List of Publications by Year in descending order

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605 papers	37,691 citations	3933 88 h-index	4432 172 g-index
609 all docs	609 docs citations	609 times ranked	15128 citing authors

#	Article	IF	Citations
1	Fermi.jl: A Modern Design for Quantum Chemistry. Journal of Chemical Theory and Computation, 2022, 18, 677-686.	5.3	8
2	A Cationic Magnesium-Based Dithiolene Radical. Organometallics, 2022, 41, 527-531.	2.3	0
3	Mini-Review on Structureâ€“Reactivity Relationship for Aromatic Molecules: Recent Advances. ACS Omega, 2022, 7, 8199-8208.	3.5	2
4	Coupled Cluster Externally Corrected by Adaptive Configuration Interaction. Journal of Chemical Theory and Computation, 2021, 17, 182-190.	5.3	11
5	Fluorine Migration from Carbon to Iron and Fluorineâ€“Iron Dative Bonds in Octafluorocyclohexadiene Iron Carbonyl Chemistry. Organometallics, 2021, 40, 397-407.	2.3	2
6	Arbitrary-Order Derivatives of Quantum Chemical Methods via Automatic Differentiation. Journal of Physical Chemistry Letters, 2021, 12, 3232-3239.	4.6	16
7	Highly Strained Pn(CH)3 (Pn = N, P, As, Sb, Bi) Tetrahedranes: Theoretical Characterization. Journal of Physical Chemistry A, 2021, 125, 2612-2621.	2.5	2
8	Group 15 and 16 Nitreneâ€Like Pnictinidenes. Chemistry - A European Journal, 2021, 27, 14461-14471.	3.3	4
9	Four isomers of In ₂ H ₂ : a careful comparison between theory and experiment. Molecular Physics, 2021, 119, .	1.7	5
10	Kinetic Stability of Pentazole. Journal of Physical Chemistry A, 2021, 125, 9092-9098.	2.5	5
11	Contrasting the Mechanism of H₂Activation by Monomeric and Potassiumâ€Stabilized Dimeric Al^IComplexes: Do Potassium Atoms Exert any Cooperative Effect?. Chemistry - A European Journal, 2021, 27, 17369-17378.	3.3	9
12	Cumulants as the Variables of Density Cumulant Theory: A Path to Hermitian Triples. Journal of Chemical Physics, 2021, 155, 244105.	3.0	0
13	Substituent Effects on Aluminyl Anions and Derived Systems: A High-Level Theory. Journal of Physical Chemistry A, 2021, 125, 10379-10391.	2.5	1
14	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
15	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene (c-C₃H₂): the importance of numerical stability. Molecular Physics, 2020, 118, e1589007.	1.7	7
16	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. Journal of Chemical Physics, 2020, 152, 024302.	3.0	8
17	A Stable Naked Dithiolene Radical Anion and Synergic THF Ring-Opening. Journal of the American Chemical Society, 2020, 142, 17301-17305.	13.7	11
18	Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides Be₂H₂, Mg₂H₂, Ca₂H₂, Sr₂H₂, and Ba₂H₂. Proposals for Observations. Inorganic Chemistry, 2020, 59, 10404-10408.	4.0	3

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19	Comparative Study of the Thermal Stabilities of the Experimentally Known High-Valent Fe(IV) Compounds Fe(1-norbornyl)4 and Fe(cyclohexyl)4. Journal of Physical Chemistry A, 2020, 124, 6867-6876.	2.5	2
20	Reduced Density Matrix Cumulants: The Combinatorics of Size-Consistency and Generalized Normal Ordering. Journal of Chemical Theory and Computation, 2020, 16, 6150-6164.	5.3	11
21	Assessing the orbital-optimized unitary Ansatz for density cumulant theory. Journal of Chemical Physics, 2020, 153, 244102.	3.0	2
22	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
23	Unusual Structures of the Parent Molecules Diarsene, Distibene, and Dibismuthene: Toward Their Observation. Chemistry - A European Journal, 2020, 26, 14159-14166.	3.3	2
24	Energetics and mechanisms for the acetonyl radical + O2 reaction: An important system for atmospheric and combustion chemistry. Journal of Chemical Physics, 2020, 152, 114301.	3.0	5
25	Substituted Ortho-Benzynes: Properties of the Triple Bond. Journal of Organic Chemistry, 2020, 85, 9905-9914.	3.2	6
26	Conclusive determination of ethynyl radical hydrogen abstraction energetics and kinetics*. Molecular Physics, 2020, 118, e1769214.	1.7	7
27	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO₂ by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	2.5	18
28	A remarkable case of basis set dependence: the false convergence patterns of the methyl anion. Molecular Physics, 2019, 117, 1069-1077.	1.7	3
29	Unsaturation in binuclear iron carbonyl complexes of the split (3 + 2) fiveâ€electron donor hydrocarbon ligand bicyclo[3.2.1]octaâ€2,6â€dienâ€4â€yl: Role of agostic hydrogen atoms. International Journal of Quantum Chemistry, 2019, 119, e26010.	2.0	0
30	Dispersion Effects in Stabilizing Organometallic Compounds: Tetra-1-norbornyl Derivatives of the First-Row Transition Metals as Exceptional Examples. Journal of Physical Chemistry A, 2019, 123, 9514-9519.	2.5	11
31	Characterization of the 2-methylvinoxy radical + O2 reaction: A focal point analysis and composite multireference study. Journal of Chemical Physics, 2019, 151, 124302.	3.0	11
32	Ï€â€Hydrogen Bonding Probes Chemical Reactivity: Bromination of a CC Double Bond and Electrophilic Aromatic Benzylation. ChemistrySelect, 2019, 4, 10934-10942.	1.5	2
33	Substituent effects on the aromaticity of benzeneâ€"An approach based on interaction coordinates. Journal of Chemical Physics, 2019, 150, 214108.	3.0	8
34	Ethyl + O₂ in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical. Journal of Physical Chemistry A, 2019, 123, 3558-3568.	2.5	16
35	Cyclobutyne: Minimum or Transition State?. Journal of Organic Chemistry, 2019, 84, 5548-5553.	3.2	3
36	The Nature of Lithium Bonding in C₂H₂Li₂, C₆Li₆, and Lithium Halide Dimers. Organometallics, 2019, 38, 4708-4716.	2.3	1

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37	Ï€-Hydrogen Bonding Probes the Reactivity of Aromatic Compounds: Nitration of Substituted Benzenes. Journal of Physical Chemistry A, 2019, 123, 1069-1076.	2.5	7
38	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. Journal of Chemical Theory and Computation, 2018, 14, 1333-1350.	5.3	41
39	Spinâ€“Orbit Coupling via Four-Component Multireference Methods: Benchmarking on p-Block Elements and Tentative Recommendations. Journal of Chemical Theory and Computation, 2018, 14, 1235-1246.	5.3	15
40	The Structure and Clâ€“O Dissociation Energy of the ClOO Radical: Finally, the Right Answers for the Right Reason. Journal of Physical Chemistry A, 2018, 122, 2604-2610.	2.5	5
41	Hyperconjugative effects in Ï€â€hydrogen bonding: Theory and experiment. Journal of Computational Chemistry, 2018, 39, 527-534.	3.3	6
42	Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. Journal of Physical Chemistry A, 2018, 122, 9498-9511.	2.5	4
43	Metalâ€“Metal (MM) Bond Distances and Bond Orders in Binuclear Metal Complexes of the First Row Transition Metals Titanium Through Zinc. Chemical Reviews, 2018, 118, 11626-11706.	47.7	106
44	Fundamental Vibrational Analyses of the HCN Monomer, Dimer and Associated Isotopologues. ChemPhysChem, 2018, 19, 3257-3265.	2.1	6
45	Reinterpretation of the electronic absorption spectrum of the methylene amidogen radical (H2CN). Journal of Chemical Physics, 2018, 149, 094302.	3.0	1
46	High-level theoretical characterization of the vinoxy radical (â€¢CH2CHO) + O2 reaction. Journal of Chemical Physics, 2018, 148, 184308.	3.0	18
47	Nucleophilic Influences and Origin of the S N 2 Allylic Effect. Chemistry - A European Journal, 2018, 24, 11637-11648.	3.3	17
48	Quantification of Aromaticity of Heterocyclic Systems Using Interaction Coordinates. Journal of Physical Chemistry A, 2018, 122, 6953-6960.	2.5	22
49	Prediction and Characterization of Alkalineâ€Earth (M=Be, Mg, Ca, Sr, and Ba) Metallacyclopentadienes and Relevant Derivatives. ChemistrySelect, 2017, 2, 1442-1453.	1.5	7
50	The fate of the tert-butyl radical in low-temperature autoignition reactions. Journal of Chemical Physics, 2017, 146, 194304.	3.0	17
51	Metalâ€“metal bonding in biscycloheptatrienyl dimetal compounds of the secondâ€row transition metals. International Journal of Quantum Chemistry, 2017, 117, e25374.	2.0	0
52	Enhanced Relative Stability of Metallabenzenes versus Metallocenes upon Ring Perfluorination: Nickel, Palladium, and Platinum Systems. European Journal of Inorganic Chemistry, 2017, 2017, 4714-4721.	2.0	1
53	Bis(azulene) â€œsubmarineâ€•metal dimer sandwich compounds (C₁₀H₈)₂M₂ (Mâ€‰=â€‰Ti, V, Cr, Mn, Fe, Co, Ni): Parallel and opposed orientations. Journal of Computational Chemistry, 2016, 37, 250-260.	3.3	6
54	1,1â€Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure. ChemPhysChem, 2016, 17, 1623-1629.	2.1	2

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55	Infrared laser spectroscopy of the n-propyl and i-propyl radicals: Stretch-bend Fermi coupling in the alkyl CH stretch region. Journal of Chemical Physics, 2016, 145, 224304.	3.0	19
56	Characterizing a nonclassical carbene with coupled cluster methods: cyclobutylidene. Physical Chemistry Chemical Physics, 2016, 18, 24560-24568.	2.8	2
57	The Recently Synthesized Dimagnesiabutadiene and the Analogous Dimetallaâ€Beryllium, â€Calcium, â€Strontium, and â€Barium Compounds. Chemistry - A European Journal, 2016, 22, 15019-15026.	3.3	9
58	The methylsulfinyl radical CH₃SO examined. Physical Chemistry Chemical Physics, 2016, 18, 22293-22299.	2.8	14
59	Toward unsaturated stannylenes Y₂Zî€Sn: and related compounds with triplet electronic ground states. RSC Advances, 2016, 6, 53749-53759.	3.6	4
60	Chlorine peroxide (Cl₂O₂) and its isomers: structures, spectroscopy, formation and thermochemistry. Molecular Physics, 2016, 114, 1135-1147.	1.7	7
61	Catenanes: A molecular mechanics analysis of the (C₁₃H₂₆)₂ Structure 13â€13 D2. Journal of Computational Chemistry, 2016, 37, 124-129.	3.3	3
62	Ïƒ Bond activation through tunneling: formation of the boron hydride cations BH_n⁺ (n = 2, 4, 6). Physical Chemistry Chemical Physics, 2016, 18, 4063-4070.	2.8	4
63	The Reaction between Bromine and the Water Dimer and the Highly Exothermic Reverse Reaction. Journal of Computational Chemistry, 2016, 37, 177-182.	3.3	3
64	Exploring mechanisms of a tropospheric archetype: CH3O2 + NO. Journal of Chemical Physics, 2015, 143, 234302.	3.0	23
65	From Gasâ€Phase to Liquidâ€Water Chemical Reactions: The Fluorine Atom Plus Water Trimer System. Angewandte Chemie - International Edition, 2015, 54, 11223-11226.	13.8	11
66	Major differences between trifluorophosphine and carbonyl ligands in binuclear cyclopentadienyliron complexes. New Journal of Chemistry, 2015, 39, 3708-3718.	2.8	1
67	Triple decker sandwiches and related compounds of the first row transition metals with cyclopentadienyl and hexafluorobenzene rings: remarkable effects of fluorine substitution. Physical Chemistry Chemical Physics, 2015, 17, 20100-20113.	2.8	3
68	Carbonyl migration from phosphorus to the metal in binuclear phosphaketenyl metal carbonyl complexes to give bridging diphosphido complexes. New Journal of Chemistry, 2015, 39, 1390-1403.	2.8	9
69	Examining the ground and first excited states of methyl peroxy radical with high-level coupled-cluster theory. Molecular Physics, 2015, 113, 2992-2998.	1.7	13
70	Peroxyacetyl radical: Electronic excitation energies, fundamental vibrational frequencies, and symmetry breaking in the first excited state. Journal of Chemical Physics, 2015, 142, 054303.	3.0	10
71	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
72	Protonated Digermane, Distannane, and Diplumbane: Can They Be Made in the Laboratory?. European Journal of Inorganic Chemistry, 2014, 2014, 5015-5020.	2.0	3

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73	Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O4+. Journal of Chemical Physics, 2014, 141, 074111.	3.0	14
74	The exothermic HCl + OHÂ·(H2O) reaction: Removal of the HCl + OH barrier by a single water molecule. Journal of Chemical Physics, 2014, 140, 124316.	3.0	8
75	The LiÂ·Â·Â·HF van der Waals minimum and the barrier to the deep HFâ€“Li potential well. Molecular Physics, 2014, 112, 770-773.	1.7	3
76	Metal triangles versus metal chains and terminal versus bridging hydrogen atoms in trinuclear osmium carbonyl hydride chemistry. New Journal of Chemistry, 2014, 38, 1433-1440.	2.8	2
77	From spiropentane to butterfly and tetrahedral structures in tetranuclear iron carbonyl carbide chemistry. New Journal of Chemistry, 2014, 38, 3762-3769.	2.8	3
78	Novel germanetellones: XYGeî€Te (X, Y = H, F, Cl, Br, I and CN) â€“ structures and energetics. Comparison with the first synthetic successes. Dalton Transactions, 2014, 43, 4151.	3.3	3
79	Features of the potential energy surface for the SiO + OH â†' SiO2+ H reaction: relationship to oxygen isotopic partitioning during gas phase SiO2formation. RSC Advances, 2014, 4, 47163-47168.	3.6	7
80	Spinâ€“orbit corrected potential energy surface features for the I (2P3/2) + H2O â†' HI + OH forward and reverse reactions. Physical Chemistry Chemical Physics, 2014, 16, 2641.	2.8	13
81	Additionâ€“Elimination versus Direct Substitution Mechanisms for Arene Chlorination. European Journal of Organic Chemistry, 2014, 2014, 6918-6924.	2.4	18
82	Conical Intersections and Lowâ€Lying Electronic States of Tetrafluoroethylene. ChemPhysChem, 2014, 15, 2359-2366.	2.1	2
83	Streptococcal Hyaluronate Lyase Reveals the Presence of a Structurally Significant Cï£¿Hâ‹…â‹…â‹…O Hydrogen Bond. Chemistry - A European Journal, 2014, 20, 990-998.	3.3	3
84	Binuclear methylaminobis(difluorophosphine) iron carbonyls: phosphorusâ€“nitrogen bond cleavage in preference to ironâ€“iron multiple bond formation. New Journal of Chemistry, 2013, 37, 3294.	2.8	6
85	Metallametallocenes: Sandwich Compounds of the Firstâ€Row Transition Metals (M, Mâ€² = Fe, Co, Ni) Containing a Metallacyclopentadiene Ring. European Journal of Inorganic Chemistry, 2013, 2013, 2070-2077.	2.0	8
86	Density cumulant functional theory: The DC-12 method, an improved description of the one-particle density matrix. Journal of Chemical Physics, 2013, 138, 024107.	3.0	17
87	Moving on from F+H₂: The More Challenging Reaction between Atomic Fluorine and Methylamine. ChemPhysChem, 2013, 14, 896-899.	2.1	4
88	A new type of sandwich compound: homoleptic bis(trimethylenemethane) complexes of the first row transition metals. New Journal of Chemistry, 2013, 37, 1545.	2.8	14
89	Tetragermacyclobutadiene: Energetically Disfavored with Respect to Its Structural Isomers. Chemistry - A European Journal, 2013, 19, 7487-7495.	3.3	6
90	The ethyl radical in superfluid helium nanodroplets: Rovibrational spectroscopy and ab initio computations. Journal of Chemical Physics, 2013, 138, 194303.	3.0	26

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91	Does the metalâ€“metal sextuple bond exist in the bimetallic sandwich compounds Cr₂(C₆H₆)₂, Mo₂(C₆H₆)₂, and W₂(C₆H₆)₂?^{â€}. Molecular Physics, 2013, 111, 2523-2535.	1.7	11
92	Coaxial versus perpendicular structures for a range of binuclear cyclopentadienylpalladium derivatives. New Journal of Chemistry, 2013, 37, 775.	2.8	14
93	The alkaline earth dimer cations (Be₂ ⁺, Mg₂ ⁺,) Tj ETQq1 1 0.784314 rgBT /Over Coupled cluster and full configuration interaction studies^{â€}. Molecular Physics, 2013, 111, 2292-2298.	1.7	54
94	Structureâ€“reactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 37-55.	14.6	31
95	Orbital-optimized density cumulant functional theory. Journal of Chemical Physics, 2013, 139, 204110.	3.0	28
96	Communication: Some critical features of the potential energy surface for the Cl + H2O â†' HCl + OH forward and reverse reactions. Journal of Chemical Physics, 2013, 139, 041101.	3.0	29
97	Binuclear pentalene manganese carbonyl complexes: conventionaltransand unconventionalcisstructures. Molecular Physics, 2012, 110, 1637-1650.	1.7	8
98	Arbitrary order El'yashevichâ€“WilsonBtensor formulas for the most frequently used internal coordinates in molecular vibrational analyses. Journal of Chemical Physics, 2012, 137, 164103.	3.0	2
99	The lowest-lying electronic singlet and triplet potential energy surfaces for the HNOâ€“NOH system: Energetics, unimolecular rate constants, tunneling and kinetic isotope effects for the isomerization and dissociation reactions. Journal of Chemical Physics, 2012, 136, 164303.	3.0	28
100	Analytic gradients for density cumulant functional theory: The DCFT-06 model. Journal of Chemical Physics, 2012, 137, 054105.	3.0	18
101	In search of the next Holy Grail of polyoxide chemistry: Explicitly correlated ab initio full quartic force fields for HOOH, HOOOH, HOOOOH, and their isotopologues. Journal of Chemical Physics, 2012, 136, 084302.	3.0	30
102	Binuclear iron boronyl carbonyls isoelectronic with the well-known decacarbonyldimanganese. New Journal of Chemistry, 2012, 36, 1022.	2.8	14
103	Symmetric and asymmetric triple excitation corrections for the orbital-optimized coupled-cluster doubles method: Improving upon CCSD(T) and CCSD(T)Î›: Preliminary application. Journal of Chemical Physics, 2012, 136, 204114.	3.0	52
104	Fundamental vibrational frequencies and spectroscopic constants for the methylperoxyl radical, CH₃O₂, and related isotopologues ¹³CH₃OO, CH₃ ¹⁸O¹⁸O, and CD₃OO. Molecular Physics, 2012, 110, 2419-2427.	1.7	13
105	Electron Attachment to Solvated dGpdG: Effects of Stacking on Baseâ€Centered and Phosphateâ€Centered Valenceâ€Bound Radical Anions. Chemistry - A European Journal, 2012, 18, 5232-5238.	3.3	7
106	The Beryllium Pentamer: Trailing an Uneven Sequence of Dissociation Energies. ChemPhysChem, 2012, 13, 1255-1260.	2.1	5
107	Telluroformaldehyde and its derivatives: structures, ionization potentials, electron affinities and singletâ€“triplet gaps of the X2CTe and XYCTe (X,YÂ=ÂH, F, Cl, Br, I and CN) species. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	10
108	New Structural Features in Tetranuclear Iron Carbonyl Thiocarbonyls: Exotriangular Iron Atoms and Sixâ€Electronâ€Donating Thiocarbonyl Groups Bridging Four Iron Atoms. European Journal of Inorganic Chemistry, 2012, 2012, 1104-1113.	2.0	4

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109	Open chains versus closed rings: comparison of binuclear butadiene iron carbonyls with their cyclobutadiene analogues. New Journal of Chemistry, 2011, 35, 920.	2.8	9
110	Ground and excited state properties of photoactive platinum(iv) diazido complexes: Theoretical considerations. Dalton Transactions, 2011, 40, 7571.	3.3	30
111	Quadratically convergent algorithm for orbital optimization in the orbital-optimized coupled-cluster doubles method and in orbital-optimized second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 104103.	3.0	104
112	The Beryllium tetramer: Profiling an elusive molecule. Journal of Chemical Physics, 2011, 134, 074110.	3.0	20
113	Mononuclear bis(pentalene) sandwich compounds of the first-row transition metals: variable hapticity of the pentalene rings and intramolecular coupling reactions. New Journal of Chemistry, 2011, 35, 1718.	2.8	8
114	Is There an Entrance Complex for the F+NH₃ Reaction?. Chemistry - an Asian Journal, 2011, 6, 3152-3156.	3.3	13
115	Unsaturation in homoleptic tetranuclear iridium carbonyls: a comparison of density functional theory with the MP2 method in metal cluster structures. Theoretical Chemistry Accounts, 2011, 130, 393-400.	1.4	4
116	Binuclear Pentalene Iron Carbonyl Complexes. European Journal of Inorganic Chemistry, 2011, 2011, 2746-2755.	2.0	9
117	Edgeâ€Bridging and Faceâ€Bridging Hydrogen Atoms in Trinuclear Rhenium Carbonyl Hydrides. European Journal of Inorganic Chemistry, 2011, 2011, 4626-4636.	2.0	2
118	From acetylene complexes to vinylidene structures: The GeC₂H₂ system. Journal of Computational Chemistry, 2011, 32, 15-22.	3.3	3
119	The Inherent Competition between Addition and Substitution Reactions of Br₂ with Benzene and Arenes. Angewandte Chemie - International Edition, 2011, 50, 6809-6813.	13.8	39
120	Large-scale symmetry-adapted perturbation theory computations via density fitting and Laplace transformation techniques: Investigating the fundamental forces of DNA-intercalator interactions. Journal of Chemical Physics, 2011, 135, 174107.	3.0	174
121	Binuclear Cyclopentadienylmanganese Carbonyl Thiocarbonyls: Four-Electron Donor Bridging Thiocarbonyl Groups of Two Types and a Bridging Acetylenedithiolate Ligand. European Journal of Inorganic Chemistry, 2010, 2010, 4175-4186.	2.0	6
122	Chromium-Chromium Bonding in Binuclear Azulene Chromium Carbonyl Complexes. European Journal of Inorganic Chemistry, 2010, 2010, 5161-5173.	2.0	11
123	Hydroxyl Radical Reactions with Adenine: Reactant Complexes, Transition States, and Product Complexes. Chemistry - A European Journal, 2010, 16, 11848-11858.	3.3	39
124	The ten chemically transparent dinitronaphthalene isomers and their radical anions. Molecular Physics, 2010, 108, 2491-2509.	1.7	4
125	Perturbative triples corrections in state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2010, 132, 074107.	3.0	96
126	Triplet states of cyclopropenylidene and its isomers. Journal of Chemical Physics, 2010, 132, 044308.	3.0	16

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127	The barrier height, unimolecular rate constant, and lifetime for the dissociation of HN2. Journal of Chemical Physics, 2010, 132, 064308.	3.0	35
128	Vertical detachment energies of anionic thymidine: Microhydration effects. Journal of Chemical Physics, 2010, 133, 144305.	3.0	11
129	The mixed sandwich compounds C5H5MC7H7of the first row transition metals: variable hapticity of the seven-membered ring. Molecular Physics, 2010, 108, 883-894.	1.7	10
130	Unsaturation and variable hapticity in binuclear azulene manganese carbonyl complexes. Dalton Transactions, 2010, 39, 10702.	3.3	7
131	Quantum Mechanical Modeling for the GeX2/GeHX + GeH4 Reactions (X = H, F, Cl, and Br). Journal of Physical Chemistry A, 2010, 114, 4210-4223.	2.5	2
132	Dimerization of a fluorocarbyne complex to a tetrahedrane derivative: Fluorocarbyne and difluoroacetylene cobalt carbonyl complexes. Dalton Transactions, 2010, 39, 5242.	3.3	5
133	Density cumulant functional theory: First implementation and benchmark results for the DCFT-06 model. Journal of Chemical Physics, 2010, 133, 174122.	3.0	26
134	The quest for trifluorophosphine as a bridging ligand in homoleptic binuclear and tetranuclear cobalt complexes. Molecular Physics, 2010, 108, 2477-2489.	1.7	5
135	Neutral homoleptic tetranuclear iron carbonyls: why havenâ€™t they been synthesized as stable molecules?. New Journal of Chemistry, 2010, 34, 208-214.	2.8	6
136	Binuclear manganesecarbonyl thiocarbonyls: metalâ€“metal multiple bonds versus four-electron donorthiocarbonyl groups. New Journal of Chemistry, 2010, 34, 92-102.	2.8	9
137	Fe3(BF)3(CO)8 structures with face-semibridging fluoroborylene ligands and a bicapped tetrahedral Fe3B3 cluster isoelectronic with Os6(CO)18. New Journal of Chemistry, 2010, 34, 2813.	2.8	6
138	Noncovalent Interactions of a Benzo[a]pyrene Diol Epoxide with DNA Base Pairs: Insight into the Formation of Adducts of (+)-BaP DE-2 with DNA. Journal of Physical Chemistry A, 2010, 114, 2038-2044.	2.5	33
139	Terminal versus bridging cyclobutadiene rings in binuclear nickel carbonyl derivatives: A cube-antiprism twist of the cyclobutadiene rings in the perpendicular structures. New Journal of Chemistry, 2010, 34, 1885.	2.8	4
140	The subtleties of explicitly correlated Z-averaged perturbation theory: Choosing an R12 method for high-spin open-shell molecules. Journal of Chemical Physics, 2009, 131, 244116.	3.0	13
141	Characterization of the HSiNî—¸HNSi system in its electronic ground state. Journal of Chemical Physics, 2009, 130, 104301.	3.0	10
142	A laboratory and theoretical study of protonated carbon disulfide, HSCS+. Journal of Chemical Physics, 2009, 130, 234304.	3.0	14
143	Vanadium Carbonyl Nitrosyl Compounds: The Carbonyl Nitrosyl Chemistry of an Oxophilic Early Transition Metal. European Journal of Inorganic Chemistry, 2009, 2009, 1647-1656.	2.0	9
144	(Cyclopentadienyl)nitrosylmanganese Compounds: The Original Molecules Containing Bridging Nitrosyl Groups. European Journal of Inorganic Chemistry, 2009, 2009, 3982-3992.	2.0	3

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145	Inhibition of Alkyne Cyclotrimerization to Arenes on a Metal Site by Fourâ€Electron Donation through Simultaneous Sigma and Pi Bonding: The Tris(alkyne)Tungsten Carbonyls. European Journal of Inorganic Chemistry, 2009, 2009, 5439-5448.	2.0	2
146	The highly unsaturated dimetal hexacarbonyls of manganese and rhenium: Alternatives to a formal metalâ€“metal quintuple bond. International Journal of Quantum Chemistry, 2009, 109, 3082-3092.	2.0	6
147	The interplay between metalâ€“metal bonds, fourâ€electron donor carbonyl groups, and fiveâ€electron donor nitrosyl groups in highly unsaturated binuclear rhenium carbonyl nitrosyls. International Journal of Quantum Chemistry, 2009, 109, 2273-2285.	2.0	0
148	Electrophile Affinity: A Reactivity Measure for Aromatic Substitution. Journal of the American Chemical Society, 2009, 131, 14722-14727.	13.7	60
149	Analytic gradients for the state-specific multireference coupled cluster singles and doubles model. Journal of Chemical Physics, 2009, 131, 064109.	3.0	68
150	Enthalpy of formation and anharmonic force field of diacetylene. Journal of Chemical Physics, 2009, 130, 044301.	3.0	41
151	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
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