Jeanet Conradie

List of Publications by Citations

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	Catalytic generation of N2O3 by the concerted nitrite reductase and anhydrase activity of hemoglobin. *Nature Chemical Biology*, **2007**, 3, 785-94	11.7	189
334	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
333	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
332	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
331	Synthesis and molecular structure of gold triarylcorroles. *Inorganic Chemistry*, **2011**, 50, 12844-51	5.1	91
330	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
329	Cyclic voltammetry of ferrocene-containing β-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
328	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
327	Banana peel as a biosorbent for the decontamination of water pollutants. A review. *Environmental Chemistry Letters*, **2020**, 18, 1085-1112	13.3	65
326	Synthetic, electrochemical and structural aspects of a series of ferrocene-containing dicarbonyl β-diketonato rhodium(I) complexes. *Inorganica Chimica Acta*, **2005**, 358, 2530-2542	2.7	65
325	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
324	Oxidative Addition of CH3I and CO Migratory Insertion in a Series of Ferrocene-Containing Carbonyl Phosphine β-Diketonato Rhodium(I) Complexes. *Organometallics*, **2009**, 28, 1018-1026	3.8	62
323	Ruthenocene-Containing β-Diketones: Synthesis, pKa? Values, Keto−Enol Isomerization Kinetics, and Electrochemical Aspects. *Organometallics*, **2008**, 27, 353-362	3.8	57
322	Electronic Absorption and Resonance Raman Signatures of Hyperporphyrins and Nonplanar Porphyrins. *Journal of Physical Chemistry B*, **2003**, 107, 3613-3623	3.4	54
321	A thermally stable {FeNO}8 complex: properties and biological reactivity of reduced MNO systems. *Chemical Science*, **2012**, 3, 364-369	9.4	52
320	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
319	Electrochemical and density functional theory modeled reduction of enolized 1,3-diketones. *Electrochimica Acta*, **2011**, 56, 6211-6218	6.7	48

318	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
317	Synthesis and characterisation of ferrocene-containing β-diketonato complexes of rhodium(I) and rhodium(III). *Inorganica Chimica Acta*, **2002**, 328, 191-203	2.7	47
316	A Metallocorrole with Orthogonal Pyrrole Rings. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1865-1870	2.3	46
315	Understanding the Jahn–Teller Effect in Octahedral Transition-Metal Complexes: A Molecular Orbital View of the Mn(β-diketonato)3 Complex. *Journal of Chemical Education*, **2013**, 90, 1692-1696	2.4	43
314	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
313	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
312	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
311	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
310	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
309	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
308	Electrochemical behaviour of Tris(β-diketonato)iron(III) complexes: A DFT and experimental study. *Electrochimica Acta*, **2015**, 152, 512-519	6.7	38
307	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
306	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
305	Solvation energies of the proton in methanol revisited and temperature effects. *Physical Chemistry Chemical Physics*, **2018**, 20, 29184-29206	3.6	38
304	Density functional theory calculations of Rh-β-diketonato complexes. *Dalton Transactions*, **2015**, 44, 1503-15	4.3	36
303	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
302	Electrochemical and Computational Chemistry Study of Mn(β-diketonato)3 complexes. *Electrochimica Acta*, **2015**, 158, 418-426	6.7	35
301	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

300	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
299	Iron(III)-nitro porphyrins: theoretical exploration of a unique class of reactive molecules. *Inorganic Chemistry*, **2006**, 45, 4902-9	5.1	35
298	Cobalt- and Rhodium-Corrole-Triphenylphosphine Complexes Revisited: The Question of a Noninnocent Corrole. *Inorganic Chemistry*, **2017**, 56, 14788-14800	5.1	34
297	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
296	Low-energy states of manganese-oxo corrole and corrolazine: multiconfiguration reference ab initio calculations. *Inorganic Chemistry*, **2012**, 51, 4002-6	5.1	32
295	Structures, relative stability and binding energies of neutral water clusters, (H2O)2□0. *New Journal of Chemistry*, **2019**, 43, 13020-13037	3.6	31
294	Stable eight-coordinate iron(III/II) complexes. *Inorganic Chemistry*, **2010**, 49, 2032-4	5.1	31
293	Molecular structures of free-base corroles: nonplanarity, chirality, and enantiomerization. *Journal of Physical Chemistry A*, **2015**, 119, 3452-7	2.8	30
292	Mono- and diboron corroles: factors controlling stoichiometry and hydrolytic reactivity. *Inorganic Chemistry*, **2014**, 53, 5486-93	5.1	30
291	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
290	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
289	Synthesis, crystal structure and electrochemistry of tetrahedral mono-□diketonato titanocenyl complexes. *Inorganica Chimica Acta*, **2007**, 360, 2277-2283	2.7	30
288	XPS Fe 2p peaks from iron tris(□diketonates): Electronic effect of the □diketonato ligand. *Polyhedron*, **2016**, 119, 142-150	2.7	30
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286	Corroles cannot ruffle. *Inorganic Chemistry*, **2011**, 50, 3247-51	5.1	29
285	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
284	Electrochemical behaviour and structure of novel phosphine- and phosphite-substituted tungsten(0) Fischer carbene complexes. *Electrochimica Acta*, **2014**, 130, 104-118	6.7	28
283	A Frontier orbital energy approach to redox potentials. *Journal of Physics: Conference Series*, **2015**, 633, 012045	0.3	28

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281	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
280	Electrochemical and density functional theory study of bis(cyclopentadienyl) mono(□diketonato) titanium(IV) cationic complexes. *Electrochimica Acta*, **2010**, 56, 257-264	6.7	27
279	Structures and infrared spectroscopy of large sized protonated ammonia clusters. *Journal of Chemical Physics*, **2018**, 149, 244301	3.9	27
278	Significance of the electron-density of molecular fragments on the properties of manganese(III) □diketonato complexes: an XPS and DFT study. *RSC Advances*, **2017**, 7, 27718-27728	3.7	26
277	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
276	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
275	Exploration of the potential energy surface of the ethanol hexamer. *Journal of Chemical Physics*, **2019**, 150, 124308	3.9	25
274	Substitution and Isomerization of Asymmetric □Diketonato Rhodium(I) Complexes: A Crystallographic and Computational Study. *Organometallics*, **2010**, 29, 2446-2458	3.8	25
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
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271	Molecular structure and conformation of dinitrosylheme. *Journal of the American Chemical Society*, **2003**, 125, 4968-9	16.4	24
270	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
269	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
268	Exploration of the potential energy surfaces of small ethanol clusters. *Physical Chemistry Chemical Physics*, **2020**, 22, 13201-13213	3.6	22
267	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
266	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
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263	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
262	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
261	Large-Sized Ammonia Clusters and Solvation Energies of the Proton in Ammonia. *Journal of Computational Chemistry*, **2020**, 41, 21-30	3.5	20
260	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
259	Electrochemical study of □diketonatobis(triphenylphosphite)rhodium(I) complexes. *Electrochimica Acta*, **2011**, 56, 9287-9294	6.7	19
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256	Electronic properties of Fe charge transfer complexes □A combined experimental and theoretical approach. *Electrochimica Acta*, **2016**, 216, 339-346	6.7	18
255	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
254	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
253	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
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251	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
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248	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
247	Solvent effects on the structures of the neutral ammonia clusters. *Computational and Theoretical Chemistry*, **2020**, 1191, 113042	2	15

246	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
245	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
244	Electronic structure of an iron-porphyrin-nitrene complex. *Inorganic Chemistry*, **2010**, 49, 243-8	5.1	15
243	Correlation between the FeNO angle and d-p mixing in {FeNO}7 complexes. *Inorganic Chemistry*, **2011**, 50, 4223-5	5.1	15
242	Density Functional Theory Study of Substitution at the Square-Planar Acetylacetonato-dicarbonyl-rhodium(I) Complex. *Organometallics*, **2009**, 28, 3710-3715	3.8	15
241	Electrochemical and DFT study of the reduction of substituted phenanthrolines. *Polyhedron*, **2017**, 122, 147-154	2.7	14
240	Binding energies and isomer distribution of neutral acetonitrile clusters. *International Journal of Quantum Chemistry*, **2020**, 120, e26221	2.1	14
239	Theoretical infrared spectrum of the ethanol hexamer. *International Journal of Quantum Chemistry*, **2020**, 120, e26234	2.1	14
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236	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
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233	Redox behaviour of bis(-diketonato)copper(II) complexes. *Journal of Electroanalytical Chemistry*, **2019**, 837, 76-85	4.1	14
232	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
231	Singlet-Triplet Gaps of Cobalt Nitrosyls: Insights from Tropocoronand Complexes. *Inorganic Chemistry*, **2015**, 54, 7362-7	5.1	13
230	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
229	Global and local minima of protonated acetonitrile clusters. *New Journal of Chemistry*, **2020**, 44, 17558-17569	3.3	13

228	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
227	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
226	Synthesis and XPS characterization of Si-supported chromium(0) Fischer aminocarbene complexes. *Journal of Organometallic Chemistry*, **2017**, 836-837, 62-67	2.3	12
225	Oxidation potential of [Rh(β-diketonato)(P(OPh)3)2] complexes: Relationships with experimental, electronic and calculated parameters. *Electrochimica Acta*, **2013**, 110, 718-725	6.7	12
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223	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
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219	Structures of water clusters in the solvent phase and relative stability compared to gas phase. *Polyhedron*, **2021**, 193, 114856	2.7	12
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217	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
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213	Structures of the solvated copper(II) ion in ammonia at various temperatures. *New Journal of Chemistry*, **2020**, 44, 3637-3653	3.6	11
212	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
211	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

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208	Rhodium-rhodium interactions in [Rh(□diketonato)(CO)2] complexes. *Journal of Molecular Structure*, **2017**, 1144, 280-289	3.4	10
207	Structural and electronic features of triphenylstibine-functionalized Fischer carbene complexes of molybdenum(0). *Polyhedron*, **2017**, 133, 307-318	2.7	10
206	Energetics of Saddling versus Ruffling in Metalloporphyrins: Unusual Ruffled Dodecasubstituted Porphyrins. *ACS Omega*, **2017**, 2, 6708-6714	3.9	10
205	Comparison of X-ray photoelectron spectroscopy multiplet splitting of Cr 2p peaks from chromium tris(□diketonates) with chemical effects. *Journal of Electron Spectroscopy and Related Phenomena*, **2016**, 206, 46-51	1.7	10
204	Isocorroles as Homoaromatic NIR-Absorbing Chromophores: A First Quantum Chemical Study. *Scientific Reports*, **2018**, 8, 11952	4.9	10
203	Femtosecond laser spectroscopy and DFT studies of photochromic dithizonatomercury complexes. *Journal of Physical Chemistry A*, **2014**, 118, 844-55	2.8	10
202	Characterization of [Rh(PhCOCHCOCH2CH2CH3)(CO)2] by X-ray crystallography, a computational and a statistical study. *Polyhedron*, **2011**, 30, 660-665	2.7	10
201	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
200	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
199	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
198	Water-ammonia and water-acetonitrile proton transfer free energy. *Journal of Molecular Liquids*, **2020**, 318, 114300	6	10
197	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
196	Synthesis, electrochemical and DFT study of octahedral bis(□diketonato)-titanium(IV) complexes. *Inorganica Chimica Acta*, **2016**, 453, 247-256	2.7	10
195	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
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191	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
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