to define morphological change of rock-salt crystals with additives? A first principles study. <i>CrystEngComm</i> , 2013, 15, 2631.	1.3	17
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38920	Molecular structural, non-linear optical, second order perturbation and Fukui studies of Indole-3-Aldehyde using density functional calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 106, 299-309.	2.0	27
38921	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order. <i>Journal of Chemical Physics</i> , 2013, 138, 074108.	1.2	84
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42403	Conformational analysis and vibrational study of daidzein by using FT-IR and FT-Raman spectroscopies and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 120, 405-415.	2.0	37
42404	Quantum chemical calculations of conformation, vibrational spectroscopic, electronic, NBO and thermodynamic properties of 2,2-dichloro-N-(2,3-dichlorophenyl) acetamide and 2,2-dichloro-N-(2,3-dichlorophenyl) acetamide. <i>Computational and Theoretical Chemistry</i> , 2014, 1032, 27-41.	1.1	10
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43697	Amplified Vibrational Circular Dichroism as a Probe of Local Biomolecular Structure. <i>Journal of the American Chemical Society</i> , 2014, 136, 3530-3535.	6.6	53
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44111	Molecular insight of isotypes specific β -tubulin interaction of tubulin heterodimer with noscapinoids. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 751-763.	1.3	32

#	ARTICLE	IF	CITATIONS
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44126	Experimental Measurement and Theory of Substituent Effects in Î€-Hydrogen Bonding: Complexes of Substituted Phenols with Benzene. <i>Journal of Organic Chemistry</i> , 2014, 79, 6823-6831.	1.7	23
44127	Redox Reactions of Nickel, Copper, and Cobalt Complexes with â€œNoninnocentâ€•Dithiolate Ligands: Combined in Situ Spectroelectrochemical and Theoretical Study. <i>Organometallics</i> , 2014, 33, 4846-4859.	1.1	29
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44182	Feeling and investigating blue: On the enthalpy of formation of indigo. <i>Journal of Chemical Thermodynamics</i> , 2014, 73, 69-75.	1.0	3
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44197	Substituent effects in <i>trans</i> - <i>p</i> , <i>p</i> -disubstituted azobenzenes: X-ray structures at 100 K and DFT-calculated structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2014, 70, 575-579.	0.2	5
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44218	Spectroscopic, crystallographic and theoretical studies of lasalocid complex with ammonia and benzylamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 297-307.	2.0	4
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44226	Fused Azacalix[4]arenes. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 745-752.	1.2	9
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44738	Electronic structure of low work function electrodes modified by C ₁₆ H ₃₃ SH. <i>Materials Research Bulletin</i> , 2014, 58, 19-23.	2.7	3
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44743	Investigation of intense femto-second laser ionization and dissociation of methane with time-dependent density-functional approach. <i>Chemical Physics Letters</i> , 2014, 604, 60-67.	1.2	12
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44746	First-principle study of atomic oxygen and nitrogen adsorption on (111) β -cristobalite as a model of thermal protection coverage. <i>Acta Astronautica</i> , 2014, 100, 40-46.	1.7	13
44747	Study of conformational stability, structural, electronic and charge transfer properties of cladrin using vibrational spectroscopy and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 615-628.	2.0	5
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44751	Vibrational spectroscopic study and NBO analysis on tranexamic acid using DFT method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 184-192.	2.0	76
44752	Comparative experimental and theoretical studies of N-(4-Methylbenzylidene)-N ² -(2-carboxyphenyl) hydrazine novel Schiff base. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 490-497.	2.0	7
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44755	The theoretical assessment and prediction of CBr bond dissociation enthalpies. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 116-124.	1.1	14
44756	The molecular conformation of butyl acrylate – A vibrational spectroscopy and computational study. <i>Vibrational Spectroscopy</i> , 2014, 73, 56-66.	1.2	6
44757	Neutral heteroleptic rhenium-based M ₃ L ₃ L ² type metallacycles: Synthesis, structural characterization and DFT/TDDFT studies. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 224-232.	0.8	20
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44761	Synthesis, experimental spectra (IR & Raman and NMR), vibrational analysis and theoretical DFT investigations of N-(5-(4-methylbenzoyl)-2-oxo-4-(4-methylphenyl)pyrimidine-1(2H)-yl)-4-methylbenzamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 22-34.	2.0	4
44762	Quantum chemical and spectroscopic investigations of 3-methyladenine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 653-664.	2.0	39
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44774	Theoretical study on mechanism of reactions of triarylphosphines with S-nitrosated proteins. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 11-18.	1.1	0
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44779	Intramolecular resonance-assisted hydrogen bonds: A theoretical description by means of atomic charges and charge fluxes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 465-472.	2.0	8
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44809	Fine-Tuning Dual Emission and Aggregation-Induced Emission Switching in NPI-BODIPY Dyads. <i>Chemistry - A European Journal</i> , 2014, 20, 9052-9062.	1.7	55
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44817	Isothermal Cold Crystallization Kinetics Study of Sildenafil. <i>Crystal Growth and Design</i> , 2014, 14, 3199-3209.	1.4	30
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47363	Theoretical study on catalyzed selective photoreduction mechanism for 4-bromobenzaldehyde in two different solvents. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19997-20005.	1.3	2
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47983	Dithiafulvalene functionalized diketopyrrolopyrrole based sensitizers for efficient hydrogen production. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13710-13718.	1.3	22
47984	Benzothiadiazole-based organic dyes with pyridine anchors for dye-sensitized solar cells: effect of donor on optical properties. <i>Tetrahedron</i> , 2015, 71, 4203-4212.	1.0	38
47985	Physicochemical properties of the ternary complexes of Pt(<i>scp</i>) with uracil and small peptide moieties: an experimental and computational study. <i>New Journal of Chemistry</i> , 2015, 39, 5208-5217.	1.4	3
47986	A family of unsymmetrical hydroxyl-substituted BEDT-TTF donors: syntheses, structures and preliminary thin film studies. <i>RSC Advances</i> , 2015, 5, 40205-40218.	1.7	5
47987	Conformational Stability and Thermal Pathways of Relaxation in Triclosan (Antibacterial/Excipient/Contaminant) in Solid-State: Combined Spectroscopic (¹ H NMR) and Computational (Periodic DFT) Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4864-4874.	1.1	21
47988	Metal complexation studies of amylopectin-graft-poly[(N,N-dimethylacrylamide)-co-(acrylic acid)]: a biodegradable synthetic graft copolymer. <i>Polymer International</i> , 2015, 64, 1336-1351.	1.6	18
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47991	Dual wavelength asymmetric photochemical synthesis with circularly polarized light. <i>Chemical Science</i> , 2015, 6, 3853-3862.	3.7	58
47992	Syntheses, structural diversity and properties of three coordination polymers built by chlorophenyl imidazole dicarboxylate. <i>Supramolecular Chemistry</i> , 2015, 27, 141-150.	1.5	4
47993	Synthesis, spectral analysis (FT-IR, ¹ H NMR, ¹³ C NMR and UV-visible) and quantum chemical studies on molecular geometry, NBO, NLO, chemical reactivity and thermodynamic properties of novel 2-amino-4-(4-(dimethylamino)phenyl)-5-oxo-6-phenyl-5,6-dihydro-4H-pyrano[3,2-c]quinoline-3-carbonitrile. <i>Journal of Molecular Structure</i> , 2015, 1095, 112-124.	1.8	31
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48001	Stereoselective Syntheses of (+)-2- <i>epi</i> -Deoxoprosopinine, ($\hat{\alpha}$)-Deoxoprosophylline, (+)- <i>cis</i> -195A, and 2,5-Di- <i>epi</i> - <i>cis</i> -195A from a Common Chiral Nonracemic Building Block. <i>Journal of Organic Chemistry</i> , 2015, 80, 5236-5251.	1.7	13
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48014	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1948-1956.	1.1	23
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48027	A Trimetal Carbene with Reactivity Reminiscent of Fischer-Tropsch Catalysis. <i>Organometallics</i> , 2015, 34, 1651-1660.	1.1	5
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48030	A highly selective CHEF-type chemosensor for monitoring Zn^{2+} in aqueous solution and living cells. <i>RSC Advances</i> , 2015, 5, 41905-41913.	1.7	59
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48033	Structure and Conformation of Protonated d-(+)-Biotin in the Unsolvated State. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6198-6203.	1.2	10
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48041	High-conductance surface-anchoring of a mechanically flexible platform-based porphyrin complex. <i>New Journal of Physics</i> , 2015, 17, 013012.	1.2	17
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48047	Effect of branched and cycloalkyl functionalities on CO ₂ separation performance of poly(IL) membranes. <i>Separation and Purification Technology</i> , 2015, 155, 89-95.	3.9	27
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48066	An introduction to applied quantum mechanics in the Wigner Monte Carlo formalism. <i>Physics Reports</i> , 2015, 577, 1-34.	10.3	47
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48084	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1481-1492.	2.3	90
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48086	Polymorphic phase transition mechanism of compressed coesite. <i>Nature Communications</i> , 2015, 6, 6630.	5.8	47
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48089	FT-IR, FT-Raman, UV/Vis spectra and fluorescence imaging studies on 2-(bromoacetyl)benzo(b)furan by ab initio DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 147, 212-224.	2.0	8

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48092	Molecular thermodynamics of metabolism: quantum thermochemical calculations for key metabolites. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10438-10453.	1.3	16
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48097	Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach. <i>Journal of Chemical Physics</i> , 2015, 142, 064109.	1.2	60
48098	Regioselective synthesis and ab initio calculations of fused heterocycles thermally and under microwave irradiation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 148, 175-183.	2.0	6
48099	In situ prepared copper nanoparticles on modified KIT-5 as an efficient recyclable catalyst and its applications in click reactions in water. <i>Journal of Molecular Catalysis A</i> , 2015, 402, 100-108.	4.8	83
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49047	Relationship Between the Free Radical Polymerization Rates of Methacrylates and the Chemical Properties of their Monomeric Radicals. <i>Macromolecular Chemistry and Physics</i> , 2015, 216, 334-343.	1.1	2
49048	Oxidative addition of SiH ₄ and GeH ₄ to Ir(PPh ₃) ₂ (CO)Cl: structural and spectroscopic evidence for the formation of products derived from cis oxidative addition. <i>Dalton Transactions</i> , 2015, 44, 2801-2808.	1.6	2
49049	Studies on Orientation of Cyclization in Thiazolo-Quinazoline Heterocyclic System Through NMR, DFT, and X-ray Diffraction. <i>Journal of Heterocyclic Chemistry</i> , 2015, 52, 1046-1054.	1.4	2
49050	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. <i>Superlattices and Microstructures</i> , 2015, 79, 79-85.	1.4	12
49051	DFT electronic structure calculations, spectroscopic studies, and normal coordinate analysis of 2-[(5-nitro-1,3-thiazol-2-yl)carbamoyl]phenyl acetate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 743-752.	2.0	7
49052	Five-coordinate Indium(III) Porphyrins with Hydroxy and Carboxy BODIPY as Axial Ligands: Synthesis, Characterization and Photophysical Studies. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 468-477.	1.0	20
49053	Toward the construction of parameter-free doubly hybrid density functionals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 589-595.	1.0	22
49054	Molybdenum L-edge XAS Spectra of MoFe Nitrogenase. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2015, 641, 65-71.	0.6	36
49055	Cyclometalated Fe(II) Complexes as Sensitizers in Dye-Sensitized Solar Cells. <i>Inorganic Chemistry</i> , 2015, 54, 560-569.	1.9	78
49056	³ He NMR studies on helium-pyrrole, helium-indole, and helium-carbazole systems: a new tool for following chemistry of heterocyclic compounds. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 103-109.	1.1	9
49057	Triphenylacetic Acid Amides: Molecular Propellers with Induced Chirality. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 738-749.	1.2	20
49058	Molecular insight into the interaction mechanisms of amino-2H-imidazole derivatives with BACE1 protease: A QM/MM and QTAIM study. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 389-397.	1.0	20
49059	A novel fluorescent nano-chemosensor for cesium ions based on naphthalene macrocyclic derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 279-285.	2.0	10
49060	Designing Stable Radicals with Highly Electrophilic or Nucleophilic Character: Thiadiazinyl as a Case Study. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 506-513.	1.2	13
49061	Access to Novel Graphene-Like Sheet of Hydroboron: First-Principles Investigation. <i>Chemistry - an Asian Journal</i> , 2015, 10, 362-369.	1.7	2
49062	Mechanistic aspects of the reaction of uranium atom with H ₂ O in the gas phase. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2015, 304, 489-499.	0.7	9
49063	Nonfluorobutanesulfonyl Azide as a Shelf-Stable Highly Reactive Oxidant for the Copper-Catalyzed Synthesis of 1,3-Diyne from Terminal Alkynes. <i>Journal of Organic Chemistry</i> , 2015, 80, 1098-1106.	1.7	24

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49069	Influence of Ligand Substitution Pattern on Structure in Cobalt(II) Complexes of Bulky <i>N</i>, <i>Nâ€²</i> Diarylformamidinate <i>N</i>, <i>O</i> Oxides. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 73-82.	1.0	15
49070	Effect of Solvent and Protonation/Deprotonation on Electrochemistry, Spectroelectrochemistry and Electronâ€Transfer Mechanisms of Nâ€Confused Tetraarylporphyrins in Nonaqueous Media. <i>Chemistry - A European Journal</i> , 2015, 21, 2651-2661.	1.7	24
49071	Rhenabenzenes and Unexpected Coupling Products from the Reactions of Rhenacyclobutadienes with Ethoxyethyne. <i>Organometallics</i> , 2015, 34, 167-176.	1.1	27
49072	Mechanistic Details and Reactivity Descriptors in Oxidation and Acid Catalysis of Methanol. <i>ACS Catalysis</i> , 2015, 5, 666-682.	5.5	49
49073	Correlations between hardness, electrostatic interactions, and thermodynamic parameters in the decomposition reactions of 3-buten-1-ol, 3-methoxy-1-propene, and ethoxyethene. <i>Structural Chemistry</i> , 2015, 26, 547-554.	1.0	3
49074	Deep-blue emitting pyreneâ€benzimidazole conjugates for solution processed organic light-emitting diodes. <i>RSC Advances</i> , 2015, 5, 8727-8738.	1.7	31
49075	Scalar Relativistic Calculations of Hyperfine Coupling Constants Using <i>Ab Initio</i> Density Matrix Renormalization Group Method in Combination with Third-Order Douglasâ€Krollâ€Hess Transformation: Case Studies on 4d Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 73-81.	2.3	17
49076	Study of Properties on Different B_nN_n Nano Structures in Point of Theoretical Calculations. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015, 23, 239-244.	1.0	0
49077	Structure evolution of nanoparticulate Fe₂O₃. <i>Nanoscale</i> , 2015, 7, 2960-2969.	2.8	47
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49080	NMR, DFT and luminescence studies of the complexation of V(v) oxoions in solution with 8-hydroxyquinoline-5-sulfonate. <i>New Journal of Chemistry</i> , 2015, 39, 1488-1497.	1.4	11
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49083	Quantum Chemistry in Proton-Conductors. <i>Advances in Quantum Chemistry</i> , 2015, , 31-67.	0.4	15
49084	Reactions of Ti, Zr, and Hf Atoms with Hydrogen Sulfide: Argon Matrix Infrared Spectra and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2244-2252.	1.1	8
49085	Protein-Like Dynamics of Polycarbonate Polymers in Water. <i>Journal of Physical Chemistry B</i> , 2015, 119, 316-329.	1.2	5
49086	Effect of alkyl substituents in BODIPYs: a comparative DFT computational investigation. <i>RSC Advances</i> , 2015, 5, 2706-2714.	1.7	25
49087	Organic Thin Film Transistors Based on Highly Dipolar Donor-Acceptor Polymethine Dyes. <i>Advanced Functional Materials</i> , 2015, 25, 44-57.	7.8	42
49088	Spin effects in thermoelectric phenomena in SiC nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1925-1933.	1.3	11
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49090	Reaching for two new stable ambiphilic quinoline-derived <i>N</i> -heterocyclic carbenes at DFT level. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 224-230.	1.0	2
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49093	Photolysis of acetophenone derivatives with β -cyclopropyl substituents. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 137-146.	0.9	1
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49095	2-((E)-(2-aminophenylimino)methyl)-6-isopropyl-3-methylphenol based fluorescent receptor for dual Ni ²⁺ and Cu ²⁺ recognition: Nanomolar detection. <i>Polyhedron</i> , 2015, 87, 79-85.	1.0	15
49096	Electrochemical behaviour of Tris(β^2 -diketonato)iron(III) complexes: A DFT and experimental study. <i>Electrochimica Acta</i> , 2015, 152, 512-519.	2.6	52
49097	Synthesis, crystal structure, computational and photophysical studies of new hydrazone-thiazole derivatives decorated with N-methyl tetrahydrocarbazole pendant. <i>Journal of Molecular Structure</i> , 2015, 1080, 137-144.	1.8	7
49098	Quantum mechanical and experimental analyses of TNT metabolite 2-hydroxylamino-4,6-dinitrotoluene. <i>Journal of Molecular Structure</i> , 2015, 1080, 145-152.	1.8	4
49099	Coordination of noble metals by an ambiphilic PBiP pincer ligand: Metallophilic Bi-Cu and Bi-Ag interactions. <i>Journal of Organometallic Chemistry</i> , 2015, 784, 62-68.	0.8	20

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49101	Vibrational spectroscopic and DFT calculation studies of 2-amino-7-bromo-5-oxo-[1]benzopyrano [2,3-b]pyridine-3 carbonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 252-263.	2.0	44
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49107	Push-pull molecular structures based on angular benzobisthiazolium acceptor: synthesis, photophysical properties and theoretical studies. <i>Tetrahedron</i> , 2015, 71, 315-323.	1.0	4
49108	Rational design of biaryl pharmacophore inserted noscapine derivatives as potent tubulin binding anticancer agents. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 249-270.	1.3	35
49109	Photo- and Electrocatalytic Reduction of CO ₂ by [Re(CO) ₃ (L) ₂ (Imine)(4-piperidinyl-1,8-naphthalimide)]Cl Complexes. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 296-304.		45
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49112	Poly(sulfobetaine methacrylate)s as Electrode Modifiers for Inverted Organic Electronics. <i>Journal of the American Chemical Society</i> , 2015, 137, 540-549.	6.6	62
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49116	DFT calculations of thiosemicarbazide, arylisothiocyanates, and 1-aryl-2,5-dithiohydrazodicarbonamides as corrosion inhibitors of copper in an aqueous chloride solution. <i>Journal of Industrial and Engineering Chemistry</i> , 2015, 26, 291-308.	2.9	83
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49121	Understanding Zinc(II) Chelation with Quercetin and Luteolin: A Combined NMR and Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 83-95.	1.2	68
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49130	Raman microimaging of murine lungs: insight into the vitamin A content. <i>Analyst</i> , 2015, 140, 2171-2177.	1.7	18
49131	Novel Dengue Virus NS2B/NS3 Protease Inhibitors. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 1100-1109.	1.4	108
49132	A DFT investigation of structure, spectroscopic properties and tautomerism of the anticonvulsant drug Lyrica. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 637-642.	2.0	15
49133	Structural Stability, Acidity, and Halide Selectivity of the Fluoride Riboswitch Recognition Site. <i>Journal of the American Chemical Society</i> , 2015, 137, 299-306.	6.6	26
49134	Indolizine-Based Donors as Organic Sensitizer Components for Dye-Sensitized Solar Cells. <i>Advanced Energy Materials</i> , 2015, 5, 1401629.	10.2	71
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49137	A Combined Experiment and Computation Study of the Fused Polycyclic Benzimidazole Derivatives. <i>Journal of Fluorescence</i> , 2015, 25, 127-136.	1.3	1
49138	Composite Method for Implicit Representation of Solvent in Dimethyl Sulfoxide and Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5173-5180.	1.1	22
49139	Approximate quantum trajectory dynamics for reactive processes in condensed phase. <i>Molecular Simulation</i> , 2015, 41, 86-106.	0.9	7
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49148	A Combined Experimental and Computational Investigation on the Unusual Molecular Mechanism of the Lossen Rearrangement Reaction Activated by Carcinogenic Halogenated Quinones. <i>Journal of Organic Chemistry</i> , 2015, 80, 180-189.	1.7	24
49149	Theoretical prediction of detonation performance and stability for energetic polydinitroaminoprismanes. <i>RSC Advances</i> , 2015, 5, 7766-7772.	1.7	13
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49174	Protocols Utilizing Constant pH Molecular Dynamics to Compute pH-Dependent Binding Free Energies. <i>Journal of Physical Chemistry B</i> , 2015, 119, 861-872.	1.2	29
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49263	Extinction coefficients of CC and CC bands in ethyne and ethene molecules interacting with Cu ⁺ and Ag ⁺ in zeolites – IR studies and quantumchemical DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1988-1992.	2.0	4
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49285	Uranyl extraction by N,N-dialkylamide ligands studied using static and dynamic DFT simulations. <i>Dalton Transactions</i> , 2015, 44, 2623-2638.	1.6	17
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49292	Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. <i>Journal of Computational Chemistry</i> , 2015, 36, 151-163.	1.5	26
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49296	Structure and bonding analysis of intermediate model heme-imidazole and heme-thiolate enzymes complexed with formate, acetate and nitrate: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 137-143.	1.1	1
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49303	Spectroscopic (FT-IR, ¹ H, ¹³ C NMR, UV), DOS and orbital overlap population analysis of copper complex of (E)-4-(2-(4-nitrophenyl) diazenyl)-N, N bis ((pyridin-2-yl) methyl) benzamine by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1932-1940.	2.0	3
49304	FTIR, FT-Raman, UV-Visible spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 961-978.	2.0	49
49305	Vibrational spectroscopic investigations of 4,4-dimethyl-2-oxazoline: A density functional theory approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1530-1542.	2.0	8
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49307	Ab initio study of two quinoline derivatives as corrosion inhibitor in acidic media: electronic structure, inhibitor-metal interaction, and nuclear quadrupole resonance parameters. <i>Research on Chemical Intermediates</i> , 2015, 41, 6789-6802.	1.3	16
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49315	Identifying dominant conformations of N-acetyl-l-cysteine methyl ester and N-acetyl-l-cysteine in water: VCD signatures of the amide I and the CO stretching bands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 131-140.	2.0	8

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49317	The $F^+ + CH_3I \rightarrow FCH_3 + I^+$ entrance channel potential energy surface. <i>International Journal of Mass Spectrometry</i> , 2015, 377, 222-227.	0.7	19
49318	1,3,4-Thiadiazolidine-2,5-dione: Crystal Structure, Calculation of Aromaticity and Photodecomposition Quantum Yield. <i>Journal of Heterocyclic Chemistry</i> , 2015, 52, 392-396.	1.4	1
49319	An NMR and Computational Study of Azolo[<i>c</i>]pyrimidines with Special Emphasis on Pyrazolo[1,5- <i>a</i>]pyrimidines. <i>Journal of Heterocyclic Chemistry</i> , 2015, 52, 336-345.	1.4	14
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49333	FTIR, Raman and NMR spectroscopic and DFT theoretical studies on poly(N-vinylimidazole). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 134, 267-275.	2.0	51

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49536	Accurate Equilibrium Structures for Piperidine and Cyclohexane. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1486-1493.	1.1	17
49537	Experimental and theoretical binding affinity between polyvinylpyrrolidone and selected phenolic compounds from food matrices. <i>Food Chemistry</i> , 2015, 168, 464-470.	4.2	28
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50520	Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2155-2164.	1.2	22
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53150	First Principle Analysis of (10-Boranyl anthracene-9-yl)borane-Based Molecular Single-Electron Transistor for High-Speed Low-Power Electronics. <i>IEEE Transactions on Electron Devices</i> , 2016, 63, 1232-1238.	1.6	14
53151	Reaction of TiCl ₄ with diethyl ether. Experimental and quantum-chemical study. <i>Russian Journal of General Chemistry</i> , 2016, 86, 9-17.	0.3	0
53152	Structure and charge density distribution of amine azide based hypergolic propellant molecules: a theoretical study. <i>Canadian Journal of Chemistry</i> , 2016, 94, 126-136.	0.6	5
53153	Interaction of L-proline with group IIB (Zn ²⁺ , Cd ²⁺ , Tl ⁺) complexes. <i>Canadian Journal of Chemistry</i> , 2016, 94, 501-508.	0.6	6
53154	Performance of Minnesota functionals on predicting core-level binding energies of molecules containing main-group elements. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	23
53155	Second- and third-order nonlinear optical properties of unsubstituted and mono-substituted chalcones. <i>Chemical Physics Letters</i> , 2016, 648, 91-96.	1.2	57
53156	Color tuning of cyclometalated 2-phenylbenzo[d]oxazole-based iridium(III) complexes through modification of different N ^O ancillary ligands. <i>Inorganica Chimica Acta</i> , 2016, 445, 22-27.	1.2	6
53157	Enantiospecific formation of a metal-mediated base pair inside a DNA duplex. <i>Inorganica Chimica Acta</i> , 2016, 452, 181-187.	1.2	28
53158	Supramolecular nickel complex based on thiosemicarbazone. Synthesis, transfer hydrogenation and unexpected thermal behavior. <i>Polyhedron</i> , 2016, 110, 188-196.	1.0	11
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53160	Hydrogen Bond Basicity Prediction for Medicinal Chemistry Design. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4278-4288.	2.9	48
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53164	Comparative study of H ₂ adsorption on B ₂₄ N ₂₄ , Al ₂₄ N ₂₄ and B ₁₂ Al ₁₂ N ₂₄ clusters. <i>Computational Materials Science</i> , 2016, 117, 71-75.	1.4	21
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53166	Potential energy profile, structural, vibrational and reactivity descriptors of trans-2-methoxycinnamic acid by FTIR, FT-Raman and quantum chemical studies. <i>Journal of Molecular Structure</i> , 2016, 1113, 42-54.	1.8	16

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53171	Layered double hydroxide and sulindac coiled and scrolled nanoassemblies for storage and drug release. <i>RSC Advances</i> , 2016, 6, 16419-16436.	1.7	45
53172	A theoretical study of the regio- and stereoselectivities of non-polar 1,3-dipolar cycloaddition reaction between C-diethoxyphosphoryl-N-methylnitrene and N-(2-fluorophenyl)acrylamide. <i>Molecular Physics</i> , 2016, 114, 663-670.	0.8	9
53173	Efficient way of designing fullerene derivatives based on simplified DFT calculations and QSPR modeling. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 152, 125-133.	1.8	9
53174	Theoretical predictions on structures and p-, s-orbital aromaticities of the Hg ₃ B ₃ + ³⁺ , Hg ₃ B ₃ X (X = Li, Na, and K) and Hg ₃ B ₃ Mg + clusters. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 66-71.	1.1	0
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53181	Benzimidazole-BODIPY as optical and fluorometric pH sensor. <i>Dyes and Pigments</i> , 2016, 128, 165-169.	2.0	58
53182	The structure and properties of 5,6-dinitro-1H-benzotriazole. <i>Journal of Molecular Structure</i> , 2016, 1113, 153-161.	1.8	8
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53188	Solvent sensitive intramolecular charge transfer dynamics in the excited states of 4-N,N-dimethylamino-4-nitrobiphenyl. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7661-7671.	1.3	62
53189	Rhodamine-modified upconversion nanoprobe for distinguishing Cu ²⁺ from Hg ²⁺ and live cell imaging. <i>New Journal of Chemistry</i> , 2016, 40, 3543-3551.	1.4	27
53190	Cost-effective solar concentrators based on red fluorescent Zn(salicylaldiminato) complex. <i>RSC Advances</i> , 2016, 6, 17474-17482.	1.7	34
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53216	DFT study on deprotonation and protonation of porphyrins: How many protons can the porphyrin core take up?. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 38-46.	1.1	8
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53219	Synthesis and reactivity of molybdenum(0) complexes containing sterically expanded arene ligands. <i>Polyhedron</i> , 2016, 114, 385-392.	1.0	2
53220	Novel Di- and Trinuclear Palladium Complexes Supported by <i>N,N'</i> -Diphosphanyl NHC Ligands and <i>N,N'</i> -Diphosphanylimidazolium Palladium, Gold, and Mixed-Metal Copper "Gold Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 1219-1229.	1.9	32

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53224	CO ₂ Absorption Using Fluorine Functionalized Ionic Liquids: Interplay of Hydrogen and π -Hole Interactions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1243-1260.	1.1	21
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53236	Electrochromic behaviour of triazine based ambipolar compounds. <i>Electrochimica Acta</i> , 2016, 192, 283-295.	2.6	23
53237	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.	1.8	5
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53241	Gauging the Performance of Density Functionals for Lanthanide-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1259-1266.	2.3	39
53242	Mixed-Valence Cations of Di(carbazol-9-yl) Biphenyl, Tetrahydropyrene, and Pyrene Derivatives. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3156-3166.	1.5	19
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53271	Dissipative Particle Dynamics interaction parameters from ab initio calculations. <i>Chemical Physics Letters</i> , 2016, 645, 20-26.	1.2	32
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53791	Electronic influences of bridging and chelating diimine ligand coordination in formamidinate-bridged Rh ₂ (II,II) dimers. <i>Polyhedron</i> , 2016, 103, 172-177.	1.0	11
53792	Interactions of zinc octacarboxyphthalocyanine with selected amino acids and with albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 155, 54-60.	2.0	9
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53797	Nucleotides containing variously modified sugars: energetics, structure, and mechanical properties. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1615-1628.	1.3	6

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53806	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	0.8	21
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53815	The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 754-770.	2.0	11

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53835	Experimental and theoretical investigations of natural rubber (cis-1,4-polyisoprene) using Coloumb attenuating and Hartree-Fock theoretical methods. <i>Optik</i> , 2016, 127, 279-287.	1.4	2
53836	Mechanistic aspects of CO ₂ activation mediated by phenyl yttrium cation: A combined experimental/theoretical study. <i>Journal of Catalysis</i> , 2016, 343, 68-74.	3.1	9
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53853	Infrared, Raman and NMR spectral analysis, vibrational assignments, normal coordinate analysis, and quantum mechanical calculations of 2-Amino-5-ethyl-1,3,4-thiadiazole. <i>Journal of Molecular Structure</i> , 2016, 1103, 70-81.	1.8	11
53854	Theoretical and experimental investigations on molecular structure of bis(2-methoxy-4-allylphenyl)oxalate. <i>Journal of Molecular Structure</i> , 2016, 1103, 156-165.	1.8	7
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53860	Experimental and theoretical study of ornidazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 496-504.	2.0	12
53861	Density functional theory investigation of nonsymmetrically substituted uranyl-salophen complexes. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2016, 307, 407-417.	0.7	15
53862	Synthesis of new coumarins complemented by quantum chemical studies. <i>Research on Chemical Intermediates</i> , 2016, 42, 3905-3918.	1.3	14
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53864	Efficient removal of both basic and non-basic nitrogen compounds from fuels by deep eutectic solvents. <i>Green Chemistry</i> , 2016, 18, 157-164.	4.6	96
53865	DPP containing D-A organic dyes toward highly efficient dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2016, 125, 27-35.	2.0	25
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53871	Electronic Structure of Crystalline Buckyballs: fcc-C60. <i>Journal of Electronic Materials</i> , 2016, 45, 339-348.	1.0	26
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53882	N-heterocyclic phosphonium and phosphido nickel complexes supported by a pincer ligand framework. <i>Dalton Transactions</i> , 2016, 45, 1918-1929.	1.6	25
53883	Sensing properties of BN nanotube toward carcinogenic 4-chloroaniline: A computational study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 76, 6-11.	1.3	131
53884	Electroswitchable optical device enabling both luminescence and coloration control consisted of fluoran dye and 1,4-benzoquinone. <i>Solar Energy Materials and Solar Cells</i> , 2016, 145, 42-53.	3.0	38
53885	Molecular modeling and docking calculations of 4-acyloxy-biphenyl-4-â€“N</i>-butylcarbamates as potential inhibitors of human butyrylcholinesterase. <i>Canadian Journal of Chemistry</i> , 2016, 94, 72-77.	0.6	4
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53890	Electronic structure and spectroscopy of homoleptic compounds of dimolybdenum using TDDFT. <i>Canadian Journal of Chemistry</i> , 2016, 94, 20-27.	0.6	0
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53892	The investigation of excited state proton transfer mechanism in water-bridged 7-azaindole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 147-151.	2.0	26
53893	E-Bodipy fluorescent chemosensor for Zn ²⁺ ion. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 331, 233-239.	2.0	11
53894	Theoretical and experimental NMR studies on muscimol from fly agaric mushroom (<i>Amanita muscaria</i>). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 216-225.	2.0	8
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53897	Theoretical Investigation for Exploring the Antioxidant Potential of Chlorogenic Acid: A Density Functional Theory Study. <i>International Journal of Food Properties</i> , 2016, 19, 745-751.	1.3	41
53898	Density functional theory calculations on conformational, spectroscopic and electrical properties of 3-(2,3-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one: a potential nonlinear optical material. <i>Indian Journal of Physics</i> , 2016, 90, 79-89.	0.9	6
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53901	Molecular structure and vibrational spectroscopic studies of prothionamide by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 152, 262-271.	2.0	4
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53910	Experimental and theoretical study on cation-π interaction of Ag ⁺ with [6]helicene. <i>Structural Chemistry</i> , 2016, 27, 627-635.	1.0	7
53911	Ab initio investigations on planar (MgO) _n clusters (n = 1-5) and their hydrogen adsorption behaviour. <i>Molecular Simulation</i> , 2016, 42, 208-214.	0.9	14
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53913	Thermodynamic and electrochemical study of some dihydroxybenzenes in the presence of different nucleophiles. <i>Monatshefte für Chemie</i> , 2016, 147, 329-339.	0.9	8
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55110	Hydrolysis in Acidic Environment and Degradation of Satraplatin: A Joint Experimental and Theoretical Investigation. <i>Inorganic Chemistry</i> , 2017, 56, 6013-6026.	1.9	20
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55112	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2789-2803.	2.3	23

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55367	DFT Studies of Ru-Catalyzed C=O versus C-H Bond Functionalization of Aryl Ethers with Organoboronates. <i>Organometallics</i> , 2017, 36, 2354-2363.	1.1	20
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55369	Tailoring protein nanomechanics with chemical reactivity. <i>Nature Communications</i> , 2017, 8, 15658.	5.8	26
55370	Mechanism of microtubule stabilization by taccalonolide A _J . <i>Nature Communications</i> , 2017, 8, 15787.	5.8	58
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55373	Direct versus ligand-exchange synthesis of [PtAg ₂₈ (BDT) ₁₂ (TPP) ₄] ⁴⁺ nanoclusters: effect of a single-atom dopant on the optoelectronic and chemical properties. <i>Nanoscale</i> , 2017, 9, 9529-9536.	2.8	62
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55375	Interaction of pure and metal atom substituted carbon nanocages with CNCl: a DFT study. <i>Russian Journal of Physical Chemistry B</i> , 2017, 11, 354-360.	0.2	14
55376	A DFT Exploration of Efficient Catalysts Based on Metal-Salen Monomers for the Cycloaddition Reaction of CO ₂ to Propylene Oxide. <i>ChemistrySelect</i> , 2017, 2, 4533-4537.	0.7	15
55377	Reaction Kinetics of Phenolic Antioxidants toward Photoinduced Pyranine Free Radicals in Biological Models. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6331-6340.	1.2	7
55378	Access to Benzo[<i>a</i>]carbazoles and Indeno[1,2- <i>c</i>]quinolines by a Gold(I)-Catalyzed Tunable Domino Cyclization of Difunctional 1,2-Diphenylethyne. <i>Organic Letters</i> , 2017, 19, 3402-3405.	2.4	28
55379	Introducing boranorcaradienes with more stability than their corresponding borepins: Reversal of tautomerization <i>via</i> substituents at theoretical levels. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3714.	0.9	3
55380	Visible absorbing croconium dyes with intramolecular hydrogen bonding: A combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2017, 1146, 684-691.	1.8	8
55381	Synthesis, structure, photo- and electroluminescent properties of bis{(4-methyl-N-[2-[(E)-2-pyridyliminomethyl]phenyl])benzenesulfonamide}zinc(II). <i>Polyhedron</i> , 2017, 133, 231-237.	1.0	25
55382	Mixed ligand metal-complexes of tridentate N, N, S pyrazole containing Schiff base and 2-amino-1-ethylbenzimidazole: Synthesis, structure, spectroscopic studies and quantum-chemical calculations. <i>Polyhedron</i> , 2017, 133, 245-256.	1.0	16

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55388	One-pot synthesis of aryl-substituted 1,2,3-triphospholide anions. <i>Journal of Organometallic Chemistry</i> , 2017, 844, 1-7.	0.8	14
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55392	Cure kinetics of epoxy/β-cyclodextrin-functionalized Fe ₃ O ₄ nanocomposites: Experimental analysis, mathematical modeling, and molecular dynamics simulation. <i>Progress in Organic Coatings</i> , 2017, 110, 172-181.	1.9	62
55393	Brønsted acid mediated cyclizations of ortho-aryl(ethynyl)pyrimidines. <i>Tetrahedron</i> , 2017, 73, 3939-3948.	1.0	14
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55399	Gas phase anion photoelectron spectroscopy and theoretical investigation of gold acetylide species. <i>Journal of Chemical Physics</i> , 2017, 146, 194303.	1.2	15
55400	Stabilities, electronic and magnetic properties of Cu-doped nickel clusters: a DFT investigation. <i>Molecular Physics</i> , 2017, 115, 2495-2507.	0.8	13

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55420	Halogen atom transfer mechanism of iron-catalyzed direct arylation to form biaryl using Density Functional Theory calculations. <i>Journal of Organometallic Chemistry</i> , 2017, 844, 8-15.	0.8	7
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55426	Characterization of Protonated Model Disaccharides from Tandem Mass Spectrometry and Chemical Dynamics Simulations. <i>ChemPhysChem</i> , 2017, 18, 2812-2823.	1.0	22
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55431	Geometric and Electronic Structure Analysis of the Three-Membered Electron-Transfer Series [(1/4-CNR) ₂ [CpCo] ₂] ^{<i>n</i>} (<i>n</i> = 0, 1 ⁺ , 2 ⁺) and Its Relevance to the Classical Bridging-Carbonyl System. <i>Organometallics</i> , 2017, 36, 2126-2140.	1.1	10
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55434	H-Bond assisted mechanoluminescence of borylated aryl amines: tunable emission and polymorphism. <i>Journal of Materials Chemistry C</i> , 2017, 5, 6537-6546.	2.7	39
55435	Metal-Dependent Strengthening and Weakening of M ⁺ -H and M ⁺ -C Bonds by an Oxo Ligand: Thermal Gas-Phase Activation of Methane by [OMH] ⁺ and [MH] ⁺ (M=Mo, Ti). <i>Chemistry - A European Journal</i> , 2017, 23, 12346-12352.	1.7	7
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55439	Molecular structure, supramolecular association and anion sensing by chlorodiorganotin(IV) methylferrocenyldithiocarbamates. <i>Journal of Molecular Structure</i> , 2017, 1145, 197-203.	1.8	5
55440	Structural, electronic and spectral properties of carborane-containing boron dipyrromethenes (BODIPYs): A first-principles study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 149-154.	2.0	6
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55448	Light penetration-coupled photoisomerization modeling for photodeformation of diarylethene single crystal: upscaling isomerization to macroscopic deformation. <i>Scientific Reports</i> , 2017, 7, 967.	1.6	10
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55453	Spectral, DFT and X-ray diffraction studies on regioselective synthesis of thiazolo-quinazoline system. <i>Journal of Molecular Structure</i> , 2017, 1145, 268-277.	1.8	4
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58260	Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF ₂ , FeF ₂ ·Ethane, and FeF ₂ ·Ethylene. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2563-2579.	1.1	12
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58311	Ionic Liquid Facilitated Dehydrogenation of <i>tert</i> -Butylamine Borane. <i>ACS Omega</i> , 2018, 3, 2273-2281.	1.6	8
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58349	Pd ^{IV} Species Mediation in Pd ^{II} -Catalyzed Direct Alkylation of Arenes with Oxiranes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 3142-3148.	1.7	24
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58352	Tris-amidoximate uranyl complexes via U^{2+} binding mode coordinated in aqueous solution shown by X-ray absorption spectroscopy and density functional theory methods. <i>Journal of Synchrotron Radiation</i> , 2018, 25, 514-522.	1.0	12
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58364	Ab Initio Study of Decay Dynamics of 1-Nitronaphthalene Initiated from the S ₂ ($\tilde{\epsilon}^*$) T ₁ ETQ _{0,0} 0 rgBT ₅ /Overlock	1.1	5
58365	Exploring the Binding of Barbitol to a Synthetic Macrocyclic Receptor. A Charge Density Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3031-3044.	1.1	3
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58484	Synthesis, Structure, Bonding, and Reactivity of Metal Complexes Comprising Diborane(4) and Diborene(2): $[\{\text{Cp}^*\text{Mo}(\text{CO})_2\}_2\{\text{B}_2\text{H}_4\}^2\text{H}_4]$ and $[\{\text{Cp}^*\text{M}(\text{CO})_2\}_2\text{B}_2\text{H}_4\text{M}(\text{CO})_4]$, M=Mo,W. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8079-8083.		47
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58763	Highly selective and sensitive determination of Cu ²⁺ in drink and water samples based on a 1,8-diaminonaphthalene derived fluorescent sensor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 195, 142-147.	2.0	43
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58766	Noncollinear Two-Component Quasirelativistic Description of Spin Interactions in Exchange-Coupled Systems. Mapping Generalized Broken-Symmetry States to Effective Spin Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1267-1276.	2.3	3
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58770	Highly selective hydrazone based reversible colorimetric chemosensors for expeditious detection of CN ⁻ in aqueous media. <i>Inorganica Chimica Acta</i> , 2018, 474, 22-29.	1.2	34
58771	Hypervalent benzophenones. <i>Journal of Organometallic Chemistry</i> , 2018, 858, 89-96.	0.8	2
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58807	Characterization of Interactions between Curcumin and Different Types of Lipid Bilayers by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2341-2354.	1.2	45
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58852	Polarizable Density Embedding Coupled Cluster Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1351-1360.	2.3	20
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58854	Mechanism and Origins of Regio- and Enantioselectivities of Iridium-Catalyzed Hydroarylation of Alkenyl Ethers. <i>Journal of Organic Chemistry</i> , 2018, 83, 2937-2947.	1.7	42
58855	Nickel(III)-mediated oxidative cascades from a thiol-bearing nickel(II) precursor to the nickel(IV) product. <i>Dalton Transactions</i> , 2018, 47, 3796-3802.	1.6	8
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58857	Solid Electrolyte Layers by Solution Deposition. <i>Advanced Materials Interfaces</i> , 2018, 5, 1701328.	1.9	42
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58865	Tuning Aromaticity of para-Substituted Benzene Derivatives with an External Electric Field. <i>ChemPhysChem</i> , 2018, 19, 590-595.	1.0	12

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58867	Mechanistic Unveiling of C=C Double-Bond Rotation and Origins of Regioselectivity and Product Selectivity of Pd-Catalyzed Olefinic C-H Functionalization of <i>N</i> -Methoxy Cinnamamide. <i>Journal of Organic Chemistry</i> , 2018, 83, 2067-2076.	1.7	13
58868	Ethanol Conversion to Ethylene and Acetaldehyde over Rhodium(I) Exchanged Faujasite Zeolite. A QM/MM and Microkinetic Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2783-2795.	1.5	8
58869	Cyclolinear Oligo- and Poly(iminoborane)s: The Missing Link in Inorganic Main-Group Macromolecular Chemistry. <i>Chemistry - A European Journal</i> , 2018, 24, 5883-5894.	1.7	39
58870	Theoretical Study and Experimental Analysis on 2-(1-Ethyl-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl)-2-oxoacetic Acid (3) Using the DFT Approach. <i>Journal of Solution Chemistry</i> , 2018, 47, 172-197.	0.6	1
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58872	Effect of Transition Metal Fragments on the Reverse Fritsch-Buttenberg-Wiechell Type Ring Contraction Reaction of Metallabenzynes to Metal-Carbene Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2160-2167.	1.1	2
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58874	New 1,2-Dihydropyridine-Based Fluorophores and Their Applications as Fluorescent Probes. <i>ACS Omega</i> , 2018, 3, 856-862.	1.6	10
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58878	DFT/TDDFT, NPA, and AIM-based study of the molecular switching properties of photocyclization and metallochromism of the DAE complexes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	9
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58881	Chiral Phosphoric Acid Catalyzed Enantioselective Ring Expansion Reaction of 1,3-Dithiane Derivatives: Case Study of the Nature of Ion-Pairing Interaction. <i>Journal of the American Chemical Society</i> , 2018, 140, 2629-2642.	6.6	42
58882	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. <i>Nature Communications</i> , 2018, 9, 415.	5.8	527
58883	Reactions of a series of ZnL, CuL and NiL Schiff base and non-Schiff base complexes with MCl ₂ salts (M = Cu, Ni, Mn): syntheses, structures, magnetic properties and DFT calculations. <i>New Journal of Chemistry</i> , 2018, 42, 3683-3691.	1.4	12

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59265	Theoretical studies on copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate under ligand-free conditions. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 50-57.	0.8	10
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59299	Vibrational (FT-IR and FT-Raman), electronic (UV-vis) and quantum chemical investigations on pyrogallol: A study on benzenetriol dimers. <i>Vibrational Spectroscopy</i> , 2018, 95, 16-22.	1.2	42

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59676	The effect of TiO ₂ nanotube morphological engineering and ZnS quantum dots on the water splitting reaction: A theoretical and experimental study. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 6838-6850.	3.8	9
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59679	Quantum chemical calculations, molecular dynamic (MD) simulations and experimental studies of using some azo dyes as corrosion inhibitors for iron. Part 2: Bis-azo dye derivatives. <i>Journal of Molecular Structure</i> , 2018, 1163, 397-417.	1.8	101
59680	New asymmetric and symmetric 2-((pyridin-4-yl)methylenamino)-3 aminomaleo nitrile and 2,3-bis((pyridin-4-yl)methylenamino)maleonitrile Schiff bases: Synthesis, experimental characterization along with theoretical studies. <i>Journal of Molecular Structure</i> , 2018, 1163, 388-396.	1.8	7
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59682	Photophysical and electrochemical properties of organic molecules: Solvatochromic effect and DFT studies. <i>Optical Materials</i> , 2018, 77, 211-220.	1.7	15
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59689	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. <i>Nature Chemical Biology</i> , 2018, 14, 345-351.	3.9	34
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59695	Room temperature control of spin states in a thin film of a photochromic iron(II) complex. <i>Materials Horizons</i> , 2018, 5, 506-513.	6.4	43

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59697	Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. <i>Journal of Chemical Physics</i> , 2018, 148, 104110.	1.2	56
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59715	Excited states study reveals the twisted geometry induced large stokes shift in DCM fluorescent dye. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 354, 127-138.	2.0	14
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59723	Structure and absolute configuration of some 5-chloro-2-methoxy-N-phenylbenzamide derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 213-221.	2.0	10
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59725	Photoexcitation effect on the adsorption of hazardous gases on silica surface. <i>Journal of Hazardous Materials</i> , 2018, 341, 93-101.	6.5	36
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59729	Spectroscopic and DFT studies of bis-3-hydroxypyridinium and bis-3-hydroxymethylpyridinium dibromides with tetramethylene linker. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 456-468.	2.0	3
59730	Synthesis of rhodamine based organic nanorods for efficient chemosensor probe for Al (III) ions and its biological applications. <i>Sensors and Actuators B: Chemical</i> , 2018, 254, 795-804.	4.0	65
59731	DFT study of small aluminum and boron hydrides: isomeric composition and physical properties. <i>Structural Chemistry</i> , 2018, 29, 49-68.	1.0	14

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59733	QSAR, DFT and molecular modeling studies of peptides from HIV-1 to describe their recognition properties by MHC-I. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 2312-2330.	2.0	10
59734	Coumarin-based random copolymer. <i>Journal of Thermoplastic Composite Materials</i> , 2018, 31, 729-744.	2.6	1
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59745	Surface Active Ionic Liquids as Catalyst for CO ₂ Conversion to Propylene Carbonate. <i>Catalysis Letters</i> , 2018, 148, 108-118.	1.4	51
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59753	A new low temperature solid modification in 1-isothiocyanato-4-(trans-4-propylcyclohexyl)benzene (3CHBT) probed by Raman spectroscopy and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 188-196.	2.0	2
59754	A facile and regioselective one-pot synthesis of novel pyrazolo[1,5-a]pyridine-2,3-dione. <i>Molecular Diversity</i> , 2018, 22, 37-46.	2.1	1
59755	Evaluation of estrogenic activity of red clover (<i>Trifolium pratense</i> L.) sprouts cultivated under different conditions by content of isoflavones, calorimetric study and molecular modelling. <i>Food Chemistry</i> , 2018, 245, 324-336.	4.2	31
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59766	Reaction of 2-propanol with ozone in aqueous media. <i>Water Research</i> , 2018, 128, 171-182.	5.3	12
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59769	Synthesis, X-ray structure, spectroscopic, DFT study and catalytic activity of cis-[RuCl ₂ (L)(EPh ₃)] complexes (E = P, As, Sb; L = NN ² N ³ tridentate azoimine-quinoline ligands). <i>Inorganica Chimica Acta</i> , 2018, 471, 186-193.		5
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59771	DNA/BSA binding interactions and VHPO mimicking potential of vanadium(IV) complexes: Synthesis, structural characterization and DFT studies. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4125.	1.7	14
59772	Mechanism and selectivity of rhodium-catalyzed C-H bond arylation of indoles. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25526.	1.0	7
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59779	Metal chelating ability and antioxidant properties of Curcumin-metal complexes - A DFT approach. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 1-14.	1.3	81
59780	Molecular structure, electronic properties, and charge transfer analysis of clopenthixol as a nano-drug with quantum chemical calculations. <i>Canadian Journal of Physics</i> , 2018, 96, 312-327.	0.4	6
59781	Novel enamines as non-cytotoxic compounds with mild antibacterial activity: Synthesis and structure-activity correlations. <i>Journal of Molecular Structure</i> , 2018, 1154, 636-642.	1.8	10
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59783	Development of Solid Catalyst-Solid Substrate Reactions for Efficient Utilization of Biomass. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 29-43.	2.0	63
59784	Molecular acidity: An accurate description with information-theoretic approach in density functional reactivity theory. <i>Journal of Computational Chemistry</i> , 2018, 39, 117-129.	1.5	67
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59787	The concern of emergence of multi-station reaction pathways that might make stepwise the mechanism of the 1,3-dipolar cycloadditions of azides and alkynes. <i>Journal of Molecular Structure</i> , 2018, 1155, 58-64.	1.8	13
59788	Laboratory spectroscopy of methoxymethanol in the millimeter-wave range. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5509-5516.	1.3	21
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59790	Proton sensitive charge-transfer excited states in bis-terdentate cyclometalated Ir(III) complexes: Spectroscopic and theoretical investigation. <i>Inorganica Chimica Acta</i> , 2018, 471, 8-16.	1.2	6
59791	A new barbiturate-based centrosymmetric compound: Joint experimental/DFT investigation of the structural, spectroscopic and surface properties. <i>Journal of Molecular Structure</i> , 2018, 1155, 278-287.	1.8	6
59792	Carbon-bromine bond cleavage – A perspective from bromine and carbon kinetic isotope effects on model debromination reactions. <i>Chemosphere</i> , 2018, 193, 17-23.	4.2	4
59793	Lycopene-rich extract from red guava (<i>Psidium guajava</i> L.) displays cytotoxic effect against human breast adenocarcinoma cell line MCF-7 via an apoptotic-like pathway. <i>Food Research International</i> , 2018, 105, 184-196.	2.9	43
59794	Dissecting the concave-convex interaction in corannulene and sumanene dimers: SAPT(DFT) analysis and performance of DFT dispersion-corrected methods. <i>Journal of Computational Chemistry</i> , 2018, 39, 93-104.	1.5	12
59795	A DFT study on TNGU isomers and aluminized cis-TNGU composites. <i>Defence Technology</i> , 2018, 14, 109-118.	2.1	4
59796	Hydrogen bonded 2-methyl-1H-imidazol-3-ium 3,5-dinitrobenzoate 3,5-dinitrobenzoic acid, a new optical crystal: Evaluation of properties by structural, spectral, quantum chemical calculations, Z-scan and Hirshfeld studies. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 114, 228-239.	1.9	12
59797	A comparative structural, spectroscopic, optical and photoluminescence studies by DFT of Fe(II) difluoro(oxalato)borate complex. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 352, 43-54.	2.0	10
59798	A reinvestigation of mono- and bis-ethynyl phosphonium salts: structural and computational studies and new reactivity. <i>Canadian Journal of Chemistry</i> , 2018, 96, 8-17.	0.6	4
59799	Theoretical study of the CO formation mechanism in the CO ₂ gasification of lignite. <i>Fuel</i> , 2018, 211, 353-362.	3.4	26
59800	Condensation product of 2-hydroxy-1-naphthaldehyde and 2-aminophenol: Selective fluorescent sensor for Al ³⁺ ion and fabrication of paper strip sensor for Al ³⁺ ion. <i>Inorganica Chimica Acta</i> , 2018, 469, 202-208.	1.2	23
59801	Cd(II) and Ni(II) complexes from aroyl hydrazones: Unravelling the intermolecular interactions and electronic, crystal structures through experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2018, 469, 264-279.	1.2	23
59802	Crystal structures, vibrational spectra and DFT calculations of five halogeno-derivatives of 7-azaindole (3Br7AI, 4Br7AI, 4Cl7AI, 3Br4Cl7AI and 5Br3Cl7AI): a comparative study. <i>Journal of Molecular Structure</i> , 2018, 1152, 386-398.	1.8	5
59803	Synthesis, characterization and computational studies of 3-[(E)-(2-hydroxyphenyl)imino]methyl}benzene-1,2-diol and molecular structure of its zwitterionic form. <i>Journal of Molecular Structure</i> , 2018, 1152, 21-28.	1.8	5

#	ARTICLE	IF	CITATIONS
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59806	Controlling the electronic properties of the graphene nanoflakes by BN impurities. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 86-93.	1.3	17
59807	Enhancement of the photovoltaic performance in D 3 A porphyrin-based DSCs by incorporating an electron withdrawing triazole spacer. <i>Polyhedron</i> , 2018, 140, 9-18.	1.0	16
59808	Aromatic hydrazones derived from nicotinic acid hydrazide as fluorimetric pH sensing molecules: Structural analysis by computational and spectroscopic methods in solid phase and in solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 259-267.	2.0	21
59809	Investigation of electronic structure of tri- and tetranuclear molybdenum clusters by X-ray photoelectron and emission spectroscopies and quantum chemical methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 347-352.	2.0	8
59810	Isocyano-functionalized, 1,8-naphthalimide-based chromophore as efficient ratiometric fluorescence probe for Hg ²⁺ in aqueous medium. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 3074-3084.	4.0	27
59811	A highly sensitive and selective fluorescent chemosensor for the sequential recognition of Zn ²⁺ and S ²⁻ in living cells and aqueous media. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 3108-3116.	4.0	37
59812	Theoretical investigation of twisted charge-transfer-promoted intramolecular proton transfer in the excited state of 4- ² -dimethylaminoflavonol in a highly polar solvent. <i>Journal of Luminescence</i> , 2018, 194, 785-790.	1.5	41
59813	Tuning the photophysical properties of heteroleptic Ir(III) complexes through ancillary ligand substitution: Experimental and theoretical investigation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 350, 130-141.	2.0	7
59814	Stone-Wales defects in nitrogen-doped C ₂₀ fullerenes: Insight from ab initio calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 96, 6-10.	1.3	15
59815	Conformational behavior, redox and spectroscopic properties of gold dithiolene complexes: [Au(iPr-thiazYdt) ₂] ¹ (Y = O, S, Se). <i>Inorganica Chimica Acta</i> , 2018, 469, 255-263.	1.2	3
59816	A dual sensor selective for Hg ²⁺ and cysteine detection. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2756-2763.	4.0	63
59817	Effects of wheat gluten protein on the properties of starch based sustainable wood polymer nanocomposites. <i>European Polymer Journal</i> , 2018, 100, 137-145.	2.6	17
59818	Solution and Solid-State Study of the Spin-Crossover [Fe ^{II} (R ¹) ₃](BF ₄) ₂ Complexes (R = Me, Et, Vinyl). <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 414-428.	1.0	28
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59820	Reaction mechanism, rate constants, and product yields for the oxidation of Cyclopentadienyl and embedded five-member ring radicals with hydroxyl. <i>Combustion and Flame</i> , 2018, 187, 147-164.	2.8	24
59821	Synthesis, spectroscopic characterization, first order nonlinear optical properties and DFT calculations of novel Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) complexes with 1,3-diphenyl-4-phenylazo-5-pyrazolone ligand. <i>Journal of Molecular Structure</i> , 2018, 1153, 248-261.	1.8	33

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59823	Mixed valent/geometry, linear, tetranuclear nickel complex bearing ONO pincer ligand exhibiting hitherto unknown ligation mode. <i>Polyhedron</i> , 2018, 143, 157-164.	1.0	1
59824	Interactions of Glycopolymers with Assemblies of Peptide Amphiphiles via Dynamic Covalent Bonding. <i>ACS Biomaterials Science and Engineering</i> , 2018, 4, 2061-2066.	2.6	5
59825	Accurate density functional prediction of molecular electron affinity with the scaling corrected Kohn-Sham frontier orbital energies. <i>Molecular Physics</i> , 2018, 116, 927-934.	0.8	10
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59827	A combined experimental (IR, Raman and UV-Vis) and quantum chemical study of canadine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 249-258.	2.0	4
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59830	Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO, and molecular docking analysis of N-ethyl-N-nitrosourea, a potential anticancer agent. <i>Journal of Molecular Structure</i> , 2018, 1154, 39-50.	1.8	31
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59832	A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor. <i>Molecular Physics</i> , 2018, 116, 323-337.	0.8	1
59833	A sobering assessment of small-molecule force field methods for low energy conformer predictions. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25512.	1.0	43
59834	Primary Formation Path of Formaldehyde in Hydrothermal Vents. <i>Origins of Life and Evolution of Biospheres</i> , 2018, 48, 1-22.	0.8	6
59835	Fluorescent pyridopyrimidine fused pyranones - design, synthesis, fluorescent whitening and DFT studies. <i>Journal of Luminescence</i> , 2018, 194, 248-256.	1.5	12
59836	Structural investigation of anhydrous nitrofurantoin and its monohydrate based on terahertz/Raman vibrational spectroscopy and density functional theory. <i>Journal of Molecular Structure</i> , 2018, 1153, 170-178.	1.8	7
59837	Systematically tuning of optoelectronic properties from electron donating to accepting substituents on bicarbazole/cyanobenzene hybrids: Host to dopant materials for phosphorescent and delayed fluorescence OLEDs. <i>Organic Electronics</i> , 2018, 52, 22-31.	1.4	13
59838	Role of the Diphosphine Chelate in Emissive, Charge-Neutral Iridium(III) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 624-635.	1.7	12
59839	Aluminum doping makes boron nitride nanotubes (BNNTs) an attractive adsorbent of hydrazine (N ₂ H ₄). <i>Structural Chemistry</i> , 2018, 29, 375-382.	1.0	18

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59843	Structural, photophysical, and theoretical studies of imidazole-based excited-state intramolecular proton transfer molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 325-335.	2.0	10
59844	Ferrocene- ϵ -substituted bis(ethynyl)anthracene compounds as anticancer agents. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4071.	1.7	7
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59846	Workflows and performances in the ranking prediction of 2016 D3R Grand Challenge 2: lessons learned from a collaborative effort. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 129-142.	1.3	8
59847	Experimental and DFT studies of PM2.5 removal by chemical agglomeration. <i>Fuel</i> , 2018, 212, 27-33.	3.4	34
59848	Synthesis, spatial and electronic structure of 1-(+)-neomenthyl-1,2-diphosphole and 1-(+)-neomenthyl-1,2,4-triphosphole tungstenpentacarbonyl complexes. <i>Journal of Organometallic Chemistry</i> , 2018, 867, 125-132.	0.8	11
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59854	A binding-block ion selective mechanism revealed by a Na/K selective channel. <i>Protein and Cell</i> , 2018, 9, 629-639.	4.8	14
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59856	Dicyanovinylcoumarin as a turn-on fluorescent sensor for cyanide ion. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 351, 108-114.	2.0	25
59857	Theoretical studies on the electronic and optoelectronic properties of [A ₂ AP(w)/A [*] AP(WC)/C ₂ AP(w)/C [*] AP(WC)/C.A(w)/C [*] AP(WC)] ⁻ Au@sub.88</sub>mismatch nucleobase complexes. <i>Molecular Physics</i> , 2018, 116, 263-272.		

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59861	Replacement of oxidizable residues predicted by QM-MM simulation of a fungal laccase generates variants with higher operational stability. <i>Journal of Inorganic Biochemistry</i> , 2018, 178, 125-133.	1.5	8
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59863	A turn-on supramolecular fluorescent probe for sensing benzimidazole fungicides and its application in living cell imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 372-376.	2.0	16
59864	One-dimensional diamondoid polyaniline-like nanothreads from compressed crystal aniline. <i>Chemical Science</i> , 2018, 9, 254-260.	3.7	66
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59866	Probing the activity of pure and N-doped fullerenes towards oxygen reduction reaction by density functional theory. <i>Carbon</i> , 2018, 126, 53-57.	5.4	76
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59871	Experimental and theoretical analysis of a rare nitrate bridged 3d-4f complex containing LaZn ₂ core synthesized from a Zn(II) metalloligand. <i>Journal of Molecular Structure</i> , 2018, 1153, 85-95.	1.8	8
59872	In Situ Analysis of Chain Orientation Behavior in Thin Film Aromatic Polyimides by Variable Temperature pMAIRS during Thermal Imidization. <i>Macromolecular Chemistry and Physics</i> , 2018, 219, 1700370.	1.1	21
59873	Rapid and sensitive detection of pyrimethanil residues on pome fruits by Surface Enhanced Raman Scattering. <i>Food Chemistry</i> , 2018, 244, 16-24.	4.2	45
59874	Coordination mode of the N-[bis(diethylamino)phosphoryl]benzenesulfonamide ligand in Lu(III) and Ag(I) complexes. Mass spectra, thermal properties and DFT calculations. <i>Polyhedron</i> , 2018, 139, 98-106.	1.0	5
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59878	Synthesis, molecular, electronic structure, linear and non-linear optical and phototransient properties of 8-methyl-1,2-dihydro-4H-chromeno[2,3-b]quinoline-4,6(3H)-dione (MDCQD): Experimental and DFT investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 478-490.	2.0	29
59879	Synthesis and characterization of Ni(II) complexes bearing of 2-((1 <i>H</i>)-benzimidazol-2-yl)phenol derivatives as highly active catalysts for ethylene oligomerization. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4015.	1.7	15
59880	DFT Study on Planar (CaO) <i>n</i> Rings (<i>n</i> =1-5) and Their Hydrogen Storage Behavior: CaO Versus MgO Clusters. <i>Journal of Cluster Science</i> , 2018, 29, 57-65.	1.7	8
59881	Rational Design and Synthesis of Unsaturated Se-Containing Osmacycles with π -Aromaticity. <i>Chemistry - A European Journal</i> , 2018, 24, 2389-2395.	1.7	35
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59887	Mechanistic, energetic and structural studies of carbon nanotubes functionalised with dihydroartemisinin drug in gas and solution phases. <i>Physics and Chemistry of Liquids</i> , 2018, 56, 610-618.	0.4	3
59888	Ensemble docking to difficult targets in early-stage drug discovery: Methodology and application to fibroblast growth factor 23. <i>Chemical Biology and Drug Design</i> , 2018, 91, 491-504.	1.5	25
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59895	Synthesis and studies on gelation ability of phenol based maleate amphiphile and its application in nutraceutical release. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2018, 537, 310-317.	2.3	6
59896	Extraction of actinides by Tri-n-butyl phosphate derivatives: Effect of substituents. <i>Inorganica Chimica Acta</i> , 2018, 469, 123-132.	1.2	22
59897	Dual fluorescence of (E)-N-(4-(dimethylamino)benzylidene)-2H-1,2,4-triazol-3-amine (DMABA-Amtr): A ground state perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 601-607.	2.0	3
59898	DFT modeling of structures and redox potentials of wild-type, Nickel-substituted and mutated (N47S/M121L, HPAz) Azurin. <i>Inorganica Chimica Acta</i> , 2018, 470, 360-364.	1.2	2
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59905	Infrared multiple photon dissociation spectroscopy of cationized canavanine: Side-chain substitution influences gas-phase zwitterion formation. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 158-173.	0.7	7
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59914	Synthesis, molecular structure and photochemical properties of tricarbonyl and dicarbonyl derivatives of 1N- and 2N-cymantrenylalkyl-1,2,3-triazoles. <i>Journal of Organometallic Chemistry</i> , 2018, 867, 71-78.	0.8	3
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59916	A density functional theory study on the structural and electronic properties of $\text{Pb}_x\text{Sb}_y\text{Se}_z$ ($x + y + z = 1$). <i>Journal of Computational Chemistry</i> , 2018, 39, 1-10.	1.0	0
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59937	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene – A frequently used benzene derivative. <i>Journal of Molecular Structure</i> , 2018, 1151, 245-255.	1.8	51
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61122	Synthesis, spectral and electrochemical properties of selected boron ketiminates with aminocoumarin fragment. <i>Monatshefte für Chemie</i> , 2018, 149, 1795-1811.	0.9	3
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61134	Mechanism and kinetic analysis of PCDD/Fs formation from aliphatic hydrocarbons (C ₂ H ₂ , C ₂ H ₄ , C ₃ H ₆), Tj ETQq1 1 0.784314 rgBT /Dv	0.8	0
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61916	A mononuclear nonheme {FeNO} ⁶ complex: synthesis and structural and spectroscopic characterization. <i>Chemical Science</i> , 2018, 9, 6952-6960.	3.7	11
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66900	Effects of solvents on the excited state intramolecular proton transfer and hydrogen bond mechanisms of alizarin and its isomers. <i>Journal of Molecular Liquids</i> , 2020, 301, 112415.	2.3	56
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66913	Selective Oxidation of H ₂ and CO by NiIr Catalyst in Aqueous Solution: A DFT Mechanistic Study. <i>Inorganic Chemistry</i> , 2020, 59, 1014-1028.	1.9	8
66914	Accurate Water Properties from an Efficient ab Initio Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 974-987.	2.3	15
66915	AMBER Force Field Parameters for Cobalt-Containing Biological Systems: A Systematic Derivation Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 777-787.	1.2	5
66916	Does gold behaves as hydrogen? A joint theoretical and experimental study. <i>Nanoscale Advances</i> , 2020, 2, 844-850.	2.2	3

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66918	Theoretical study of Schiff bases reactivity prediction of corrosion inhibition effect. <i>Molecular Simulation</i> , 2020, 46, 207-212.	0.9	2
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66929	Rational modifications of PCN-700 to induce electrical conductivity: a computational study. <i>Dalton Transactions</i> , 2020, 49, 102-113.	1.6	8
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66934	QSAR study of <i>N</i> -substituted oseltamivir derivatives as potent avian influenza virus H5N1 inhibitors using quantum chemical descriptors and statistical methods. <i>New Journal of Chemistry</i> , 2020, 44, 1747-1760.	1.4	26

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66969	Towards a white-emitting phosphor Ca ₁₀ V ₆ O ₂₅ based material. <i>Journal of Luminescence</i> , 2020, 220, 116990.	1.5	5
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66972	Photochromic properties of some azomaleimide derivatives and DFT quantum chemical study of thermal cis-trans isomerization pathways. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 390, 112300.	2.0	12
66973	Tin(IV) complex of 3,4-dihydroxybenzaldehyde 4-ethylthiosemicarbazone: Synthesis, spectral studies and molecular modeling. <i>Journal of Saudi Chemical Society</i> , 2020, 24, 236-243.	2.4	5
66974	Theoretical study of hydrogen bonding in complex alcohol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2020, 300, 112331.	2.3	3
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70595	NMR structural characterization from one-bond ¹³ C- ¹³ C couplings: Complete assignment of a hydrogen-poor depsidone. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 23-33.	1.1	4
70596	Complex of 4-(2-aminophenyl)-1,2,3-thiadiazole with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone: Experimental study and investigation at different exchange-correlation functionals. DOS, NBO, QTAIM and RDG analyses. <i>Journal of Molecular Structure</i> , 2021, 1223, 128855.	1.8	12
70597	Spectral, modeling and anticancer activity studies on the newly synthesized N-allyl-2-(2,4-dinitrophenyl)hydrazine-1-carbothioamide and some bivalent metal complexes. <i>Journal of Molecular Structure</i> , 2021, 1223, 128949.	1.8	7
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70600	Assessing conformer energies using electronic structure and machine learning methods. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26381.	1.0	40
70601	Synthesis, characterisation and comparative study of the hydroxyl, acrylate and vinyl-ether terminated cyanobiphenyl bridged with different spacer lengths. <i>Liquid Crystals</i> , 2021, 48, 168-181.	0.9	2
70602	Highly efficient capture of odorous sulfur-based VOCs by ionic liquids. <i>Journal of Hazardous Materials</i> , 2021, 402, 123507.	6.5	20
70603	Mechanistic investigation on ethanol- α -butadiene conversion reaction over metal oxide clusters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26494.	1.0	13
70604	Metal-ion-assisted structural and anomeric analysis of Amadori compounds by electrospray ionization mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e8960.	0.7	4
70605	Mechanistic insight into the performance enhancement of Si anode of a lithium-ion battery with a fluoroethylene carbonate electrolyte additive. <i>Journal of Applied Electrochemistry</i> , 2021, 51, 143-154.	1.5	12
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70608	Cu ²⁺ cation-exchange in Zn _x Cd _{1-x} S thin films for neuromorphic devices. <i>Applied Surface Science</i> , 2021, 537, 147921.	3.1	3
70609	Coordination complexes of di(2-pyridyl)ketone with copper(I) and their formation in solution and under solvent-free conditions. <i>Inorganica Chimica Acta</i> , 2021, 514, 119951.	1.2	5
70610	Synthesis, characterization and density functional theory of copper(II) complex and cobalt(II) coordination polymer for detection of nitroaromatic explosives. <i>Inorganica Chimica Acta</i> , 2021, 515, 120048.	1.2	7
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70615	Theoretical investigation of structure, anticancer activity and molecular docking of thiourea derivatives. <i>Journal of Molecular Structure</i> , 2021, 1225, 129118.	1.8	38
70616	Synthesis, spectroscopic, DFT, HSA binding and docking studies of new 1,5-bis(4-chlorophenyl)-3-(2-(4-methylpiperazin-1-yl)quinolin-3-yl)pentane-1,5-dione. <i>Journal of Molecular Structure</i> , 2021, 1223, 129260.	1.8	4

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70618	Synthesis, X-ray and complete assignments of ¹ H and ¹³ C nuclear magnetic resonance data for novel dichloro-1,4-dihydro-1,4-epoxynaphthalene derivatives. <i>Journal of Molecular Structure</i> , 2021, 1224, 129287.	1.8	2
70619	Synthesis of 1-aryl-3-methylsulfanyl-5-amino-1,2,4-triazoles and their analysis by spectroscopy, X-ray crystallography and theoretical calculations. <i>Journal of Molecular Structure</i> , 2021, 1226, 129317.	1.8	14
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70624	DFT computational study towards investigating psychotropic drugs, promazine and trifluoperazine adsorption on graphene, fullerene and carbon cyclic ring nanoclusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119012.	2.0	28
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70626	Investigation of inclusion complex of metformin into selective cyclic peptides as novel drug delivery system: Structure, electronic properties, AIM and NBO study via DFT. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 67-75.	0.8	7
70627	Synthesis and Reactivity of Heteroleptic Ga(III) Allyl Cation Analogues. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1986-1991.	7.2	22
70628	Thermal, optical, etching, structural studies and theoretical calculations of [1-(2,2,6,6-tetramethylpiperidin-1-yl)ethane-1-thione] (1-TMPP). <i>Journal of Molecular Structure</i> , 2021, 1224, 129077.	1.8	11
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70630	N-substitution in isatin thiosemicarbazones decides nuclearity of Cu(II) complexes: Spectroscopic, molecular docking and cytotoxic studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118963.	2.0	33
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70633	Computational study of the substitution of early actinides and Ce into zirconolite. <i>Journal of Nuclear Materials</i> , 2021, 543, 152525.	1.3	4
70634	Rapid detection of trace formaldehyde in food based on surface-enhanced Raman scattering coupled with assembled purge trap. <i>Food Chemistry</i> , 2021, 340, 127930.	4.2	28

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70636	Synthesis, spectra, electronic structure, molecular docking and cytotoxicity investigation on 2-(piperidin-1-ylmethyl)-isoindoline-1,3-dione "A Mannich base system. <i>Journal of Molecular Structure</i> , 2021, 1224, 129151.	1.8	5
70637	Synthesis, crystal structure, DNA interaction, DFT analysis and molecular docking studies of copper(ii) complexes with 1-methyl-l-tryptophan and phenanthroline units. <i>Journal of Molecular Structure</i> , 2021, 1224, 129236.	1.8	14
70638	Catalytic oxidative coupling of o-phenylenediamine, in-vitro antibacterial and antitumor activities of a gold(III)-bipyridine complex. <i>Journal of Molecular Structure</i> , 2021, 1223, 129264.	1.8	8
70639	Morphologically controlled eco-friendly synthesis of a novel 2D Hg(II) metal-organic coordination polymer: Biological activities and DFT analysis. <i>Journal of Molecular Structure</i> , 2021, 1226, 129335.	1.8	9
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70641	Binding of SARS-CoV-2 to Cell Receptors: A Tale of Molecular Evolution. <i>ChemBioChem</i> , 2021, 22, 724-732.	1.3	27
70642	Experimental and computational thermochemical study of dimethoxyacetophenones. <i>Journal of Chemical Thermodynamics</i> , 2021, 152, 106257.	1.0	3
70643	Flat crown ethers with planar tetracoordinate carbon atoms. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26479.	1.0	17
70644	Tunable luminescence in Ce ³⁺ /Mn ²⁺ co-doped ZrO ₂ nanophosphor integrated with theoretical studies on possible (ZrO ₂) _n clusters using DFT method. <i>Journal of Alloys and Compounds</i> , 2021, 853, 157378.	2.8	4
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70646	Experimental and theoretical study of CO ₂ sorption in biocompatible and biodegradable cholinium-based ionic liquids. <i>Separation and Purification Technology</i> , 2021, 254, 117609.	3.9	24
70647	Simple 3,6-disubstituted Carbazoles as Potential Hole Transport Materials: Photophysical, Electrochemical and Theoretical Studies. <i>Photochemistry and Photobiology</i> , 2021, 97, 289-300.	1.3	13
70648	Sensing behavior of pristine and doped C ₇₀ fullerenes to mercaptopurine drug: a DFT/TDDFT investigation. <i>Structural Chemistry</i> , 2021, 32, 457-468.	1.0	10
70649	Presence of excited electronic states on terbium incorporation in CaMoO ₄ : Insights from experimental synthesis and first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 149, 109790.	1.9	8
70650	Determination of rate constants for a thermoneutral H-abstraction reaction: Allylic hydrogen abstraction from 1,5-hexadiene by allyl radical. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 861-869.	2.4	5
70651	Experimental and theoretical spectroscopic characterization, NLO response, and reactivity of the pharmacological agent spilanthal and analogues. <i>Journal of Molecular Structure</i> , 2021, 1227, 129423.	1.8	9
70652	Synthesis, crystal structure, spectroscopic studies, NBO, AIM and SQMFF calculations of new pyridazinone derivative. <i>Journal of Molecular Structure</i> , 2021, 1223, 129213.	1.8	42

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70653	Adsorption of nitrosamine conformers on the C ₂₄ , B ₁₂ N ₁₂ , Be ₁₂ O ₁₂ and Al ₁₂ P ₁₂ nanocages and their conversion to nitrogen and water molecules: A DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 127, 114506.	1.3	6
70654	Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions. <i>Synlett</i> , 2021, 32, 561-572.	1.0	8
70655	Exploring the effect of oligothiophene and acene cores on the optoelectronic properties and enhancing p- and n-type ability of semiconductor materials. <i>Journal of Sulfur Chemistry</i> , 2021, 42, 180-192.	1.0	16
70656	Temozolomide binding to Cucurbit[7]uril: QAIM, NCI-RDG and NBO analyses. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2021, 99, 61-77.	0.9	16
70657	Self-consistent electrostatic embedding for liquid phase polarization. <i>Journal of Molecular Liquids</i> , 2021, 322, 114550.	2.3	7
70658	Conformer selective monohydrated clusters of 1,2,3,4-tetrahydroisoquinoline in SO: I-Potential energy surface studies, vibrational signatures and NBO analysis. <i>Journal of Molecular Structure</i> , 2021, 1225, 129177.	1.8	8
70659	Quantification of Noncovalent Interactions in Azide-Pnictogen, Chalcogen, and Halogen Contacts. <i>Chemistry - A European Journal</i> , 2021, 27, 4627-4639.	1.7	25
70660	Feasibility of Ca ₁₂ O ₁₂ Nanocluster in Lithium and Sodium Atom/Ion Batteries: DFT Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2021, 31, 1006-1014.	1.9	5
70661	A novel method for the synthesis and characterization of 10-hexyl-3-(1-hexyl-4,5-diphenyl-1H-imidazo[5,1-b]pyridin-2-yl)propan-1-amine molecular docking studies. <i>Research on Chemical Intermediates</i> , 2021, 47, 759-794.	1.3	12
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70665	Theoretical evaluation of the antioxidant activity of some stilbenes using the Density Functional Theory. <i>Journal of Molecular Structure</i> , 2021, 1229, 129496.	1.8	4
70666	Markovnikov versus anti-Markovnikov addition and C-H activation: Pd-Cu synergistic catalysis. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	23
70667	Halogen Complexes of Anionic N-Heterocyclic Carbenes. <i>Chemistry - A European Journal</i> , 2021, 27, 4349-4363.	1.7	25
70668	The influence of Ĩ-linkers configuration on properties of 10-hexylphenoxazine donor-based sensitizer for dye-sensitized solar cell application – Theoretical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107779.	1.3	9
70669	DFT computational investigation of the reaction behavior of polyamidoamine dendrimer as nanocarrier for delivery of melphalan anticancer drug. <i>Journal of Molecular Liquids</i> , 2021, 323, 114625.	2.3	8
70670	Quantum study of DHA, DPA and EPA anticancer fatty acids for microscopic explanation of their biological functions. <i>Journal of Molecular Liquids</i> , 2021, 325, 114646.	2.3	6

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70672	Titanium (IV) complexes of some tetraâ€dentate symmetrical bisâ€Schiff bases of 1,6â€hexanediamine: Synthesis, characterization, and in silico prediction of potential inhibitor against coronavirus (SARSâ€CoVâ€2). <i>Applied Organometallic Chemistry</i> , 2021, 35, e6067.	1.7	18
70673	Two dinuclear copper (II) and nickel (II) complexes based on 4â€(diethylamino)salicylaldehyde: Xâ€ray structures, spectroscopic, electrochemical, antibacterial, Hirshfeld surfaces analyses, and timeâ€dependent density functional theory calculations. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	15
70674	Building up Pt^{II}â€Thiosemicarbazoneâ€Lysineâ€sC18 Conjugates. <i>ChemBioChem</i> , 2021, 22, 694-704.	1.3	8
70675	Computational and Experimental Study of Turboâ€Organomagnesium Amide Reagents: Cubane Aggregates as Reactive Intermediates in Pummerer Coupling. <i>Chemistry - A European Journal</i> , 2021, 27, 2767-2773.	1.7	4
70676	Germaborenes: Borylene Transfer Agents for the Synthesis of Iminoboranes. <i>Chemistry - A European Journal</i> , 2021, 27, 1981-1983.	1.7	15
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70679	Negative-mode mass spectrometric study on dc corona, ac corona and dielectric barrier discharge ionization in ambient air containing H ₂ O ₂ , 2,4,6-trinitrotoluene (TNT), and 1,3,5-trinitroperhydro-1,3,5-triazine (RDX). <i>International Journal of Mass Spectrometry</i> , 2021, 459, 116440.	0.7	10
70680	Exploring reaction pathways for the structural rearrangements of the Mn cluster induced by water binding in the S ₃ state of the oxygen evolving complex of photosystem II. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 405, 112905.	2.0	12
70681	Curvature effects of electron-donating polymers on the device performance of non-fullerene organic solar cells. <i>Journal of Power Sources</i> , 2021, 482, 229045.	4.0	12
70682	Synthesis, X-ray crystallography, vibrational spectroscopy, thermal and DFT studies of (E)-6-(4-methylstyryl)-4,5-dihydropyridazin-3(2H)-one. <i>Journal of Molecular Structure</i> , 2021, 1225, 129180.	1.8	16
70683	Studies of crystal growth, structural, spectral and optical properties of solution grown 2-phenylethylammonium p-nitrophenolate monohydrate single crystals for efficient nonlinear optical applications. <i>Journal of Molecular Structure</i> , 2021, 1225, 129304.	1.8	10
70684	Synthesis, spectroscopic characterization and antibacterial evaluation by chalcones derived of acetophenone isolated from <i>Croton anisodontus</i> M&A. <i>Journal of Molecular Structure</i> , 2021, 1226, 129403.	1.8	25
70685	Morphology design and control of a novel 3D potassium metal-organic coordination polymer compound: Crystallography, DFT, thermal, and biological studies. <i>Journal of Molecular Structure</i> , 2021, 1228, 129434.	1.8	16
70686	Multi-spectroscopic (FT-IR, FT-Raman, ¹ H NMR and ¹³ C NMR) investigations on syringaldehyde. <i>Journal of Molecular Structure</i> , 2021, 1229, 129490.	1.8	19
70687	Hole transport materials for perovskite solar cells: A computational study. <i>Materials Chemistry and Physics</i> , 2021, 258, 123863.	2.0	21
70688	A Raman spectroscopy and rheology study of the phase transitions of the ionic liquid choline acetate. <i>Journal of Molecular Liquids</i> , 2021, 322, 114530.	2.3	12

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70690	Ultrahigh Thermoresistant Lightweight Bioplastics Developed from Fermentation Products of Cellulosic Feedstock. <i>Advanced Sustainable Systems</i> , 2021, 5, 2000193.	2.7	16
70691	Experimental and DFT investigation of ceria-nanocomposite decorated AC derived from groundnut shell for efficient removal of methylene-blue from wastewater effluent. <i>Applied Surface Science</i> , 2021, 536, 147749.	3.1	40
70692	Pd(II) complexes with ONN pincer ligand: Tailored synthesis, characterization, DFT, and catalytic activity toward the Suzuki-Miyaura reaction. <i>Journal of Molecular Structure</i> , 2021, 1225, 129071.	1.8	13
70693	Synthesis, characterization, anti-proliferative activity and chemistry computation of DFT theoretical methods of hydrazine-based Schiff bases derived from methyl acetoacetate and 1-hydroxyacetophenone. <i>Journal of Molecular Structure</i> , 2021, 1225, 129086.	1.8	12
70694	Drug design of new sigma-1 antagonists against neuropathic pain: A QSAR study using partial least squares and artificial neural networks. <i>Journal of Molecular Structure</i> , 2021, 1223, 129156.	1.8	5
70695	Synthesis, molecular docking and modeling of new acenaphthenequinones clubbed of anticancer. <i>Journal of Molecular Structure</i> , 2021, 1224, 129215.	1.8	4
70696	Synthesis, spectroscopy, crystal structure, TGA/DTA study, DFT and molecular docking investigations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one. <i>Journal of Molecular Structure</i> , 2021, 1228, 129435.	1.8	55
70697	Electronic and adsorption properties of extended chevron and cove-edged graphene nanoribbons. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 126, 114438.	1.3	13
70698	Cu (II) and Co (II/III) complexes of N,O-chelated Schiff base ligands: DNA interaction, protein binding, cytotoxicity, cell death mechanism and reactive oxygen species generation studies. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	11
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70700	Diverse interactions of aggregated insulin with selected coumarin dyes: Time dependent fluorogenicity, simulation studies and comparison with thioflavin T. <i>Dyes and Pigments</i> , 2021, 184, 108796.	2.0	1
70701	Calculation of donor numbers: Computational estimates for the Lewis basicity of solvents. <i>Journal of Molecular Liquids</i> , 2021, 322, 114506.	2.3	24
70702	Spectroscopic, quantum chemical, hydrogen bonding, reduced density gradient analysis and anti-inflammatory activity study on piper amide alkaloid piperine and wisanine. <i>Journal of Molecular Structure</i> , 2021, 1225, 129146.	1.8	16
70703	Electronic and molecular characterization of an air-stable Cr(II) complex containing azo-anion-radicals. <i>Journal of Molecular Structure</i> , 2021, 1223, 129247.	1.8	3
70704	Lack of the π -long-distance π ™ dynamical co-operative interactions due to low symmetry of hydrogen-bonded malonic acid aggregates in molecular crystals. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118993.	2.0	2
70705	Enhancement of hydrogen storage capacities of Co and Pt functionalized h-BN nanosheet: Theoretical study. <i>Vacuum</i> , 2021, 183, 109838.	1.6	15
70706	The Size-Accelerated Kinetic Resolution of Secondary Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 774-778.	7.2	17

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70708	A Novel Fluorescent Probe Based on Pyrazole-Pyrazoline for Fe (III) Ions Recognition. <i>Journal of Fluorescence</i> , 2021, 31, 29-38.	1.3	21
70709	Clumped 13CH ₂ D and 12CHD ₂ compositions of methyl groups from wood and synthetic monomers: Methods, experimental and theoretical calibrations, and initial results. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 297, 233-275.	1.6	8
70710	Synthesis, crystal structure, DFT studies and Hirshfeld surface analysis of novel isoxazole derivatives. <i>Journal of Molecular Structure</i> , 2021, 1228, 129450.	1.8	7
70711	Biological activities, DFT calculations and docking of imines tetradentates ligands, derived from salicylaldehydic compounds as metallo-beta-lactamase inhibitors. <i>Journal of Molecular Structure</i> , 2021, 1228, 129463.	1.8	7
70712	Enhancement of one- and two-photon absorption and visualization of intramolecular charge transfer of pyrenyl-contained derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118897.	2.0	26
70713	An algorithm to correct for the CASSCF active space in multiscale QM/MM calculations based on geometry ensembles. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26533.	1.0	5
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70715	Computational insights into electrocatalytic CO ₂ reduction facilitated by Mn(I) half sandwich-based catalysts: Role of substitution and solvent. <i>Electrochimica Acta</i> , 2021, 366, 137463.	2.6	2
70716	Relative cross sections and appearance energies in electron impact ionization and dissociation of mono-halogenated biphenyls. <i>International Journal of Mass Spectrometry</i> , 2021, 459, 116452.	0.7	3
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70852	Rapid Evaluation of the Mechanism of Buchwald-Hartwig Amination and Aldol Reactions Using Intramolecular ¹³ C Kinetic Isotope Effects. <i>ACS Catalysis</i> , 2021, 11, 60-67.	5.5	9
70854	Using high-throughput virtual screening to explore the optoelectronic property space of organic dyes; finding diketopyrrolopyrrole dyes for dye-sensitized water splitting and solar cells. <i>Sustainable Energy and Fuels</i> , 2021, 5, 704-719.	2.5	15
70855	A force field for bio-polymers in ionic liquids (BILFF) – part 1: [EMIm][OAc]/water mixtures. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1242-1253.	1.3	8
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70858	Cellulose conversion to biofuel precursors using conjugated ionic liquid catalyst: An experimental and DFT study. <i>Applied Catalysis A: General</i> , 2021, 610, 117951.	2.2	11
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70861	Hydrogen bonding effects on acidity enhancement of barbiturates and their metabolites in gas and solution phase, a DFT study. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113112.	1.1	1
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70864	New cobalt(II) Schiff base complex: Synthesis, characterization, DFT calculation and antimicrobial activity. <i>Inorganic Chemistry Communication</i> , 2021, 127, 108350.	1.8	12
70865	Theoretical insight into oxidation catalysis of chromite spinel MCr ₂ O ₄ (M = Mg, Co, Cu, and Zn): Volcano plot for oxygen-vacancy formation and catalytic activity. <i>Journal of Catalysis</i> , 2021, 393, 30-41.	3.1	11
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70873	Investigation of Aviation Lubricant Aging under Engine Representative Conditions. <i>Tribology Transactions</i> , 2021, 64, 501-512.	1.1	7
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70936	Scalable, safer and greener syntheses of vinylimidazoles via reactive distillation of hydroxyethylimidazole intermediates. <i>Polymer International</i> , 2021, 70, 582-593.	1.6	1
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70955	Ab-initio search for efficient red thermally activated delayed fluorescence molecules for organic light emitting diodes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118952.	2.0	5
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70968	Molecular structure, spectral (FT-IR, FT-Raman, Uv-Vis, and fluorescent) properties and quantum chemical analyses of azomethine derivative of 4-aminoantipyrine. <i>Journal of Molecular Structure</i> , 2021, 1227, 129512.	1.8	17
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74058	Molecular structure, hydrogen bond strength, and infrared Fourier transform vibrational assignment of 2,6-dimethylheptane-3,5-dione. <i>Journal of Molecular Structure</i> , 2021, 1243, 130803.	1.8	1
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74069	Molecular structure, spectral and thermal properties and in silico biological activity of new bis-phthalimidopropylalkylammonium conjugates of bile acids. <i>Journal of Molecular Structure</i> , 2021, 1243, 130814.	1.8	1
74070	Synthesis and characterization for new Mn(II) complexes; conductometry, DFT, antioxidant activity via enhancing superoxide dismutase enzymes that confirmed by in-silico and in-vitro ways. <i>Journal of Molecular Structure</i> , 2021, 1243, 130855.	1.8	7
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74072	Ionic liquid screening for dichloromethane absorption by multi-scale simulations. <i>Separation and Purification Technology</i> , 2021, 275, 119187.	3.9	16

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74073	On structure and hyperhalogen properties of hetero-binuclear superatoms $M_2(BO_2)^+$ ($M = Na, Mg$); T_j $ETQ_{0,0} \text{ rgBT}_2$ /Overlock	1.0	0
74074	Utilization of asymmetrical electron transport as strategy for modelling and design of efficient single molecule diodes: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113441.	1.1	5
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74076	Predicting ion mobility as a function of the electric field for small ions in light gases. <i>Analytica Chimica Acta</i> , 2021, 1184, 339019.	2.6	9
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74078	Synthesis, characterization, surface analysis, optical activity and solvent effects on the electronic absorptions of Schiff base-functionalized amino thiophene derivatives: Experimental and TD-DFT investigations. <i>Journal of Molecular Structure</i> , 2021, 1244, 131267.	1.8	6
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74083	Development of metal free melamine modified graphene oxide for electrochemical sensing of epinephrine. <i>FlatChem</i> , 2021, 30, 100288.	2.8	25
74084	Novel bisthiazole ligand and its copper(II) complex with unusual seven membered ring: Synthesis, characterization, experimental and theoretical study of the effect of ligand flexibility, and antimicrobial activity. <i>Polyhedron</i> , 2021, 209, 115490.	1.0	4
74085	Synthesis optimization, DFT and physicochemical study of chitosan sulfates. <i>Journal of Molecular Structure</i> , 2021, 1245, 131083.	1.8	54
74086	p-Block Heterobenzenes: Recurring Features in Structural, Vibrational, Electronic and Topological Properties. <i>Journal of Molecular Structure</i> , 2021, 1245, 131258.	1.8	1
74087	Synthesis, characterization, molecular structure, and computational studies on 4(1H)-pyran-4-one and its derivatives. <i>Journal of Molecular Structure</i> , 2021, 1245, 131077.	1.8	2
74088	Increasing the sensitivity of the molecular probes for the substituent effects α The SESE approach. <i>Journal of Molecular Structure</i> , 2021, 1246, 131186.	1.8	1
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74090	Influence of progressive halogenation of Zn(II)-tetraarylporphyrins and their free bases on the structure and spectral-fluorescence properties of tetrapyrrolic macrocycle. <i>Inorganica Chimica Acta</i> , 2021, 528, 120620.	1.2	1

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74092	Synthesis, spectroscopic characterization, molecular docking studies and DFT calculation of novel Mannich base 1-((4-ethylpiperazin-1-yl)(2-hydroxyphenyl)methyl)naphthalen-2-ol. <i>Journal of Molecular Structure</i> , 2021, 1246, 131164.	1.8	31
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74094	Metal organic frameworks as sacrificial templates for preparation of hierarchical covalent organic frameworks enabling ultrafast sample treatment in nontargeted food safety analysis. <i>Chemical Engineering Journal</i> , 2021, 425, 130673.	6.6	4
74095	Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. <i>Journal of Molecular Liquids</i> , 2021, 343, 117633.	2.3	23
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74103	Vibrational and conformational analysis of structural phase transition in Estradiol 17 β valerate with temperature. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120219.	2.0	0
74104	Third-order NLO studies of 2, 4-Bis (4-fluorophenyl)-2, 3-dihydro-1H-1, 5-benzodiazepine using Z-scan technique and DFT method. <i>Journal of Molecular Structure</i> , 2021, 1246, 131169.	1.8	9
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74107	DFT and MD simulation investigation of favipiravir as an emerging antiviral option against viral protease (3CLpro) of SARS-CoV-2. <i>Journal of Molecular Structure</i> , 2021, 1246, 131253.	1.8	27
74108	Spectroscopic characterization of 4,5-diphenyl-2-(2,4,5-trimethoxyphenyl)-1H-imidazole obtained from the condensation of benzyl. Experimental and DFT approach. <i>Journal of Molecular Structure</i> , 2021, 1246, 131269.	1.8	2

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74110	Conformational equilibrium, IR and Raman vibrational spectra of the quercetin molecule in different solvents: A comprehensive quantum-chemical investigation. <i>Chemical Physics Impact</i> , 2021, 3, 100033.	1.7	2
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74112	Crystallographic, spectroscopic, TD/DFT calculations and Hirshfeld surface analysis of cadmium(II) coordination polymer containing pyridine ring. <i>Journal of Molecular Structure</i> , 2021, 1245, 131028.	1.8	16
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74117	Biotin-tagged cis-dichlorido-oxidovanadium(IV) complex for DNA crosslinking and photo-induced apoptotic cytotoxicity. <i>Inorganica Chimica Acta</i> , 2021, 528, 120629.	1.2	3
74118	Polymorph acceptor-based triads with photoinduced TADF for UV sensing. <i>Chemical Engineering Journal</i> , 2021, 425, 131549.	6.6	7
74119	Electron scattering from molecules relevant to Titan's atmosphere. <i>International Journal of Mass Spectrometry</i> , 2021, 470, 116708.	0.7	5
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74128 Synthesis, crystal structural determination and in silico biological studies of

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74159	Synthesis, biological and theoretical properties of crystal zinc complex with thiosemicarbazone of glyoxylic acid. Journal of Molecular Structure, 2022, 1248, 131470.	1.8	12
74160	Solution-processed Cd-substituted CZTS nanocrystals for sensitized liquid junction solar cells. Journal of Alloys and Compounds, 2022, 890, 161575.	2.8	9
74161	Reactivity of hemilabile 2-pyridylselenolate ligand towards [NiCl ₂ (dppe)]: Combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1248, 131368.	1.8	5
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74164	A Density Functional Theory study for adsorption and sensing of 5-Fluorouracil on Ni-doped boron nitride nanotube. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106183.	1.9	10
74165	Assessing CH ₄ /N ₂ separation potential of MOFs, COFs, IL/MOF, MOF/Polymer, and COF/Polymer composites. <i>Chemical Engineering Journal</i> , 2022, 428, 131239.	6.6	89
74166	Theoretical study of the reaction mechanism between Criegee intermediates and hydroxyl radicals in the presence of ammonia and amine. <i>Chemosphere</i> , 2022, 287, 131877.	4.2	3
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74173	Multiscale modeling studies for exploring lignocellulosic biomass structure. , 2022, , 257-289.		2
74174	Optimized molecular geometry, vibrational analysis, and Fe-O bond strength of Tris(1±-cyanoacetylacetonate)iron(III):An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2022, 1248, 131444.	1.8	4
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74176	The uptake of selenite in calcite revealed by X-ray absorption spectroscopy and quantum chemical calculations. <i>Science of the Total Environment</i> , 2022, 802, 149221.	3.9	4
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74178	Synthesis, characterization, crystal and molecular structure and theoretical study of N-(naphthalen-1-yl)-2-(piperidin-1-yl) acetamide, a selective butyrylcholinesterase inhibitor. <i>Journal of Molecular Structure</i> , 2022, 1248, 131544.	1.8	0
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74182	Synthesis, crystal structure, spectroscopic characterization, $\hat{1}\pm$ -glucosidase inhibition and computational studies of (E)-5-methyl-N $\hat{2}$ -(pyridin-2-ylmethylene)-1H-pyrazole-3-carbohydrazide. <i>Journal of Molecular Structure</i> , 2022, 1248, 131506.	1.8	13
74183	Techneium-99 decontamination from radioactive wastewater by modified bentonite: batch, column experiment and mechanism investigation. <i>Chemical Engineering Journal</i> , 2022, 428, 131333.	6.6	26
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74188	Molecular modeling and antioxidant evaluation of new di-2-thienyl ketones festooned with thiazole or pyridine moiety. <i>Journal of Molecular Structure</i> , 2022, 1247, 131287.	1.8	7
74189	Optical properties of new 5- (phenothiazinyl)methylidenebarbituric acid derivatives. <i>Journal of Molecular Structure</i> , 2022, 1247, 131334.	1.8	1
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74192	Structure and dynamics of methacrylamide, a computational and free-jet rotational spectroscopic study. <i>Journal of Molecular Structure</i> , 2022, 1248, 131391.	1.8	3
74193	The NVO defects in diamond: A quantum mechanical characterization through its vibrational and Electron Paramagnetic Resonance spectroscopies. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 160, 110304.	1.9	3
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74196	Exploring the relationship between the $\hat{1}\pm$ ON-OFF $\hat{1}\pm$ mechanism of fluorescent probes and intramolecular charge transfer properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120339.	2.0	4
74197	Excited state hydrogen atom transfer pathways in 2,7-diazaindole $\hat{1}\pm$ S1-3 ($\hat{1}\pm$ H $\hat{2}$ O and NH $\hat{3}$) clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120386.	2.0	3
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74204	[Diaquo{bis(p-hydroxybenzoato- η^1 O1)}(1-methylimidazole- η^1 N1)}copper(II)]: Synthesis, crystal structure, catalytic activity and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1247, 131323.	1.8	3
74205	Exploring packing features of N-substituted acridone derivatives: Synthesis and X-ray crystallography studies. <i>Journal of Molecular Structure</i> , 2022, 1248, 131448.	1.8	3
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74211	DFT study on the effect of functional groups of carbonaceous surface on ammonium adsorption from water. <i>Chemosphere</i> , 2022, 287, 132294.	4.2	15
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74213	Mn(II) catalyzed synthesis of 5-(4-hydroxyphenyl)-2-(N-phenylamino)-1,3,4-oxadiazole: Crystal structure, DFT, molecular docking, Hirshfeld surface analysis, and in vitro anticancer activity on DL cells. <i>Journal of Molecular Structure</i> , 2022, 1249, 131547.	1.8	10
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77973	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 255-265.	2.5	17
77974	Fragmentation pathways of deprotonated α -hydroxybenzyl alcohol. <i>Journal of Mass Spectrometry</i> , 2022, 57, e4829.	0.7	1
77975	Density functional theory-nuclear magnetic resonance-validated full structure elucidation of the ionbrunonine C, an unstable α -oxide theionbrunonine from <i>Mostuea brunonis</i> . <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 1178-1184.	1.1	1

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77977	Synthesis, structural elucidation, in vitro antibacterial activity, DFT calculations, and molecular docking aspects of mixed-ligand complexes of a novel oxime and phenylalanine. <i>Bioorganic Chemistry</i> , 2022, 121, 105685.	2.0	5
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77979	Photovoltaic parameters and computational spectroscopic investigation of third order nonlinear optical of CuPc/Si organic diode. <i>Optical Materials</i> , 2022, 126, 112071.	1.7	9
77980	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2845-2862.	2.3	18
77981	Insights into reaction mechanisms of phosphonium cation and methyleneimine: a theoretical study. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 0, , 1-7.	0.8	0
77982	Photo-switching behaviour in liquid crystalline materials incorporating a non-planar dithienylcyclopentene core and their birefringence properties. <i>Liquid Crystals</i> , 2022, 49, 1475-1487.	0.9	2
77983	Synthesis and characterization of chiral bidentate bis(N-heterocyclic carbene)-carboxylate palladium and nickel complexes. <i>Inorganica Chimica Acta</i> , 2022, 537, 120946.	1.2	4
77984	Enantioselective Cytotoxicity of Chiral Diphosphine Ruthenium(II) Complexes Against Cancer Cells. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	7
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77987	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2947-2954.	2.3	7
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77990	Slow hole transfer kinetics lead to high blend photoluminescence of unfused A ² DA ² CA type acceptors with unfavorable HOMO offset. <i>Solar Rrl</i> , 0, , .	3.1	0
77991	Enantioselective Addition of Remote Alkyl Radicals to Double Bonds by Photocatalytic Proton-Coupled Electron Transfer (PCET) Deconstruction of Unstrained Cycloalkanols. <i>Organic Letters</i> , 2022, 24, 3123-3127.	2.4	8
77992	Photochemical Hydrogen Storage with Hexaazatrinaphthylene (HATN). <i>ChemPhysChem</i> , 2022, , .	1.0	2
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77995	Insights into the C-H activation mechanism in the Rh(I)-Catalyzed alkenylation of ketone with alkyne. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113703.	1.1	1
77996	Molecular modeling and docking studies of new antimicrobial antipyrine-thiazole hybrids. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103898.	2.3	6
77997	Identification of radiation degradation products of soluble fraction of silicone foams. <i>Polymer Degradation and Stability</i> , 2022, 198, 109893.	2.7	3
77998	Thiourea derivatives acting as functional monomers of As(III) molecular imprinted polymers: A theoretical and experimental study on binding mechanisms. <i>Journal of Hazardous Materials</i> , 2022, 430, 128508.	6.5	7
77999	Arene-ruthenium(II) complexes with tetracyclic oxime derivatives: synthesis, structure and antiproliferative activity against human breast cancer cells. <i>Inorganica Chimica Acta</i> , 2022, 535, 120879.	1.2	10
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78005	Structure, stability and properties of alternating boron-nitride nanotubes (BNNTs): A density functional theory calculations. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113668.	1.1	2
78006	Optimization of energy surface of thiophene-benzothiazole derivative Schiff base molecule with fuzzy logic modelling. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113680.	1.1	3
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78008	Iridium(III)-3-hydroxy-2-(3-methyl-2-thienyl)-4-oxo-4H-1-benzopyran complex: The analytical, in-vitro antibacterial and DFT studies. <i>Inorganic Chemistry Communication</i> , 2022, 139, 109333.	1.8	3
78009	An electrochemical chiral sensor based on glutamic acid functionalized graphene-gold nanocomposites for chiral recognition of tryptophan enantiomers. <i>Journal of Electroanalytical Chemistry</i> , 2022, 913, 116283.	1.9	14
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78013	Triple proton transfer after water rearrangement in (2,6-aza)Ind ²⁺ ·(H ₂ O) ₂ . <i>Journal of Molecular Liquids</i> , 2022, 353, 118847.	2.3	2
78014	DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. <i>Separation and Purification Technology</i> , 2022, 289, 120709.	3.9	8
78015	Investigation of reaction mechanisms of CO ₂ reduction to methanol by Ni-C80 and Co-Si60 catalysts. <i>Inorganic Chemistry Communication</i> , 2022, 139, 109358.	1.8	1
78016	Aggregation induced emission (AIE)-active ferrocene conjugated linear π -extended multi donor-acceptor (D-D ² -A) chromophores: Synthesis, structural, theoretical, linear and nonlinear optical studies. <i>Dyes and Pigments</i> , 2022, 201, 110193.	2.0	17
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78019	Investigations of tetramethyl glutaramide ligand in the formation of stable gas-phase tetrapositive complexes with metal tetracations. <i>International Journal of Mass Spectrometry</i> , 2022, 475, 116818.	0.7	0
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78029	Hetero Diels-Alder cycloadduct of Anti-Tumor (E)-3-X-indoline-2-thiones with C ₂₀ fullerene as drug delivery in solution vs. gas phase: A DFT survey. <i>Inorganic Chemistry Communication</i> , 2022, 139, 109353.	1.8	4

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78041	Optical absorption and photoluminescence of partially fluorinated graphite crystallites. <i>Carbon</i> , 2022, 193, 98-106.	5.4	7
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78045	Development of magnetic nanoparticles for the intracellular delivery of miR-148b in non-small cell lung cancer. <i>Biomedical Engineering Advances</i> , 2022, 3, 100031.	2.2	9
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78061	Deep eutectic solvents with multiple hydroxyl sites for efficient and reversible absorption of SF ₆ . Journal of Molecular Liquids, 2022, 356, 119052.	2.3	2
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78063	Regulating the excited state behaviors of 2-benzooxazol-2-yl-4,6-di-tert-butyl-phenol fluorophore by solvent polarity: A theoretical simulation. Chemical Physics, 2022, 558, 111513.	0.9	7
78064	Ionic-liquid doping of carbon nanotubes with [HMIM][BF ₄] for flexible thermoelectric generators. Chemical Engineering Journal, 2022, 438, 135526.	6.6	21
78065	Mechanistic insight into the electron-donation effect of modified ZIF-8 on Ru for CO ₂ hydrogenation to formic acid. Journal of CO ₂ Utilization, 2022, 60, 101992.	3.3	14

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78067	A two-photon fluorogenic probe based on a coumarin schiff base for formaldehyde detection in living cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 274, 121074.	2.0	7
78068	Validation of hybrid WC1LYP functional for ferroelectric LiNbO3 and LiTaO3 using Compton spectroscopy and first-principles computations. <i>Materials Today Communications</i> , 2022, 31, 103288.	0.9	2
78069	Effect of halide/pseudohalide anions on the association and semimicroextraction of substituted chloroaurates with a symmetric carbocyanine dye: A complex study and analytical application. <i>Journal of Molecular Liquids</i> , 2022, 356, 119037.	2.3	0
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78073	Nanoconfinement of tetraphenylethylene in zeolitic metal-organic framework for turn-on mechanofluorochromic stress sensing. <i>Applied Materials Today</i> , 2022, 27, 101434.	2.3	11
78074	Extreme structure and spontaneous lift of spin degeneracy in doped perforated bilayer graphenes. <i>Carbon</i> , 2022, 192, 61-70.	5.4	6
78075	Synthesis, NMR, vibrational spectroscopy, thermal and DFT studies of new DABCO hexafluorophosphate based ionic liquid. <i>Journal of Molecular Structure</i> , 2022, 1258, 132682.	1.8	6
78076	A spectroscopic study of benzonitrile. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2022, 283, 108159.	1.1	3
78077	Rational design of novel potential EGFR inhibitors by 3D-QSAR, molecular docking, molecular dynamics simulation, and pharmacokinetics studies. <i>Chemical Data Collections</i> , 2022, 39, 100851.	1.1	6
78078	The His23 and Lys79 pair determines the high catalytic efficiency of the inorganic pyrophosphatase of the haloacid dehalogenase superfamily. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2022, 1866, 130128.	1.1	1
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78081	Highly improved nonlinear optical responses of reduced graphene oxide via the decoration of Ni doped ZnS nanoparticles. <i>Photonics and Nanostructures - Fundamentals and Applications</i> , 2022, 50, 101004.	1.0	4
78082	Conformational stability, quantum computational, spectroscopic, molecular docking and molecular dynamic simulation study of 2-hydroxy-1-naphthaldehyde. <i>Journal of Molecular Structure</i> , 2022, 1259, 132755.	1.8	7
78083	Piano-stool type (1-6-p-cymene)ruthenium(II) thiazole-derived motifs complexes: Synthesis, crystal structures, DFT studies, molecular docking and in-vitro binding studies with HSA and cytotoxicity. <i>Inorganica Chimica Acta</i> , 2022, 537, 120925.	1.2	2

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78085	Synthesis, antimicrobial, anticancer activities, PASS prediction, molecular docking, molecular dynamics and pharmacokinetic studies of designed methyl β -D-glucopyranoside esters. <i>Journal of Molecular Structure</i> , 2022, 1260, 132761.	1.8	27
78086	A coumarin-based fluorescence chemosensor for the determination of Al^{3+} and ClO_4^- with different fluorescence emission channels. <i>Inorganica Chimica Acta</i> , 2022, 537, 120953.	1.2	6
78087	Polyethersulfone/polyvinylpyrrolidone/boron nitride composite membranes for high proton conductivity and long-term stability high-temperature proton exchange membrane fuel cells. <i>Journal of Membrane Science</i> , 2022, 653, 120512.	4.1	19
78088	An account of chronological computational investigations to ascertain the role of π - π bonding in influencing the Lewis acidity of BX_3 ($X = F, Cl, Br$ and I): Evolution of novel parameters and relegation of π -type back bonding concept. <i>Coordination Chemistry Reviews</i> , 2022, 463, 214519.	9.5	3
78089	Theoretical and experimental investigations of a gold nanosensor based on rhodamine-modified carbon nanotubes. <i>Journal of Molecular Structure</i> , 2022, 1260, 132765.	1.8	1
78090	Deep eutectic solvent-based polymer electrolyte for solid-state lithium metal batteries. <i>Journal of Energy Chemistry</i> , 2022, 70, 363-372.	7.1	32
78091	Substitution-inert polynuclear platinum complexes and Glycosaminoglycans: A molecular dynamics study of its non-covalent interactions. <i>Journal of Inorganic Biochemistry</i> , 2022, 232, 111811.	1.5	1
78092	Refine the evaluation of photophysical properties of organometallic chromophores under confined molecular crystal conditions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121168.	2.0	1
78093	Experimental and Theoretical Vibrational Spectroscopic Investigations, DFT quantum chemical analysis, Biological activities and Molecular docking on 4,4'-Dimethoxy-2,2'-Bipyridine. <i>Journal of Molecular Structure</i> , 2022, 1260, 132846.	1.8	4
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78096	Experimental and density functional theoretical modeling of triazole pesticides extraction by Ti2C nanosheets as a sorbent in dispersive solid phase extraction method before HPLC-MS/MS analysis. <i>Microchemical Journal</i> , 2022, 178, 107331.	2.3	30
78097	Robust and predictive QSAR models for predicting the D2, 5-HT1A, and 5-HT2A inhibition activities of fused tricyclic heterocycle piperazine (piperidine) derivatives as atypical antipsychotic drugs. <i>Journal of Molecular Structure</i> , 2022, 1259, 132753.	1.8	2
78098	Radicals in ammonium tartrate at 295 K by X-radiation: Revised radical structures by EMR and DFT analyses. <i>Radiation Physics and Chemistry</i> , 2022, 196, 110097.	1.4	3
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78100	Antispasmodic activity of carnosic acid extracted from <i>rosmarinus officinalis</i> : Isolation, spectroscopic characterization, DFT studies, and in silico molecular docking investigations. <i>Journal of Molecular Structure</i> , 2022, 1260, 132795.	1.8	43
78101	Naked-eye colorimetric anion probing and fluorescent switching features of conjugated Schiff Bases derived from 4-(Trifluoromethyl) benzenesulfonamide. <i>Journal of Luminescence</i> , 2022, 247, 118849.	1.5	5

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78107	Ionic Liquid Functionalized Cu ₂ O nanoparticles. <i>Journal of Molecular Structure</i> , 2022, 1262, 132961.	1.8	5
78108	Synthesis, prototropic tautomerism studies of indenocarbothioamides and their conversion to biologically active indenothiazole derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 276, 121194.	2.0	0
78109	Highly fluorescent carbon nitride oligomer with aggregation-induced emission characteristic for plastic staining. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 276, 121238.	2.0	4
78110	Molecularly engineered organic copolymers as high capacity cathode materials for aqueous proton battery operating at sub-zero temperatures. <i>Journal of Colloid and Interface Science</i> , 2022, 619, 123-131.	5.0	14
78111	Synthesis, characterizations, crystal structure, inhibition effects and theoretical study of novel Schiff base on the corrosion of carbon steel in 1M HCl. <i>Journal of Molecular Structure</i> , 2022, 1261, 132852.	1.8	20
78112	Peptide-based colorimetric and fluorescent dual-functional probe for sequential detection of copper(II) and cyanide ions and its application in real water samples, test strips and living cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 276, 121222.	2.0	27
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78132	Simulation of Gas Production Mechanisms in Shear Deformation of Medium-Rank Coal. <i>ACS Omega</i> , 2022, 7, 342-350.	1.6	3
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81833	Molecular docking, HOMO-LUMO and quantum chemical computation analysis of anti-glyoximehydrazone derivatives containing pyrazolone moiety and their transition metal complexes. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100981.	1.3	1
81834	Revealing intrinsic changes of DNA induced by spore photoproduct lesion through computer simulation. <i>Biophysical Chemistry</i> , 2023, 296, 106992.	1.5	0
81835	Synthesis, electronic structure and interaction of rhodium(I) and iridium(I) bisimine-acenaphthalene complexes with CO ₂ . <i>Polyhedron</i> , 2023, 235, 116350.	1.0	0
81836	Theoretical study of C ₆ F ₅ -corrole molecules functionalized with aromatic groups for Photodynamic Therapy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 293, 122500.	2.0	2

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81838	Molecular spectroscopy and optical effect of Albendazole chemical compound behaves as liquid crystal: A theoretical and experimental approach. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2023, 291, 116351.	1.7	0
81839	Adsorption of 40 low molecular weight drugs on pristine and fluorinated C60 fullerenes: Ab initio, statistical and neural networks analysis. <i>Journal of Molecular Liquids</i> , 2023, 377, 121559.	2.3	1
81840	LE and ICT properties of pyrazolo[1,5-a]pyrimidines based dyes: Experiments and DFT/TDDFT calculations. <i>Journal of Luminescence</i> , 2023, 257, 119772.	1.5	3
81841	A bioinspired cobalt catalyst based on a tripodal imidazole/pyridine platform capable of water reduction and oxidation. <i>Journal of Inorganic Biochemistry</i> , 2023, 242, 112162.	1.5	0
81842	H \cdots Bond interactions in water multimers and water multimers \cdots Pyridine complexes: Natural bond orbital and reduced density gradient isosurface analyses. <i>Journal of Molecular Liquids</i> , 2023, 377, 121524.	2.3	6
81843	Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3+3] Annulation of 2-bromoenals and β -ketothioamides: A DFT study. <i>Molecular Catalysis</i> , 2023, 542, 113135.	1.0	0
81844	Theoretical investigation into activation of hydroperoxides by excited quinones under ultraviolet irradiation. <i>Chemical Engineering Journal</i> , 2023, 463, 142423.	6.6	0
81845	In silico evaluation of geroprotective phytochemicals as potential sirtuin 1 interactors. <i>Biomedicine and Pharmacotherapy</i> , 2023, 161, 114425.	2.5	2
81846	Silk fibroin-based biopolymer composite binders with gradient binding energy and strong adhesion force for high-performance micro-sized silicon anodes. <i>Journal of Energy Chemistry</i> , 2023, 80, 442-451.	7.1	5
81847	Tuning the surface electronic structure of WS ₂ with Zn- and Cu-phthalocyanine for improved hydrogen evolution reaction: Experimental and DFT investigation. <i>FlatChem</i> , 2023, 39, 100499.	2.8	4
81848	Synthesis, spectra, crystal, DFT, molecular docking and in vitro cholinesterase inhibition evaluation on two novel symmetrical Azine Schiff bases. <i>Journal of Molecular Structure</i> , 2023, 1281, 135171.	1.8	3
81849	Heterojunction solar cell based on donor-acceptor pi-conjugated naphthalene bisbenzimidazole, perylene bisbenzimidazole, and naphthalene imidazole: A spectroscopic, microscopic and DFT assessment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122516.	2.0	3
81850	Coupling of experimental and theoretical studies to apprehend the action of benzodiazepine derivative as a corrosion inhibitor of carbon steel in 1M HCl. <i>Journal of Molecular Structure</i> , 2023, 1281, 135139.	1.8	14
81851	Spectroscopic characterization of a mononuclear oxovanadium (IV) Schiff base complex. Oxidation catalysis applications and antibacterial activities. <i>Journal of Molecular Structure</i> , 2023, 1281, 135131.	1.8	3
81852	Ionic mononuclear [Fe] and heterodinuclear [Fe,Ru] bis(diphenylphosphino)alkane complexes: Synthesis, spectroscopy, DFT structures, cytotoxicity, and biomolecular interactions. <i>Journal of Inorganic Biochemistry</i> , 2023, 242, 112156.	1.5	3
81853	DFT and electrochemical study on some iron(III) complexes with 2-hydroxybenzophenones. <i>Inorganica Chimica Acta</i> , 2023, 550, 121445.	1.2	0
81854	Arylidine extensions of 3-methyl-5-oxo-4,5-dihydro-1H-pyrazol-benzenesulfonamide derivatives: Synthesis, computational simulations and biological evaluation as tumor-associated carbonic anhydrase inhibitors. <i>Bioorganic Chemistry</i> , 2023, 135, 106492.	2.0	3

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81856	3-(dimethylamino)dibenzothiophene (3-DMADBT): Synthesis, characterization, crystallographic study, Quantum chemical calculations, Hirshfeld surface analysis and FT-IR spectroscopy. <i>Journal of Molecular Structure</i> , 2023, 1281, 135142.	1.8	0
81857	3-arylthioimidazo[1,2-a]pyridine derivatives: A theoretical and experimental study of its photophysical properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 440, 114675.	2.0	1
81858	Simulation and quantitative characterisation of polyvinyl alcohol grafted ethylenediamine tetraacetic acid chelating material. <i>Materials Today Communications</i> , 2023, 35, 105720.	0.9	0
81859	Theoretical study of lithium oxide clusters adsorbed on anatase TiO ₂ surface. <i>Surfaces and Interfaces</i> , 2023, 38, 102856.	1.5	1
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81862	Judicious training pattern for superior molecular reorganization energy prediction model. <i>Journal of Energy Chemistry</i> , 2023, 81, 143-148.	7.1	0
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81865	Computational studies of chalcogen doped on graphene vs. chalcogen doped on CNT and their role in the catalytic performance of electrochemical CO ₂ reduction. <i>Materials Today Communications</i> , 2023, 35, 105631.	0.9	0
81866	Synthesis, structural characterization and antibacterial activity evaluation of novel quinolone-1,2,3-triazole-benzimidazole hybrids. <i>Journal of Molecular Structure</i> , 2023, 1282, 135179.	1.8	4
81867	4-(4-methoxyphenyl)-6-methyl-3-phenyl-4H-1,2,4-oxadiazin-5(6H)-one: Synthesis, crystal structure, Hirshfeld surface analysis, noncovalent, ADMET studies and biological evaluation. <i>Journal of Molecular Structure</i> , 2023, 1282, 135197.	1.8	1
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81869	QSAR modeling, molecular docking and molecular dynamic simulation of phosphorus-substituted quinoline derivatives as topoisomerase I inhibitors. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104783.	2.3	2
81870	Molecular dynamics simulation study of DNA conformation changes caused by the dinuclear platinum(II) complexes with the bisphosphonate group. <i>Journal of Inorganic Biochemistry</i> , 2023, 243, 112179.	1.5	1
81871	NIR light-driven photocatalytic NAD(P)H oxidation and H ₂ O ₂ generation in situ for enhanced chemodynamic therapy and immune response. <i>Nano Today</i> , 2023, 50, 101824.	6.2	8
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81874	Experimental and theoretical observations in a mixed mode dispersive solid phase extraction of exogenous surfactants from exhaled breath condensate prior to HPLC-MS/MS analysis. <i>Journal of Molecular Structure</i> , 2023, 1281, 135096.	1.8	5
81875	The interplay between spin states, geometries and biological activity of Fe(III) and Mn(II) complexes with thiosemicarbazone. <i>Polyhedron</i> , 2023, 237, 116389.	1.0	1
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81877	Luminescent furo[2,3-c]isoquinolines as fluorophores - Tuning the luminophore by donor substitution. <i>Dyes and Pigments</i> , 2023, 214, 111190.	2.0	1
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81879	Sulfido-bridged 1,2-bis(diphenylphosphino)ethane (dppe) appended trinuclear nickel(II) clusters: Crystallographic and computational analyses. <i>Inorganica Chimica Acta</i> , 2023, 551, 121471.	1.2	2
81880	Photo-oxidation of ethyl pyruvate initiated by chlorine atoms. Kinetics and reaction mechanism. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 440, 114655.	2.0	2
81881	Boron isotope fractionation between B(OH) ₃ and B(OH) ₄ ⁻ in aqueous solution: A theoretical investigation beyond the harmonic and Born-Oppenheimer approximations. <i>Chemical Geology</i> , 2023, 627, 121455.	1.4	2
81882	Interaction of bases and base pairs with polycyclic aromatic hydrocarbons as finite size model of graphene. <i>Chemical Physics Impact</i> , 2023, 6, 100199.	1.7	0
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81884	B12 and F430 models: Metal- versus ligand-centered redox in cobalt and nickel tetrahydrocorrin derivatives. <i>Journal of Inorganic Biochemistry</i> , 2023, 243, 112199.	1.5	3
81885	Engineered organotin(IV) and vanadium(V) derivatives with distinct coordination modes and luminescent properties for the efficient detection and quantification of permanganate ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122521.	2.0	1
81886	Direct observation on argon tagging nitrobenzene radical anion in gas phase: Infrared photodissociation spectroscopy and theoretical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122482.	2.0	2
81887	Structural evolution, electronic and magnetic properties investigation of V ₃ Si _n (n=14-18) clusters based on photoelectron spectroscopy and density functional theory calculations. <i>Chemical Physics Letters</i> , 2023, 820, 140423.	1.2	6
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81889	Discovery of a spirocyclic 3-bromo-4,5-dihydroisoxazole covalent inhibitor of hGAPDH with antiproliferative activity against pancreatic cancer cells. <i>European Journal of Medicinal Chemistry</i> , 2023, 254, 115286.	2.6	2
81890	Beneficial effect of in-situ citrate-grafting of hydroxyapatite surface for water treatment. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 666, 131366.	2.3	2

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81894	Know your building blocks: Time-resolved EPR spectroscopy reveals NDI-T2 and not T-NDI-T to resemble the electronic structure of PNDIT2. <i>Organic Electronics</i> , 2023, 117, 106790.	1.4	0
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81896	Environmental biotransformation mechanisms by flavin-dependent monooxygenase: A computational study. <i>Chemosphere</i> , 2023, 325, 138403.	4.2	0
81897	Ultra-low limit of luminescent detection of gossypol by terbium(III)-based metal-organic framework. <i>Journal of Hazardous Materials</i> , 2023, 452, 131289.	6.5	7
81898	Triplet state generation followed by the excited-state intramolecular proton transfer in 3-sulfanylchromen-4-one. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114700.	2.0	4
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81901	Performance enhancement of catechin-graphene quantum dot nanocomposites functionalized with carboxyl and doped/decorated with boron towards dye-sensitized solar cell applications: DFT and TD-DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 121, 108427.	1.3	5
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81903	Crystal structure, DFT calculation, molecular docking, in vitro biological activity evaluation and in silico drug-likeness prediction of (E)-N-(4-bromophenyl)-4-(2-(2-hydroxybenzylidene)) Tj ETQq0 0 0 rgBT /Overlock 108Tf 50 257 Td (hydr	10.8	57
81904	Spectroscopic, X-ray, mechanistic and DFT studies on formation of novel benzoimidazole-4-ones from cyclohexenyl carbothioamides. <i>Chemical Physics</i> , 2023, 571, 111935.	0.9	0
81905	Molecular structure of Ru(II)/diphosphine/4,6-dimethyl-2-pyrimidinethiol complexes: A combined experimental and density functional theory study. <i>Journal of Molecular Structure</i> , 2023, 1282, 135234.	1.8	0
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81908	Theoretical insights into the spectroscopic properties of ferrocenyl hetaryl ketones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122635.	2.0	0

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81910	Mononuclear copper(μ ...) complexes with mechanochromic thermally activated delayed fluorescence behaviour based on switchable hydrogen bonds. <i>Polyhedron</i> , 2023, 237, 116391.	1.0	1
81911	Photoinduced charge transfer in push-pull pyrazoline-based chromophores – Relationship between molecular structure and photophysical, photovoltaic properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122643.	2.0	1
81912	Hypochlorous acid-activated near-infrared fluorescent probe for in vivo/exogenous detection and dairy toxicity evaluation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122661.	2.0	3
81913	Modification of a commercial activated carbon with nitrogen and boron: Hydrogen storage application. <i>Journal of Energy Storage</i> , 2023, 64, 107193.	3.9	7
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81916	Full $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg" display="inline" id="d1e136"} \rangle \langle \text{mml:mi} \rangle Q \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -space analysis of molecular dynamics effect on electron momentum profile of outer-valence orbitals of oxetane. <i>Chemical Physics</i> , 2023, 571, 111922.	0.9	0
81917	Design, synthesis, and computational studies of novel imidazo[1,2-a]pyrimidine derivatives as potential dual inhibitors of hACE2 and spike protein for blocking SARS-CoV-2 cell entry. <i>Journal of Molecular Structure</i> , 2023, 1285, 135525.	1.8	3
81918	^{17}O hyperfine spectroscopy in surface chemistry and catalysis. <i>Journal of Magnetic Resonance Open</i> , 2023, 16-17, 100101.	0.5	0
81919	Solvatochromic, Halochromic and Thermochromic Effects of Copper(II) Complexes Containing N-tert-butyl 2-Picolylamine, and Halide Ion; a Computational Study. <i>Journal of Molecular Structure</i> , 2023, 1285, 135483.	1.8	2
81920	A theoretical study on the excited state behavior of a series of novel triazole pyrimidine group fluorophores: ESIPT or ICT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 297, 122706.	2.0	0
81921	On the structures of free-base lepidine and some mineral acid salts. <i>Journal of Molecular Structure</i> , 2023, 1285, 135460.	1.8	0
81922	Synthesis, molecular modelling and docking studies of new thieno[2,3-b:4,5-b \prime]dipyridine compounds as antimicrobial agents. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104839.	2.3	1
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81924	Emerging Trends of Computational Chemistry and Molecular Modeling in Froth Flotation: A Review. <i>ACS Engineering Au</i> , 2023, 3, 128-164.	2.3	4
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81929	Molecular dynamics simulations, molecular docking study, and scaled quantum calculations of 5-hydroxy-2-nitrobenzaldehyde. <i>Indian Journal of Physics</i> , 0, , .	0.9	5
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81932	Transport properties in liquids from first-principles: The case of liquid water and liquid argon. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
81933	Oâ€‘O Bond Formation and Oxygen Release in Photosystem II Are Enhanced by Spin-Exchange and Synergetic Coordination Interactions. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2684-2696.	2.3	4
81934	Antitumor and antimicrobial effect of syringic acid urea cocrystal: Structural and spectroscopic characterization, DFT calculation and biological evaluation. <i>Journal of Molecular Structure</i> , 2023, 1282, 135113.	1.8	13
81935	Ultrasound assisted synthesis of spirooxindole analogs catalyzed by Fe3O4@PPCA NPs: Experimental, theoretical and in vitro biological studies. <i>Journal of Molecular Structure</i> , 2023, 1284, 135363.	1.8	2
81936	Photophysical study on DNA & BSA binding and cytotoxic behaviour of piperidine-Pt(II) complexes: Their kinetics & mechanism and molecular docking. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114740.	2.0	2
81937	Photophysical and photochemical properties of 3-hydroxyflavone in ethanol solution: Implicit vs explicit solvent models. <i>Journal of Molecular Liquids</i> , 2023, 381, 121783.	2.3	2
81938	Synthesis, crystal structure, Hirshfeld surface analysis, DFT and antihyperglycemic activity of 9-allyl-2,3,9,10a-tetrahydrobenzo[b]cyclopenta[e][1,4]diazepin-10(1H)-one. <i>Journal of Molecular Structure</i> , 2023, 1283, 135283.	1.8	7
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81940	A density functional theory investigation on norepinephrine interaction with amino acids and alcohols. <i>Journal of Molecular Structure</i> , 2023, 1283, 135305.	1.8	1
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81942	Self-assembled crystals of nonplanar benzimidazole macrocycles: Synthesis, characterization, crystal structure, SEM, and DFT studies. <i>Journal of Molecular Structure</i> , 2023, 1284, 135367.	1.8	0
81943	Synthesis, crystal structure, DFT calculations, and Hirshfeld surface analysis of an NNN pincer type compound. <i>Journal of Molecular Structure</i> , 2023, 1283, 135252.	1.8	3
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81946	An electronic structure investigation of excited state intramolecular proton transfer in amino-benzazole derivatives: Relative energies and electron density descriptors. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114738.	2.0	2
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81953	Monitoring structural fluctuations of discotic liquid crystal during phase transitions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 295, 122619.	2.0	0
81954	Simulation of uranyl-biomolecule interaction using a cationic dummy atom model. <i>Chemical Physics Letters</i> , 2023, 822, 140479.	1.2	0
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