Jeanet Conradie

List of Publications by Year in Descending Order

335 papers	4,739 citations	35 h-index	51 g-index
348 ext. papers	5,590 ext. citations	3.7 avg, IF	6.63 L-index

#	Paper	IF	Citations
335	Polypyridyl copper complexes as dye sensitizer and redox mediator for dye-sensitized solar cells. *Electrochemistry Communications*, **2022**, 134, 107182	5.1	6
334	Data to understand the nature of non-covalent interactions in the thiophene clusters.. *Data in Brief*, **2022**, 40, 107818	1.2	0
333	Review of DFT-simulated and experimental electrochemistry properties of the polypyridyl Row-1 Mn, Fe & Co, and Group-8 Fe, Ru and Os MLCT complexes. *Electrochemistry Communications*, **2022**, 136, 107225	5.1	1
332	Non-covalent interactions in dimethylsulfoxide (DMSO) clusters and DFT benchmarking. *Journal of Molecular Liquids*, **2022**, 350, 118522	6	1
331	Data of electronic, reactivity, optoelectronic, linear and non-linear optical parameters of doping graphene oxide nanosheet with aluminum atom.. *Data in Brief*, **2022**, 41, 107840	1.2	0
330	Non-covalent interactions in small thiophene clusters. *Journal of Molecular Liquids*, **2022**, 347, 118301	6	1
329	QTAIM analysis dataset for non-covalent interactions in furan clusters.. *Data in Brief*, **2022**, 40, 107766	1.2	0
328	Electrochemical behaviour of 2-hydroxybenzophenones and related molecules. *Results in Chemistry*, **2022**, 4, 100332	2.1	1
327	DFT Study of bis(1,10-phenanthroline)copper complexes: molecular and electronic structure, redox and spectroscopic properties and application to Solar Cells. *Electrochimica Acta*, **2022**, 140276	6.7	0
326	Redox chemistry of bis(terpyridine)manganese(II) complexes □A molecular view. *Journal of Electroanalytical Chemistry*, **2022**, 913, 116272	4.1	1
325	Dimethylsulfoxide (DMSO) clusters dataset: DFT relative energies, non-covalent interactions, and cartesian coordinates.. *Data in Brief*, **2022**, 42, 108024	1.2	0
324	Iridium(VII)□corrole Terminal Carbides Should Exist as Stable Compounds. *ACS Organic & Inorganic Au*, **2022**, 2, 159-163		0
323	Electronic and structural data of 4'-substituted bis(2,2';6'2''-terpyridine)manganese in -, -, - and -cationic states from DFT calculations.. *Data in Brief*, **2022**, 42, 108221	1.2	
322	Electrochemical behaviour of copper(II) complexes containing 2-hydroxyphenones. *Electrochimica Acta*, **2022**, 140629	6.7	0
321	Structures, Temperature effect, Binding and Clustering Energies of Cu2+(MeOH)n=1-. *Journal of Molecular Liquids*, **2022**, 119439	6	0
320	Solvation energies of ferrous ion in methanol at various temperatures. *Journal of Molecular Liquids*, **2022**, 119460	6	0
319	Dye adsorption of aluminium- and zirconium-based metal organic frameworks with azobenzene dicarboxylate linkers. *Journal of Environmental Management*, **2021**, 304, 114166	7.9	2

318	Enhancement of absorption capacity, optical and non-linear optical properties of graphene oxide nanosheet. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108075	2.8	1
317	The Dog That Didn't Bark: A New Interpretation of Hypsoporphyrin Spectra and the Question of Hypsocorroles. *Journal of Physical Chemistry A*, **2021**, 125, 9962-9968	2.8	2
316	Isotherm, kinetic, thermodynamics and reusability data on the adsorption of antidepressant onto silver nanoparticle-loaded biowaste. *Data in Brief*, **2021**, 39, 107575	1.2	1
315	Structures, binding energies and non-covalent interactions of furan clusters.. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108102	2.8	1
314	Understanding Hyperporphyrin Spectra: TDDFT Calculations on Diprotonated Tetrakis(-aminophenyl)porphyrin. *Journal of Physical Chemistry A*, **2021**, 125, 9953-9961	2.8	3
313	Enhancing the loading and swelling capacity of cellulose crystal through difunctional and multifunctional epoxy crosslinkers and the effects on the elasticity and plasticity: A computational study. *Journal of Molecular Structure*, **2021**, 1228, 129436	3.4	
312	An electrochemical and computational chemistry study of substituted benzophenones. *Electrochimica Acta*, **2021**, 373, 137894	6.7	6
311	Density functional theory calculated data of the iodomethane oxidative addition to oligothiophene-containing rhodium complexes´- Importance of dispersion correction. *Data in Brief*, **2021**, 35, 106929	1.2	1
310	One-pot synthesis of zinc oxide nanoparticles via chemical precipitation for bromophenol blue adsorption and the antifungal activity against filamentous fungi. *Scientific Reports*, **2021**, 11, 8305	4.9	13
309	Proton transfer free energy and enthalpy from water to methanol. *Computational and Theoretical Chemistry*, **2021**, 1199, 113189	2	3
308	Thermodynamics, kinetics and isothermal studies of chromium (VI) biosorption onto stem bark extract coated shale and the regeneration potentials. *International Journal of Phytoremediation*, **2021**, 23, 1486-1496	3.9	4
307	Rhenium Corrole Dimers: Electrochemical Insights into the Nature of the Metal-Metal Quadruple Bond. *Inorganic Chemistry*, **2021**, 60, 8315-8321	5.1	4
306	Synthesis, characterization, electrochemistry, DFT and kinetic study of the oligothiophene-containing complex [Rh((C4H3S-C4H2S)COCHCOCF3)(CO)(PPh3)]. *Polyhedron*, **2021** , 199, 115095	2.7	0
305	stem bark extract anchored on functionalized MWCNT-spent molecular sieve nanocomposite for the biosorption of hexavalent chromium. *International Journal of Phytoremediation*, **2021**, 1-10	3.9	0
304	Functionalized MWCNTs-quartzite nanocomposite coated with Dacryodes edulis stem bark extract for the attenuation of hexavalent chromium. *Scientific Reports*, **2021**, 11, 12684	4.9	2
303	Enhanced sequestration of Cr(VI) onto plant extract anchored on carbon-coated aluminium oxide composite. *Environmental Science and Pollution Research*, **2021**, 28, 57723-57738	5.1	4
302	Accurate binding energies of ammonia clusters and benchmarking of hybrid DFT functionals. *Computational and Theoretical Chemistry*, **2021**, 1200, 113236	2	3
301	Influence of zinc and copper on the electronic, linear, and nonlinear optical properties of organometallic complexes with phenalenyl radical: a computational study. *Structural Chemistry*, **2021**, 32, 835-845	1.8	0

300	Ultrasonic aided sorption of oil from oil-in-water emulsion onto oleophilic natural organic-silver nanocomposite. *Chemical Engineering Research and Design*, **2021**, 165, 12-24	5.5	12
299	Determination of the absolute solvation free energy and enthalpy of the proton in solutions. *Journal of Molecular Liquids*, **2021**, 322, 114919	6	10
298	Structures of water clusters in the solvent phase and relative stability compared to gas phase. *Polyhedron*, **2021**, 193, 114856	2.7	12
297	Biosorption and regeneration potentials of magnetite nanoparticle loaded peel for celestine blue dye. *International Journal of Phytoremediation*, **2021**, 23, 347-361	3.9	12
296	Exploring substituents and solvent effects on the reduction potential and molecular properties of five derivatives of hydroxybenzophenone (HBP) with their possible conformations and isomers. *Structural Chemistry*, **2021**, 32, 1299-1310	1.8	2
295	Heavy-element-ligand covalence: ligand noninnocence in molybdenum and tungsten Viking-helmet Corroles. *Dalton Transactions*, **2021**, 50, 12843-12849	4.3	4
294	Structures and relative stability of hydrated ferrous ion clusters and temperature effects. *New Journal of Chemistry*, **2021**, 45, 10693-10710	3.6	3
293	Relativity as a Synthesis Design Principle: A Comparative Study of [3 + 2] Cycloaddition of Technetium(VII) and Rhenium(VII) Trioxo Complexes with Olefins. *Inorganic Chemistry*, **2021**, 60, 11090-11097	5.1	5
292	Ligand-Centered Triplet Diradical Supported by a Binuclear Palladium(II) Dipyrrindione. *Inorganic Chemistry*, **2021**, 60, 12457-12466	5.1	0
291	Hydrogen bond networks of ammonia clusters: What we know and what we don□t know. *Journal of Molecular Liquids*, **2021**, 336, 116199	6	4
290	Solvation free energy of the proton in acetonitrile. *Journal of Molecular Liquids*, **2021**, 335, 116032	6	6
289	Free energy and enthalpy data of neutral and protonated clusters in the solvent phase. *Data in Brief*, **2021**, 37, 107144	1.2	4
288	DFT study of new organic materials based on PEDOT and 4-[2-(2-N, N-dihydroxy amino thiophene) vinyl] benzenamine. *Journal of Molecular Modeling*, **2021**, 27, 275	2	0
287	Electrochemical study of the Mn(II/III) oxidation of tris(polypyridine)manganese(II) complexes. *Electrochimica Acta*, **2021**, 391, 138965	6.7	3
286	Synthesis, characterization, DFT and biological activity of oligothiophene □diketone and Cu-complexes. *Polyhedron*, **2021**, 205, 115290	2.7	4
285	DFT data to relate calculated LUMO energy with experimental reduction potentials of Cu(II)-□diketonato complexes. *Data in Brief*, **2021**, 38, 107331	1.2	1
284	Enhanced surface properties, hydrophobicity, and sorption behavior of ZnO nanoparticle-impregnated biomass support for oil spill treatment. *Environmental Science and Pollution Research*, **2021**, 28, 25283-25299	5.1	5
283	Polypyridine Os complexes electrochemical data. *Data in Brief*, **2020**, 33, 106454	1.2	

282	Solvent effects on the structures of the neutral ammonia clusters. *Computational and Theoretical Chemistry*, **2020**, 1191, 113042	2	15
281	DFT study of the influence of impurities on the structural, electronic, optoelectronic, and nonlinear optical properties of graphene nanosheet functionalized by the carboxyl group -COOH. *Journal of Molecular Modeling*, **2020**, 26, 327	2	2
280	Redox data of ferrocenylcarboxylic acids in dichloromethane and acetonitrile. *Data in Brief*, **2020**, 30, 105650	1.2	
279	Redox and Photophysical Properties of Four Subphthalocyanines Containing Ferrocenylcarboxylic Acid as Axial Ligands. *Inorganic Chemistry*, **2020**, 59, 7444-7452	5.1	8
278	Computational DFT data related to the redox behaviour of tris(Ediketonato)ruthenium(III) compounds. *Data in Brief*, **2020**, 30, 105617	1.2	1
277	Exploration of the potential energy surfaces of small ethanol clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 13201-13213	3.6	22
276	Solvent and substituent effect on electrochemistry of ferrocenylcarboxylic acids. *Journal of Electroanalytical Chemistry*, **2020**, 866, 114164	4.1	5
275	Cyclic voltammograms and electrochemical data of Fe polypyridine complexes. *Data in Brief*, **2020**, 31, 105754	1.2	3
274	Synthesis, Spectroscopy, Electrochemistry and DFT of Electron-Rich Ferrocenylsubphthalocyanines. *Molecules*, **2020**, 25,	4.8	1
273	Advances in application of cotton-based adsorbents for heavy metals trapping, surface modifications and future perspectives. *Ecotoxicology and Environmental Safety*, **2020**, 201, 110825	7	24
272	Free-base porphyrins with localized NH protons. Can substituents alone stabilize the elusive cis tautomer?. *Organic and Biomolecular Chemistry*, **2020**, 18, 2861-2865	3.9	5
271	Binding energies and isomer distribution of neutral acetonitrile clusters. *International Journal of Quantum Chemistry*, **2020**, 120, e26221	2.1	14
270	Electrochemical behaviour of bis(Ediketonato)copper(II) complexes containing Esubstituted Ediketones. *Journal of Electroanalytical Chemistry*, **2020**, 860, 113929	4.1	3
269	Synthesis, DFT and kinetic studies of chromic S-methyldithizone. *Polyhedron*, **2020**, 179, 114386	2.7	
268	Theoretical infrared spectrum of the ethanol hexamer. *International Journal of Quantum Chemistry*, **2020**, 120, e26234	2.1	14
267	Banana peel as a biosorbent for the decontamination of water pollutants. A review. *Environmental Chemistry Letters*, **2020**, 18, 1085-1112	13.3	65
266	Reduksiepotensiaal van b-diketone: Die effek van elektronskenkende, aromatiese en estersubstituentgroepe. *South African Journal of Science and Technology*, **2020**, 101-118	0.1	
265	Substituente en isomeriese effekte op die reduksieen oksidasiepotensiaal van tris(Ediketonato) mangaan(III) komplekse: DFT en MESP analises. *South African Journal of Science and Technology*, **2020**, 119-133	0.1	

264	Probing ultrafast reaction mechanisms of photo-excited dithizone through transient absorption spectroscopy and computational CASSCF studies. *Journal of the Optical Society of America B: Optical Physics*, **2020**, 37, A356	1.7	2
263	Proton transfer free energy and enthalpy data from water to ammonia, water to acetonitrile and ammonia to acetonitrile. *Data in Brief*, **2020**, 33, 106354	1.2	8
262	Structures of the solvated copper(II) ion in ammonia at various temperatures. *New Journal of Chemistry*, **2020**, 44, 3637-3653	3.6	11
261	Electrochemical behaviour of chloro- and hydroxy- subphthalocyanines. *Electrochimica Acta*, **2020**, 329, 135165	6.7	7
260	Synthesis, structure and DFT study of novel Ga(III) complexes containing a tetradentate ligand. *Journal of Molecular Structure*, **2020**, 1203, 127334	3.4	1
259	Large-Sized Ammonia Clusters and Solvation Energies of the Proton in Ammonia. *Journal of Computational Chemistry*, **2020**, 41, 21-30	3.5	20
258	The conformational search, the stability, fragment interaction and resistance to acidic attack of epoxyl-polyurethanes in different solvent media. *Structural Chemistry*, **2020**, 31, 861-875	1.8	1
257	Tris(□ketoiminato)ruthenium(III) - Structural and electronic data of the neutral, oxidized and reduced forms. *Data in Brief*, **2020**, 28, 104833	1.2	0
256	Oxidation and reduction data of subphthalocyanines. *Data in Brief*, **2020**, 28, 105039	1.2	1
255	Conformational preference of nitroformazans: A computational study. *Journal of Molecular Structure*, **2020**, 1203, 127463	3.4	1
254	Efficient synthesis of magnetic nanoparticle-Musa acuminata peel composite for the adsorption of anionic dye. *Arabian Journal of Chemistry*, **2020**, 13, 7115-7131	5.9	22
253	Nature of the copper-nitrosyl intermediates of copper nitrite reductases during catalysis. *Chemical Science*, **2020**, 11, 12485-12492	9.4	3
252	Global and local minima of protonated acetonitrile clusters. *New Journal of Chemistry*, **2020**, 44, 17558-17569	3.6	13
251	Water-ammonia and water-acetonitrile proton transfer free energy. *Journal of Molecular Liquids*, **2020**, 318, 114300	6	10
250	Cyclic Voltammetric Study of 2-Hydroxybenzophenone (HBP) Derivatives and the Correspondent Change in the Orbital Energy Levels in Different Solvents. *Electroanalysis*, **2020**, 32, 2659-2668	3	10
249	Cyclic Voltammetric and DFT Analysis of the Reduction of Manganese(III) Complexes with 2-Hydroxybenzophenones. *Electroanalysis*, **2020**, 32, 2913-2925	3	1
248	Electrochemical data of ferrocenylsubphthalocyanine dyads. *Data in Brief*, **2020**, 32, 106245	1.2	0
247	Oxidation and reduction data of four subphthalocyanines with axially coordinated ferrocenylcarboxylic acids. *Data in Brief*, **2020**, 31, 105816	1.2	1

246	Redox behaviour of [Ru(□diketonato)3] compounds. *Electrochimica Acta*, **2020**, 337, 135801	6.7	5
245	Unravelling the drugability of MSI2 RNA recognition motif (RRM) protein and the prediction of their effective antileukemia inhibitors from traditional herb concoctions. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	
244	Biogenic and chemically synthesized Solanum tuberosum peel-silver nanoparticle hybrid for the ultrasonic aided adsorption of bromophenol blue dye. *Scientific Reports*, **2020**, 10, 17094	4.9	7
243	The conformational change of Plukenetia conophora oil derivatives and their acidic resistance, intra-fragment interactions, stability in different solvent media. *Journal of Molecular Modeling*, **2020**, 26, 312	2	
242	Synthesis, characterization, and regeneration of an inorganic-organic nanocomposite (ZnO@biomass) and its application in the capture of cationic dye. *Scientific Reports*, **2020**, 10, 14441	4.9	11
241	Electrochemistry of Os Bipyridyl and Phenanthroline Complexes, Comparison with Ru and Fe. *Electroanalysis*, **2020**, 32, 2838-2851	3	6
240	X-ray diffraction and QTAIM calculations of the non-covalent intermolecular fluorine-fluorine interactions in tris(trifluoroacetylacetonato)-manganese(III). *Journal of Molecular Structure*, **2020**, 1201, 127119	3.4	2
239	A theoretical investigation of the fragment interaction and nonlinear optical and electronic properties of tris(□diketonato)iron(III) complexes. *Structural Chemistry*, **2020**, 31, 215-232	1.8	
238	Electronic effect of □diketonato ligands on the redox potential of fac and mer tris(□diketonato) iron(III) complexes: A density functional theory study and molecular electrostatic potential analysis. *International Journal of Quantum Chemistry*, **2019**, 119, e26036	2.1	6
237	Conformational study of [Cu(CF3COCHCO(C4H3X))2] (X = O or S), a combined experimental and DFT study. *Journal of Molecular Structure*, **2019**, 1198, 126916	3.4	2
236	Computational insight into the anticholinesterase activities and electronic properties of physostigmine analogs. *Future Medicinal Chemistry*, **2019**, 11, 1907-1928	4.1	2
235	Bis(acetylacetonato)copper(II) - structural and electronic data of the neutral, oxidized and reduced forms. *Data in Brief*, **2019**, 26, 104511	1.2	3
234	Theoretical Search for the Highest Valence States of the Coinage Metals: Roentgenium Heptafluoride May Exist. *Inorganic Chemistry*, **2019**, 58, 8735-8738	5.1	2
233	103Rh NMR shifts of RhI-□diketonato and RhI-□aminoketonato complexes influenced by different substituents. *Polyhedron*, **2019**, 169, 14-23	2.7	2
232	Structures of solvated ferrous ion clusters in ammonia and spin-crossover at various temperatures. *New Journal of Chemistry*, **2019**, 43, 9902-9915	3.6	9
231	Stereochemistry of Transition-Metal Dinitrosyl Complexes. A Molecular Orbital Rationale for the Attracto and Repulso Conformations. *Inorganic Chemistry*, **2019**, 58, 5943-5948	5.1	1
230	Norcorrole as a Delocalized, Antiaromatic System. *Scientific Reports*, **2019**, 9, 4852	4.9	18
229	Main-Group-Element Isophlorin Complexes Revisited: The Question of a Subvalent Central Atom. *Inorganic Chemistry*, **2019**, 58, 4634-4640	5.1	4

228	Exploration of the potential energy surface of the ethanol hexamer. *Journal of Chemical Physics*, **2019**, 150, 124308	3.9	25
227	Tris(□ketoiminato)ruthenium(III) complexes: Electrochemical and computational chemistry study. *Electrochimica Acta*, **2019**, 320, 134635	6.7	3
226	Structures, relative stability and binding energies of neutral water clusters, (H2O)2□0. *New Journal of Chemistry*, **2019**, 43, 13020-13037	3.6	31
225	Electrochemistry and spectroscopy of substituted [Ru(phen)3]2+ and [Ru(bpy)3]2+ complexes. *Electrochimica Acta*, **2019**, 320, 134540	6.7	7
224	Synthesis, crystal structures, photoluminescence, electrochemistry and DFT study of aluminium(III) and gallium(III) complexes containing a novel tetradentate Schiff base ligand. *Acta Crystallographica Section C, Structural Chemistry*, **2019**, 75, 1045-1052	0.8	
223	Electrochemical data of polypyridine complexes of Ru(II). *Data in Brief*, **2019**, 27, 104759	1.2	3
222	Iron(II) Corrole Anions. *Inorganic Chemistry*, **2019**, 58, 15225-15235	5.1	7
221	Gold dipyrrin-bisphenolates: a combined experimental and DFT study of metal-ligand interactions.. *RSC Advances*, **2019**, 10, 533-540	3.7	6
220	Computational insight into the contribution of para-substituents on the reduction potential, proton affinity, and electronic properties of nitrobenzene compounds. *Journal of Molecular Modeling*, **2019**, 25, 78	2	10
219	Redox behaviour of bis(□diketonato)copper(II) complexes. *Journal of Electroanalytical Chemistry*, **2019**, 837, 76-85	4.1	14
218	Density functional theory calculated data of different electronic states and bond stretch isomers of tris(trifluoroacetylacetonato)-manganese(III). *Data in Brief*, **2019**, 27, 104758	1.2	5
217	Synthesis, Spectroscopy and Electrochemistry in Relation to DFT Computed Energies of Ferrocene- and Ruthenocene-Containing -Diketonato Iridium(III) Heteroleptic Complexes. Structure of [(2-Pyridylphenyl)Ir(RcCOCHCOCH]. *Molecules*, **2019**, 24,	4.8	5
216	Cyclic voltammetry data of polypyridine ligands and Co(II)-polypyridine complexes. *Data in Brief*, **2019**, 22, 436-445	1.2	4
215	Jahn-Teller effect in high spin d4 and d9 octahedral metal-complexes. *Inorganica Chimica Acta*, **2019**, 486, 193-199	2.7	19
214	Electrochemical behaviour of amino substituted □amino □unsaturated ketones: A computational chemistry and experimental study. *Electrochimica Acta*, **2019**, 296, 1070-1082	6.7	2
213	Ligand Noninnocence in Cobalt Dipyrrin-Bisphenols: Spectroscopic, Electrochemical, and Theoretical Insights Indicating an Emerging Analogy with Corroles. *Inorganic Chemistry*, **2019**, 58, 7677-7689	5.1	10
212	Electrochemical and electronic properties of a series of substituted polypyridine ligands and their Co(II) complexes. *Inorganica Chimica Acta*, **2019**, 486, 26-35	2.7	11
211	Tetrahedral Pegs in Square Holes: Stereochemistry of Diboron Porphyrazines and Phthalocyanines. *Angewandte Chemie*, **2019**, 131, 3089-3093	3.6	2

210	Tetrahedral Pegs in Square Holes: Stereochemistry of Diboron Porphyrazines and Phthalocyanines. *Angewandte Chemie - International Edition*, **2019**, 58, 3057-3061	16.4	5
209	Influence of substituents on the reduction potential and pKa values of β-diketones tautomers: A theoretical study. *Electrochimica Acta*, **2019**, 297, 947-960	6.7	13
208	Synthesis, characterisation and electrochemistry of eight Fe coordination compounds containing substituted 2-(1-(4-R-phenyl-1H-1,2,3-triazol-4-yl)pyridine ligands, R = CH3, OCH3, COOH, F, Cl, CN, H and CF3. *Inorganica Chimica Acta*, **2019**, 484, 375-385	2.7	5
207	Electrochemistry of a series of symmetric and asymmetric CpNiBr(NHC) complexes: Probing the electrochemical environment due to push-pull effects. *Journal of Electroanalytical Chemistry*, **2018**, 814, 66-76	4.1	5
206	Novel dichloro(bis{2-[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) coordination compounds of seven transition metals (Mn, Fe, Co, Ni, Cu, Zn and Cd). *Polyhedron*, **2018**, 151, 243-254	2.7	6
205	Triphenylstibine-substituted Fischer carbene complexes of tungsten(0): synthesis, structure, DFT and electrochemistry. *New Journal of Chemistry*, **2018**, 42, 7301-7313	3.6	3
204	Synthesis, characterization, experimental and theoretical structure of novel Dichloro(bis{2-[1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) compounds, metal´= Mn, Co and Ni. *Journal of Molecular Structure*, **2018**, 1161, 89-99	3.4	5
203	Rhodium(triphenylphosphine)carbonyl-2,4-dioxo-3-pentyl-4-decanyloxybenzoate: synthesis, electrochemistry and oxidative addition kinetics. *New Journal of Chemistry*, **2018**, 42, 4121-4132	3.6	5
202	Iron phenanthrolines: A density functional theory study. *Inorganica Chimica Acta*, **2018**, 471, 391-396	2.7	6
201	Structures and spectroscopy of the ammonia eicosamer, (NH). *Journal of Chemical Physics*, **2018**, 149, 024304	3.9	29
200	Isocorroles as Homoaromatic NIR-Absorbing Chromophores: A First Quantum Chemical Study. *Scientific Reports*, **2018**, 8, 11952	4.9	10
199	Electronic Structure of Manganese Corroles Revisited: X-ray Structures, Optical and X-ray Absorption Spectroscopies, and Electrochemistry as Probes of Ligand Noninnocence. *Inorganic Chemistry*, **2018**, 57, 9656-9669	5.1	22
198	Orbital control over the metal vs. ligand reduction in a series of neutral and cationic bis(cyclopentadienyl) Ti(IV) complexes. *New Journal of Chemistry*, **2018**, 42, 662-670	3.6	7
197	Structural and electronic data of three first-row transition octahedral hexaaquametal(II) ions, metal=Cr, Ni or Cu. *Data in Brief*, **2018**, 21, 2051-2058	1.2	5
196	Solvation energies of the proton in methanol revisited and temperature effects. *Physical Chemistry Chemical Physics*, **2018**, 20, 29184-29206	3.6	38
195	Base-free glucose dehydration catalysed by NHC-stabilised heterohalo cyclopentadienyl Cr(III) complexes. *New Journal of Chemistry*, **2018**, 42, 19193-19204	3.6	11
194	Local versus global aromaticity in azuliporphyrin and benziporphyrin derivatives. *Organic and Biomolecular Chemistry*, **2018**, 16, 7964-7970	3.9	11
193	Electrochemical data of Co(II) complexes containing phenanthroline functionalized ligands. *Data in Brief*, **2018**, 21, 866-877	1.2	1

192	DFT and CV data of 4-phenyl-substituted dichloro(bis{2-[1-(phenyl)-1H-1,2,3-triazol-4-yl-κN]pyridine-κN})iron(II) coordination compounds. *Data in Brief*, **2018**, 21, 1458-1471	1.2	
191	Structures and infrared spectroscopy of large sized protonated ammonia clusters. *Journal of Chemical Physics*, **2018**, 149, 244301	3.9	27
190	Electrochemical properties of a series of Co(II) complexes, containing substituted phenanthrolines. *Electrochimica Acta*, **2018**, 292, 489-501	6.7	10
189	Rare and Nonexistent Nitrosyls: Periodic Trends and Relativistic Effects in Ruthenium and Osmium Porphyrin-Based {MNO} Complexes. *ACS Omega*, **2018**, 3, 10513-10516	3.9	5
188	Jahn–Teller distortion in 2-pyridyl-(1,2,3)-triazole-containing copper(II) compounds. *New Journal of Chemistry*, **2018**, 42, 16335-16345	3.6	4
187	Chemical and structural data of (1,2,3-triazol-4-yl)pyridine-containing coordination compounds. *Data in Brief*, **2018**, 20, 1397-1408	1.2	1
186	The stability, kinetics and inter-fragment electron communication of the tautomers of twelve selected β-diketone molecules: A computational study. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 25-39	2.8	4
185	Stacking of dicarbonylacetylacetonatorhodium(I) molecules. *Computational and Theoretical Chemistry*, **2017**, 1101, 30-35	2	6
184	Electrochemical study of chromium(0) Fischer carbene complexes: Trends in redox potential. *Polyhedron*, **2017**, 127, 323-330	2.7	5
183	A comparative DFT study of stacking interactions between adjacent metal atoms in linear chains of Ir and Rh acetylacetonato complexes. *Journal of Organometallic Chemistry*, **2017**, 833, 88-94	2.3	4
182	The Blue-Violet Color of Pentamethylbismuth: A Visible Spin-Orbit Effect. *ChemistryOpen*, **2017**, 6, 15-17	2.3	3
181	Synthesis and XPS characterization of Si-supported chromium(0) Fischer aminocarbene complexes. *Journal of Organometallic Chemistry*, **2017**, 836-837, 62-67	2.3	12
180	Rhodium-rhodium interactions in [Rh(β-diketonato)(CO)2] complexes. *Journal of Molecular Structure*, **2017**, 1144, 280-289	3.4	10
179	Structural and electronic features of triphenylstibine-functionalized Fischer carbene complexes of molybdenum(0). *Polyhedron*, **2017**, 133, 307-318	2.7	10
178	Significance of the electron-density of molecular fragments on the properties of manganese(III) β-diketonato complexes: an XPS and DFT study. *RSC Advances*, **2017**, 7, 27718-27728	3.7	26
177	Electrochemical and DFT study of the reduction of substituted phenanthrolines. *Polyhedron*, **2017**, 122, 147-154	2.7	14
176	Mechanistic investigation of cis and trans oxidative addition to acetylacetonato-1,5-cyclooctadieneiridium(I). *Polyhedron*, **2017**, 123, 252-258	2.7	
175	Characterization and oxidative addition reactions for iridium cod complexes. *Journal of Coordination Chemistry*, **2017**, 70, 10-24	1.6	1

174	Intra-molecular electron communication, spectroscopic and conformational stability of the newly developed urethane modified polyetheramide coatings: Computational methods. *Journal of Molecular Graphics and Modelling*, **2017**, 78, 1-13	2.8	1
173	Packing polymorphism of dicarbonyl-[2-(phenylamino)pent-3-en-4-onato]rhodium(I). *Journal of Organometallic Chemistry*, **2017**, 851, 235-247	2.3	4
172	Energetics of Saddling versus Ruffling in Metalloporphyrins: Unusual Ruffled Dodecasubstituted Porphyrins. *ACS Omega*, **2017**, 2, 6708-6714	3.9	10
171	Cobalt- and Rhodium-Corrole-Triphenylphosphine Complexes Revisited: The Question of a Noninnocent Corrole. *Inorganic Chemistry*, **2017**, 56, 14788-14800	5.1	34
170	Synthesis, characterization, computational and antimicrobial activities of a novel iridium thiourea complex. *New Journal of Chemistry*, **2017**, 41, 10919-10928	3.6	7
169	Electronic Structure of Cobalt-Corrole-Pyridine Complexes: Noninnocent Five-Coordinate Co(II) Corrole-Radical States. *Journal of Physical Chemistry A*, **2017**, 121, 9589-9598	2.8	27
168	Influence of β-octabromination on free-base triarylcorroles: Electrochemistry and protonation-deprotonation reactions in nonaqueous media. *Journal of Porphyrins and Phthalocyanines*, **2017**, 21, 633-645	1.8	1
167	Electrochemistry of triphenylstibine-functionalized Fischer carbene complexes of Molybdenum(0). *Electrochimica Acta*, **2017**, 246, 897-907	6.7	7
166	Synthesis, structure and DFT conformation analysis of CpNiX(NHC) and NiX2(NHC)2 (X´=´SPh or Br) complexes. *Journal of Molecular Structure*, **2017**, 1147, 235-243	3.4	6
165	Molybdenum(0) Fischer ethoxycarbene complexes: Synthesis, X-ray crystal structures and DFT study. *Polyhedron*, **2017**, 121, 285-296	2.7	6
164	Synthesis of Co(II)-NO(-) Complexes and Their Reactivity as a Source of Nitroxyl. *Journal of the American Chemical Society*, **2016**, 138, 12459-71	16.4	17
163	Metallocorrole Interactions with Carbon Monoxide, Nitric Oxide, and Nitroxyl-A DFT Study of Low-Energy Bound States. *Inorganic Chemistry*, **2016**, 55, 8248-50	5.1	6
162	Electronic Influence of Different β-Diketonato Ligands on the Electrochemical Behaviour of Tris(β-Diketonato)M(III) Complexes, M = Cr, Mn and Fe. *Journal of Nano Research*, **2016**, 44, 252-264	1	3
161	Electronic properties of Fe charge transfer complexes – A combined experimental and theoretical approach. *Electrochimica Acta*, **2016**, 216, 339-346	6.7	18
160	Electrochemical Behaviour of Cr and W Fischer Ethoxy Carbene Complexes: A Comparative Study. *Journal of Nano Research*, **2016**, 44, 1-9	1	2
159	The Valence States of Copernicium and Flerovium. *European Journal of Inorganic Chemistry*, **2016**, 2016, 2989-2992	2.3	6
158	Metalloporphyrin-Nitroxyl Interactions: The Low-Energy States of Reduced Manganese, Iron, and Cobalt Porphyrin Nitrosyls. *Journal of Physical Chemistry B*, **2016**, 120, 4972-9	3.4	7
157	Jahn-Teller distortion in tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedionato]manganese(III) isomers: An X-ray and computational study. *Journal of Molecular Structure*, **2016**, 1119, 48-53	3.4	7

156	Synthesis and structure of novel triphenylarsine-substituted tungsten(0) Fischer carbene complexes. *Journal of Molecular Structure*, **2016**, 1105, 205-213	3.4	5
155	Geometrical isomers of tris(β-diketonato)metal(III) complexes for M = Cr or Co: Synthesis, X-ray structures and DFT study. *Inorganica Chimica Acta*, **2016**, 447, 59-65	2.7	5
154	Orientation of trimethylolethane cyclic phosphite in rhodium complexes: Structure of [Rh(CH3COCHCOCH3)(CO)(P(OCH2)3CCH3)]. *Polyhedron*, **2016**, 111, 161-166	2.7	1
153	Comparison of X-ray photoelectron spectroscopy multiplet splitting of Cr 2p peaks from chromium tris(β-diketonates) with chemical effects. *Journal of Electron Spectroscopy and Related Phenomena*, **2016**, 206, 46-51	1.7	10
152	Characterisation and mechanistic study of the oxidative addition reactions of [Ir(cod)(sacac)]. *Journal of Organometallic Chemistry*, **2016**, 801, 80-86	2.3	2
151	Beam experiments with the Grenoble test electron cyclotron resonance ion source at iThemba LABS. *Review of Scientific Instruments*, **2016**, 87, 02A731	1.7	2
150	Synthesis and structure of dithizonato complexes of antimony(III), copper(II) and tin(IV). *Journal of Coordination Chemistry*, **2016**, 69, 788-800	1.6	2
149	Bond stretch isomers of d4 tris(benzoylacetonato-κ2O,O?)Mn(III). *Computational and Theoretical Chemistry*, **2016**, 1087, 1-5	2	4
148	Structure, substitution and hydrolysis of Bis(trifluorobenzoylacetonato-O,O?)dichloro titanium(IV): An experimental and computational study. *Inorganica Chimica Acta*, **2016**, 453, 345-356	2.7	3
147	Electrochemical and X-ray photoelectron spectroscopic insights into Molybdenum(0) Fischer ethoxycarbene complexes. *Electrochimica Acta*, **2016**, 219, 204-213	6.7	14
146	XPS Fe 2p peaks from iron tris(β-diketonates): Electronic effect of the β-diketonato ligand. *Polyhedron*, **2016**, 119, 142-150	2.7	30
145	X-ray and electronic structure of tris(benzoylacetonato-κ2O,O?)iron(III). *Journal of Molecular Structure*, **2016**, 1123, 199-205	3.4	4
144	Synthesis, electrochemical and DFT study of octahedral bis(β-diketonato)-titanium(IV) complexes. *Inorganica Chimica Acta*, **2016**, 453, 247-256	2.7	10
143	Density functional theory calculations of Rh-β-diketonato complexes. *Dalton Transactions*, **2015**, 44, 1503-15	4.5	36
142	Effect of CO substitution on the redox properties of Fischer Mo(0) carbene complexes Mo(CO)5=C(Y)(2-Furyl), Y = OEt, NHCy or NH2. *Electrochimica Acta*, **2015**, 174, 282-289	6.7	9
141	Fischer aminocarbene conformers containing a 2-thienyl or 2-furyl ring: a crystallographic, NMR, and DFT study. *Journal of Coordination Chemistry*, **2015**, 68, 2388-2408	1.6	13
140	E versus Z isomers of Fischer aminocarbene complex [Mo(CO)4(PPh3){C(NHCy)(2-furyl)}]: NH?O versus CH?O intramolecular hydrogen bonds. *Journal of Molecular Structure*, **2015**, 1094, 36-45	3.4	3
139	Tetrabenzoporphyrin and -mono-, -cis-di- and Tetrabenzotriazaporphyrin Derivatives: Electrochemical and Spectroscopic Implications of meso CH Group Replacement with Nitrogen. *Inorganic Chemistry*, **2015**, 54, 5329-41	5.1	15

138	Molecular structures of free-base corroles: nonplanarity, chirality, and enantiomerization. *Journal of Physical Chemistry A*, **2015**, 119, 3452-7	2.8	30
137	Tris(Ediketonato)chromium(III) complexes: Effect of the Ediketonate ligand on the redox properties. *Electrochimica Acta*, **2015**, 185, 288-296	6.7	27
136	Electrochemical behaviour of Tris(Ediketonato)iron(III) complexes: A DFT and experimental study. *Electrochimica Acta*, **2015**, 152, 512-519	6.7	38
135	Computational chemistry insights in the REDOX Behaviour of Cr and W Fischer carbene complexes. *Journal of Physics: Conference Series*, **2015**, 633, 012068	0.3	
134	Pentafluorosulfanyltrimethylsilane: A Nonexistent Molecule?. *European Journal of Inorganic Chemistry*, **2015**, 2015, 207-209	2.3	4
133	A Frontier orbital energy approach to redox potentials. *Journal of Physics: Conference Series*, **2015**, 633, 012045	0.3	28
132	Mechanisms of Oxygen Atom Transfer between Main-Group Elements. *European Journal of Inorganic Chemistry*, **2015**, 2015, 4138-4144	2.3	1
131	Structural investigation of trifuoromethyl substituted bis(Ediketonato)-dichlorotitanium(IV) complexes displaying a mono-dinuclear equilibrium hydrolysis reaction. *Journal of Molecular Structure*, **2015**, 1098, 267-276	3.4	4
130	Singlet-Triplet Gaps of Cobalt Nitrosyls: Insights from Tropocoronand Complexes. *Inorganic Chemistry*, **2015**, 54, 7362-7	5.1	13
129	Electrochemistry of Triphenylarsine-substituted Tungsten(0) Fischer carbene complexes. *Electrochimica Acta*, **2015**, 186, 321-327	6.7	6
128	Fischer mono- and biscarbene complexes of tungsten with mono- and dimeric heteroaromatic substituents. *Journal of Electroanalytical Chemistry*, **2015**, 739, 202-210	4.1	14
127	Observed hydrolysis of fluorine substituted bis(Ediketonato)-dichlorotitanium(IV) complexes. *Dalton Transactions*, **2015**, 44, 5106-13	4.3	6
126	Structural and conformational study of pentacarbonyl and phosphine substituted Fischer alkoxy- and aminocarbene complexes of molybdenum. *Journal of Molecular Structure*, **2015**, 1086, 190-200	3.4	11
125	Electrochemical and Computational Chemistry Study of Mn(Ediketonato)3 complexes. *Electrochimica Acta*, **2015**, 158, 418-426	6.7	35
124	Square-antiprismatic eight-coordinate complexes of divalent first-row transition metal cations: a density functional theory exploration of the electronic-structural landscape. *Inorganic Chemistry*, **2015**, 54, 1375-83	5.1	7
123	Mono- and diboron corroles: factors controlling stoichiometry and hydrolytic reactivity. *Inorganic Chemistry*, **2014**, 53, 5486-93	5.1	30
122	Electrochemical behaviour and structure of novel phosphine- and phosphite-substituted tungsten(0) Fischer carbene complexes. *Electrochimica Acta*, **2014**, 130, 104-118	6.7	28
121	Conformation analysis of triphenylphosphine in trans and cis triphenylphosphine-substituted Fischer carbene complexes. *Journal of Molecular Structure*, **2014**, 1065-1066, 29-38	3.4	17

120	Fac and mer dppe-substituted Fischer carbene complexes of chromium: X-ray, DFT and electrochemical study. *Journal of Organometallic Chemistry*, **2014**, 752, 171-182	2.3	22
119	Femtosecond laser spectroscopy and DFT studies of photochromic dithizonatomercury complexes. *Journal of Physical Chemistry A*, **2014**, 118, 844-55	2.8	10
118	X-Ray Diffraction and DFT Calculation Elucidation of the Jahn□Teller Effect Observed in Mn(dibenzoylmethanato)3. *Journal of Chemical Crystallography*, **2014**, 44, 352-359	0.5	9
117	Substitution reactions of dichlorobis(betadiketonato-O,O?)titanium(IV) complexes with aryl diolato ligands: An experimental and computational study. *Polyhedron*, **2014**, 67, 231-241	2.7	5
116	Stereochemical diversity of {MNO}(10) complexes: molecular orbital analyses of nickel and copper nitrosyls. *Inorganic Chemistry*, **2014**, 53, 4847-55	5.1	6
115	Immobilisation of iron tris(□diketonates) on a two-dimensional flat amine functionalised silicon wafer: A catalytic study of the formation of urethane, from ethanol and a diisocyanate derivative. *Polyhedron*, **2014**, 79, 52-59	2.7	16
114	Electrochemistry of Fischer alkoxycarbene complexes of chromium: The use of density functional theory to predict and understand oxidation and reduction potentials. *Electrochimica Acta*, **2013**, 114, 205-214	6.7	19
113	Oxidation potential of [Rh(□diketonato)(P(OPh)3)2] complexes□Relationships with experimental, electronic and calculated parameters. *Electrochimica Acta*, **2013**, 110, 718-725	6.7	12
112	Understanding the Jahn□Teller Effect in Octahedral Transition-Metal Complexes: A Molecular Orbital View of the Mn(□diketonato)3 Complex. *Journal of Chemical Education*, **2013**, 90, 1692-1696	2.4	43
111	Solid state packing of [Rh(□diketonato)(CO)2] complexes. Crystal structure of [Rh(PhCOCHCOC4H3S)(CO)2]. *Journal of Molecular Structure*, **2013**, 1051, 137-143	3.4	12
110	Crystal and electronic structures of tris[4,4,4-Trifluoro-1-(2-X)-1,3-butanedionato]iron(III) isomers (X=thienyl or furyl): An X-ray and computational study. *Journal of Molecular Structure*, **2013**, 1053, 134-140	3.4	17
109	Chemical and electrochemical oxidation of [Rh(□diketonato)(CO)(P(OCH2)3CCH3)]: an experimental and DFT study. *Dalton Transactions*, **2013**, 42, 8655-66	4.3	17
108	Electrochemical study of carbonyl phosphine □diketonato rhodium(I) complexes. *Electrochimica Acta*, **2013**, 113, 519-526	6.7	14
107	Characterization and oxidative addition reactions of rhodium(I) carbonyl cupferrate diphenyl-2-pyridylphoshine complexes. *Journal of Organometallic Chemistry*, **2013**, 745-746, 439-453	2.3	4
106	Conformational analysis of triphenylphosphine in square planar [Rh(□diketonato)(CO)(PPh3)] complexes. Crystal structure of [Rh(PhCOCHCO(CH2)3CH3)(CO)(PPh3)]. *Inorganica Chimica Acta*, **2013**, 395, 237-244	2.7	9
105	Characterization of acetylacetonato carbonyl diphenyl-2-pyridylphosphine rhodium(I): Comparison with other carbonyl complexes. *Journal of Molecular Structure*, **2013**, 1038, 220-229	3.4	11
104	P(OPh)3 substitution at [Rh(□diketonato)(cod)] complexes: The relationship between kinetics and frontier orbitals. *Inorganica Chimica Acta*, **2013**, 406, 211-216	2.7	4
103	A DFT study of the reactivity of □diketonato-1,5-cyclo-octadieneiridium(I) complexes. *Polyhedron*, **2013**, 51, 164-167	2.7	7

102	Determination of the relationship between theoretical vibrational frequencies and experimental IR absorbance bands in organic molecules: computational study of oxane, chromane and flavan. *Journal of Physical Organic Chemistry*, **2013**, 26, 327-334	2.1	2
101	Synthesis, Structure, and Electrochemistry of Fischer Alkoxy- and Aminocarbene Complexes of Tungsten: The Use of DFT To Predict and Understand Oxidation and Reduction Potentials. *Organometallics*, **2013**, 32, 5491-5503	3.8	39
100	Structural trends in [Rh(PhCOCHCO(CH2)nCH3)(CO)(PPh3)] (n = 0–3) and related complexes: crystal structure of [Rh(PhCOCHCO(CH2)2CH3)(CO)(PPh3)]. *Transition Metal Chemistry*, **2013**, 38, 429-440	2.1	8
99	A spectroscopic, electrochemical and DFT study of para-substituted ferrocene-containing chalcone derivatives: Structure of FcCOCHCH(p-tBuC6H4). *Polyhedron*, **2012**, 33, 257-266	2.7	42
98	Energetic Driving Force of H Spillover between Rhodium and Titania Surfaces: A DFT View. *Journal of Physical Chemistry C*, **2012**, 116, 25362-25367	3.8	15
97	Prediction of chemical and electrochemical oxidation potentials of β-diketonatobis(triphenylphosphite)rhodium(I) complexes: A DFT study. *Inorganica Chimica Acta*, **2012**, 392, 30-37	2.7	9
96	A thermally stable {FeNO}8 complex: properties and biological reactivity of reduced MNO systems. *Chemical Science*, **2012**, 3, 364-369	9.4	52
95	Low-energy states of manganese-oxo corrole and corrolazine: multiconfiguration reference ab initio calculations. *Inorganic Chemistry*, **2012**, 51, 4002-6	5.1	32
94	Reactivity of [Rh(β-diketonato)(cod)] complexes: A DFT approach. *Journal of Organometallic Chemistry*, **2012**, 719, 8-13	2.3	11
93	Conformational analysis of triphenylphosphine in square planar organometallic complexes: [(PPh3)(ML1L2L3)] and [M(acac)(L')(PPh3)]. *Dalton Transactions*, **2012**, 41, 10633-42	4.3	15
92	Reduction potentials of para-substituted nitrobenzenes—an infrared, nuclear magnetic resonance, and density functional theory study. *Journal of Physical Organic Chemistry*, **2012**, 25, 58-68	2.1	63
91	Oxidative addition of methyl iodide to [Rh(PhCOCHCOPh)(CO)(P(OCH2)3CCH3)]: an experimental and computational study. *Open Chemistry*, **2012**, 10, 256-266	1.6	5
90	The structural chemistry of metallocorroles: combined X-ray crystallography and quantum chemistry studies afford unique insights. *Accounts of Chemical Research*, **2012**, 45, 1203-14	24.3	141
89	Kinetics and mechanism of the oxidative addition of methyl iodide to [Rh(CH3COCHCOCF3)(CO)(P(OCH2)3CCH3)]: an experimental and computational study. *Reaction Kinetics, Mechanisms and Catalysis*, **2012**, 105, 233-247	1.6	13
88	First commissioning results with the Grenoble test electron cyclotron resonance ion source at iThemba LABS. *Review of Scientific Instruments*, **2012**, 83, 02A323	1.7	1
87	Relationship between electrochemical potentials and substitution reaction rates of ferrocene-containing β-diketonato rhodium(I) complexes; cytotoxicity of [Rh(FcCOCHCOPh)(cod)]. *Dalton Transactions*, **2011**, 40, 5844-51	4.3	41
86	Dithizone and its oxidation products: a DFT, spectroscopic, and X-ray structural study. *Journal of Physical Chemistry A*, **2011**, 115, 14637-46	2.8	26
85	Synthesis and molecular structure of gold triarylcorroles. *Inorganic Chemistry*, **2011**, 50, 12844-51	5.1	91

84	Iodomethane oxidative addition to -diketonatobis(triphenylphosphite)rhodium(I) complexes: A synthetic, kinetic and computational study. *Polyhedron*, **2011**, 30, 2345-2353	2.7	17
83	Electrochemical study of -diketonatobis(triphenylphosphite)rhodium(I) complexes. *Electrochimica Acta*, **2011**, 56, 9287-9294	6.7	19
82	Oxidative addition of methyl iodide to [Rh(CH3COCHCOCH3)(CO)(P(OCH2)3CCH3)]. *Inorganica Chimica Acta*, **2011**, 375, 128-134	2.7	9
81	A First TDDFT Study of Metallocorrole Electronic Spectra: Copper meso-Triarylcorroles Exhibit Hyper Spectra. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1857-1864	2.3	51
80	The Relationship between the Electrochemical and Chemical Oxidation of Ferrocene-Containing Carbonyl-Phosphane--Diketonato-Rhodium(I) Complexes Cytotoxicity of [Rh(FcCOCHCOPh)(CO)(PPh3)]. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2439-2449	2.3	30
79	A Metallocorrole with Orthogonal Pyrrole Rings. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1865-1870	2.3	46
78	Ultrafast photochemistry of dithizonatophenylmercury(II). *ChemPhysChem*, **2011**, 12, 2653-8	3.2	11
77	Correlation between the FeNO angle and d-p mixing in {FeNO}7 complexes. *Inorganic Chemistry*, **2011**, 50, 4223-5	5.1	15
76	Methyl iodide oxidative addition to [Rh(acac)(CO)(PPh3)]: an experimental and theoretical study of the stereochemistry of the products and the reaction mechanism. *Dalton Transactions*, **2011**, 40, 8226-37	4.3	24
75	Corroles cannot ruffle. *Inorganic Chemistry*, **2011**, 50, 3247-51	5.1	29
74	Electrochemical and density functional theory modeled reduction of enolized 1,3-diketones. *Electrochimica Acta*, **2011**, 56, 6211-6218	6.7	48
73	A kinetic investigation of the oxidative addition reactions of the dimeric Bu4N[Ir2(-Dcbp)(CO)2(PCy3)2] complex with iodomethane. *Journal of Organometallic Chemistry*, **2011**, 696, 1990-2002	2.3	3
72	Capturing the spin state diversity of iron(III)-aryl porphyrins: OLYP is better than TPSSh. *Journal of Inorganic Biochemistry*, **2011**, 105, 84-91	4.2	35
71	Characterization of [Rh(PhCOCHCOCH2CH2CH3)(CO)2] by X-ray crystallography, a computational and a statistical study. *Polyhedron*, **2011**, 30, 660-665	2.7	10
70	Substituent effects on metallocorrole spectra: insights from chromium-oxo and molybdenum-oxo triarylcorroles. *Journal of Porphyrins and Phthalocyanines*, **2011**, 15, 1335-1344	1.8	36
69	-octabromo-meso-tris(pentafluorophenyl)corrole: reductive demetalation-based synthesis of a heretofore inaccessible, perhalogenated free-base corrole. *Journal of Porphyrins and Phthalocyanines*, **2010**, 14, 509-512	1.8	22
68	Electronic structure of a paramagnetic {MNO}6 complex: MnNO 5,5-tropocoronand. *Inorganic Chemistry*, **2010**, 49, 2701-5	5.1	8
67	Stable eight-coordinate iron(III/II) complexes. *Inorganic Chemistry*, **2010**, 49, 2032-4	5.1	31

66	Electronic structure of an iron-porphyrin-nitrene complex. *Inorganic Chemistry*, **2010**, 49, 243-8	5.1	15
65	Understanding the unusually straight: a search for MO insights into linear {FeNO}(7) units. *Journal of Physical Chemistry B*, **2010**, 114, 8517-24	3.4	30
64	Substitution and Isomerization of Asymmetric □Diketonato Rhodium(I) Complexes: A Crystallographic and Computational Study. *Organometallics*, **2010**, 29, 2446-2458	3.8	25
63	A density functional theory study of the oxidative addition of methyl iodide to square planar [Rh(acac)(P(OPh)3)2] complex and simplified model systems. *Journal of Organometallic Chemistry*, **2010**, 695, 2126-2133	2.3	26
62	Electrochemical and density functional theory study of bis(cyclopentadienyl) mono(□diketonato) titanium(IV) cationic complexes. *Electrochimica Acta*, **2010**, 56, 257-264	6.7	27
61	Bonding in titanocenyl complexes containing O,O?-cyclic ligands. *International Journal of Quantum Chemistry*, **2010**, 110, 1100-1107	2.1	4
60	Reply to 'Nitrite□methemoglobin inadequate for hypoxic vasodilation'. *Nature Chemical Biology*, **2009**, 5, 367-367	11.7	5
59	Stereochemistry of the reaction products of the oxidative addition reaction of methyl iodide to [Rh((C4H3S)COCHCOR)(CO)(PPh3)]: A NMR and computational study. R = CF3, C6H5, C4H3S. *Inorganica Chimica Acta*, **2009**, 362, 519-530	2.7	40
58	Isomer distribution and structure of (2,2?-biphenyldiolato)bis(□diketonato)titanium(IV) complexes: A single crystal X-ray, solution NMR and computational study. *Inorganica Chimica Acta*, **2009**, 362, 3088-3096	2.7	18
57	Investigation of the electron density of iridium(I) Vaska-type complexes using DFT calculations and structural results: Structure of trans-carbonyl-chloro-bis(tricyclohexylphosphine)-iridium(I). *Inorganica Chimica Acta*, **2009**, 362, 3949-3954	2.7	9
56	A computational study and fragment analysis of the back-bonding in Titanocenyl Complexes containing a five-member L,L?-cyclic ligand, L,L?=O,O?; S,S? or Se,Se?. *Computational and Theoretical Chemistry*, **2009**, 915, 51-57		5
55	Substitution kinetics of biphenol at dichlorobis(acetylacetonato-O,O?)titanium(IV): Isolation, characterization, crystal structure and enhanced hydrolytic stability of the product bis(acetylacetonato-O,O?)(biphenyldiolato-O,O?)titanium(IV). *Polyhedron*, **2009**, 28, 209-214	2.7	12
54	Syntheses, crystal structure and theoretical modelling of tetrahedral mono-□diketonato titanocenyl complexes. *Polyhedron*, **2009**, 28, 966-974	2.7	6
53	Iodomethane oxidative addition and CO migratory insertion in monocarbonylphosphine complexes of the type [Rh((C6H5)COCHCO((CH2)nCH3))(CO)(PPh3)]: Steric and electronic effects. *Journal of Organometallic Chemistry*, **2009**, 694, 259-268	2.3	40
52	Broken-symmetry DFT spin densities of iron nitrosyls, including Roussin's red and black salts: striking differences between pure and hybrid functionals. *Journal of Physical Chemistry B*, **2009**, 113, 10540-7	3.4	40
51	Oxidative Addition of CH3I and CO Migratory Insertion in a Series of Ferrocene-Containing Carbonyl Phosphine □Diketonato Rhodium(I) Complexes. *Organometallics*, **2009**, 28, 1018-1026	3.8	62
50	Density Functional Theory Study of Substitution at the Square-Planar Acetylacetonato-dicarbonyl-rhodium(I) Complex. *Organometallics*, **2009**, 28, 3710-3715	3.8	15
49	A DFT perspective on the structures and electronic spectra of the orange and blue isomers of photochromic dithizonatophenylmercury(II). *Journal of Physical Chemistry A*, **2008**, 112, 2211-8	2.8	21

48	DFT survey of monoboron and diboron corroles: regio- and stereochemical preferences for a constrained, low-symmetry macrocycle. *Dalton Transactions*, **2008**, 4464-73	4.3	22
47	Bonding in Low-Coordinate Environments: Electronic Structure of Distorted Square-Planar Iron-Imido Complexes With Pincer-Type Ligands. *Journal of Chemical Theory and Computation*, **2008**, 4, 1576-84	6.4	3
46	Spin states at a tipping point: what determines the dz2(1) ground state of nickel(III) tetra(tbutyl)porphyrin dicyanide?. *Journal of Physical Chemistry B*, **2008**, 112, 1053-6	3.4	12
45	Not innocent: verdict from ab initio multiconfigurational second-order perturbation theory on the electronic structure of chloroiron corrole. *Journal of Physical Chemistry B*, **2008**, 112, 14099-102	3.4	82
44	Ruthenocene-Containing □Diketones: Synthesis, pKa? Values, Keto□Enol Isomerization Kinetics, and Electrochemical Aspects. *Organometallics*, **2008**, 27, 353-362	3.8	57
43	Corrole as a binucleating ligand: preparation, molecular structure and density functional theory study of diboron corroles. *Journal of the American Chemical Society*, **2008**, 130, 2888-9	16.4	38
42	A kinetic study of the oxidative addition of methyl iodide to [Rh((C4H3S)COCHCOCF3)(CO)(PPh3)] utilizing UV/vis and IR spectrophotometry and 1H, 19F and 31P NMR spectroscopy. Synthesis of [Rh((C4H3S)COCHCOCF3)(CO)(PPh3)(CH3)(I)]. *Inorganica Chimica Acta*, **2008**, 361, 208-218	2.7	34
41	Methyl iodide oxidative addition to monocarbonylphosphine [Rh((C4H3S)COCHCOR)(CO)(PPh3)] complexes utilizing UV/vis and IR spectrophotometry and NMR spectroscopy to identify reaction intermediates: R = C6H5 or C4H3S. *Inorganica Chimica Acta*, **2008**, 361, 2285-2295	2.7	38
40	Bonding in Low-Coordinate Environments: Electronic Structure of Pseudotetrahedral Iron-Imido Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 448-57	6.4	35
39	Electronic structure and FeNO conformation of nonheme iron-thiolate-NO complexes: an experimental and DFT study. *Journal of the American Chemical Society*, **2007**, 129, 10446-56	16.4	66
38	Electronic Structure of Trigonal-Planar Transition-Metal-Imido Complexes: Spin-State Energetics, Spin-Density Profiles, and the Remarkable Performance of the OLYP Functional. *Journal of Chemical Theory and Computation*, **2007**, 3, 689-702	6.4	101
37	DFT calculations on the spin-crossover complex Fe(salen)(NO): a quest for the best functional. *Journal of Physical Chemistry B*, **2007**, 111, 12621-4	3.4	166
36	Synthesis, crystal structure and electrochemistry of tetrahedral mono-□diketonato titanocenyl complexes. *Inorganica Chimica Acta*, **2007**, 360, 2277-2283	2.7	30
35	Kinetic study of the oxidative addition reaction between methyl iodide and [Rh(FcCOCHCOCF3)(CO)(PPh3)]: Structure of [Rh(FcCOCHCOCF3)(CO)(PPh3)(CH3)(I)]. *Polyhedron*, **2007**, 26, 5075-5087	2.7	47
34	□2,2?-Biphenolato-□ O:O?-□oxido-□ O:O-bis[bis(hexafluoroacetylacetonato-□ O,O?)titanium(IV)]. *Acta Crystallographica Section E: Structure Reports Online*, **2007**, 63, m664-m666		
33	Catalytic generation of N2O3 by the concerted nitrite reductase and anhydrase activity of hemoglobin. *Nature Chemical Biology*, **2007**, 3, 785-94	11.7	189
32	Trigonal bipyramidal iron(III) and manganese(III) oxo, sulfido, and selenido complexes. An electronic-structural overview. *Journal of Inorganic Biochemistry*, **2006**, 100, 707-15	4.2	10
31	Iron(III)-nitro porphyrins: theoretical exploration of a unique class of reactive molecules. *Inorganic Chemistry*, **2006**, 45, 4902-9	5.1	35

30	Methyl 4-{[(1Z)-1-benzoyl-3-oxo-3-phenylprop-1-en-1-yl]amino}benzoate. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, o4717-o4719		
29	Electronic m□ages a trois: a molecular orbital perspective of protonated ferryl intermediates and synthetic models. *Journal of Inorganic Biochemistry*, **2006**, 100, 502-6	4.2	10
28	A DFT overview of high-valent iron, cobalt and nickel tetraamidomacrocyclic ligand (TAML) complexes: the end of innocence?. *Journal of Inorganic Biochemistry*, **2006**, 100, 620-6	4.2	12
27	When being straight bends rules: a rationale for the linear FeNO unit in the low-spin square-pyramidal {FeNO}7 tetracyanonitrosylferrate(2-) anion. *Journal of Inorganic Biochemistry*, **2006**, 100, 2069-73	4.2	10
26	The challenge of being straight: explaining the linearity of a low-spin [FeNO]7 unit in a tropocoronand complex. *Inorganic Chemistry*, **2005**, 44, 8699-706	5.1	14
25	Understanding the unexpected linearity of the trans-{Mn(NO)2}8 unit in a phthalocyanine complex: some thoughts on dinitrosylheme intermediates in biology. *Journal of Inorganic Biochemistry*, **2005**, 99, 55-9	4.2	5
24	Synthetic, electrochemical and structural aspects of a series of ferrocene-containing dicarbonyl □diketonato rhodium(I) complexes. *Inorganica Chimica Acta*, **2005**, 358, 2530-2542	2.7	65
23	Models of High-Valent Heme Protein Intermediates: A Quantum Chemical Study of Iron(IV) Porphyrins with Two Univalent Axial □Bonding Ligands. *Journal of Physical Chemistry B*, **2004**, 108, 452-456	3.4	29
22	Electronic Absorption and Resonance Raman Signatures of Hyperporphyrins and Nonplanar Porphyrins. *Journal of Physical Chemistry B*, **2003**, 107, 3613-3623	3.4	54
21	Molecular structure and conformation of dinitrosylheme. *Journal of the American Chemical Society*, **2003**, 125, 4968-9	16.4	24
20	Identification of chromosomal copy number changes associated with transformation of follicular lymphoma to diffuse large B-cell lymphoma. *Human Pathology*, **2003**, 34, 915-23	3.7	24
19	Do the One-Electron Oxidized Derivatives of Some Six-Coordinate Low-Spin Iron(III) Porphyrins Feature Strong Metal□ligand Ferromagnetic Coupling?. *Journal of Physical Chemistry B*, **2003**, 107, 6486-6490	3.4	24
18	Synthesis and characterisation of ferrocene-containing □diketonato complexes of rhodium(I) and rhodium(III). *Inorganica Chimica Acta*, **2002**, 328, 191-203	2.7	47
17	Cyclic voltammetry of ferrocene-containing □diketones as a tool to obtain group electronegativities. The structure of 3-ferrocenoyl-1,1,1-trifluoro-2-hydroxyprop-2-ene. *Canadian Journal of Chemistry*, **1999**, 77, 378-386	0.9	71
16	Structure of carbonyl[(ferrocenecarbonyl)trifluoroacetonato-□,□]triphenylphosphinerhodium(I). *Acta Crystallographica Section C: Crystal Structure Communications*, **1993**, 49, 82-84		14
15	Energy-loss and straggling of hydrogen and helium ions in selenium. *Nuclear Instruments & Methods in Physics Research*, **1983**, 205, 359-363		5
14	Energy-loss and straggling of hydrogen and helium ions in silver. *Nuclear Instruments & Methods in Physics Research*, **1983**, 216, 293-298		7
13	Sequestration of thiazolyl blue tetrazolium bromide and bromophenol blue onto biochar derived from American sycamore leaves. *International Journal of Environmental Analytical Chemistry*,1-18	1.8	0

12	Populus nigra leaf-derived biochar: an efficient and reusable low-cost carbon material for the ultrasonic-assisted remediation of oil spill. *Biomass Conversion and Biorefinery*,1	2.3	0
11	Ultrasonic-assisted adsorption of eriochrome black T and celestine blue dyes onto Ipomoea batatas-derived biochar. *International Journal of Environmental Analytical Chemistry*,1-19	1.8	0
10	DFT investigation of Percyanation effect of coronene molecule: Comparative study with their Perhalogenated counterparts.. *Polymer Bulletin*,1	2.4	0
9	Potential energy surface of the thiophene pentamer and non-covalent interactions. *International Journal of Quantum Chemistry*,e26840	2.1	0
8	Treatment of motor oil-contaminated water via sorption onto natural organic lignocellulosic waste: thermodynamics, kinetics, isotherm, recycling, and reuse. *Biomass Conversion and Biorefinery*,1	2.3	0
7	Chrysophyllum albidum stem bark extract coated tillite adsorbent for the uptake of Cr(VI): thermodynamic, kinetic, isotherm, and reusability. *Biomass Conversion and Biorefinery*,1	2.3	4
6	Ananas comosus peel mediated green synthesized magnetite nanoparticles and their antifungal activity against four filamentous fungal strains. *Biomass Conversion and Biorefinery*,1	2.3	5
5	Enhanced chromium (VI) removal by Anacardium occidentale stem bark extract-coated multiwalled carbon nanotubes. *International Journal of Environmental Science and Technology*,1	3.3	2
4	Sequestered uptake of chromium(VI) by Irvingia gabonensis stem bark extract anchored silica gel. *Biomass Conversion and Biorefinery*,1	2.3	1
3	Granite-MWCNTs nanocomposite coated with Dialium guineense stem bark extract for enhanced adsorption of chromium(VI). *International Journal of Environmental Analytical Chemistry*,1-18	1.8	
2	Mo Fischer Carbene Complexes: A DFT Study on the Prediction of Redox Potentials. *Journal of the Electrochemical Society*,	3.9	3
1	Enhanced sequestration of chromium (VI) onto spent self-indicating silica gels coated with Harpephyllum caffrum stem bark extract. *International Journal of Environmental Analytical Chemistry*,1-17	1.8	4