Dylan Jayatilaka

List of Publications by Year
in descending order

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145 papers	18,326 citations	47006 47 h-index	12946 131 g-index
155 all docs	155 docs citations	155 times ranked	10495 citing authors

#	Article	IF	Citations
1	Structure Factors and Charge Density Description of Aluminum: A Quantum Crystallographic Study. Journal of Physical Chemistry A, 2022, 126, 2042-2049.	2.5	1
2	X-ray constrained wavefunctions based on Hirshfeld atoms. II. Reproducibility of electron densities in crystals of Î±-oxalic acid dihydrate. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 397-415.	1.1	9
3	X-ray constrained wavefunctions based on Hirshfeld atoms. I. Method and review. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 312-332.	1.1	10
4	Accurate crystal structures and chemical properties from NoSpherA2. Chemical Science, 2021, 12, 1675-1692.	7.4	147
5	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. Chemistry - A European Journal, 2021, 27, 3407-3419.	3.3	10
6	HgH₂meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, 54-66.	0.1	4
7	The advanced treatment of hydrogen bonding in quantum crystallography. Journal of Applied Crystallography, 2021, 54, 718-729.	4.5	11
8	CrystalExplorer: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. Journal of Applied Crystallography, 2021, 54, 1006-1011.	4.5	1,744
9	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. Structure and Bonding, 2020, , 65-144.	1.0	17
10	Roby-Gould bond indices as a tool for understanding chemical bonding from a mathematical and quantum mechanical perspective. Results in Chemistry, 2020, 2, 100053.	2.0	2
11	Hydrogen atoms in bridging positions from quantum crystallographic refinements: influence of hydrogen atom displacement parameters on geometry and electron density. CrystEngComm, 2020, 22, 4778-4789.	2.6	25
12	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. Journal of Molecular Structure, 2020, 1209, 127934.	3.6	22
13	fragHAR: towardsab initioquantum-crystallographic X-ray structure refinement for polypeptides and proteins. IUCrJ, 2020, 7, 158-165.	2.2	10
14	On the accuracy and precision of X-ray and neutron diffraction results as a function of resolution and the electron density model. IUCrJ, 2020, 7, 920-933.	2.2	23
15	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. Angewandte Chemie, 2019, 131, 16936-16940.	2.0	8
16	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. Angewandte Chemie - International Edition, 2019, 58, 16780-16784.	13.8	26
17	Relativistic quantum crystallography of diphenyl- and dicyanomercury. Theoretical structure factors and Hirshfeld atom refinement. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 705-717.	0.1	23
18	Comment on â€œInter/Intramolecular Bonds in TH₅⁺ (T = C/Si/Ge): H₂ as Tetrel Bond Acceptor and the Uniqueness of Carbon Bondsâ€• Journal of Physical Chemistry A, 2019, 123, 9242-9243.	2.5	2

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19	Tunable hydrogen storage properties of defect-engineered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="bold">C</mml:mi></mml:mrow><mml:mrow><mml:mn mathvariant="bold">4</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="bold">N</mml:mi></mml:mrow></mml:math> nanosheets under ambient conditions.	10.3	69
20	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Hostâ€“Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. Journal of the American Chemical Society, 2019, 141, 3965-3976.	13.7	35
21	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. Applied Surface Science, 2019, 471, 887-892.	6.1	39
22	A Variety of Bond Analysis Methods, One Answer? An Investigation of the Elementâ^'Oxygen Bond of Hydroxides H_nXOH. Chemistry - A European Journal, 2018, 24, 6248-6261.	3.3	33
23	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
24	Linear MgCp*₂ vs Bent CaCp*₂: London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic Câ€“HÂ·Â·Â·Ca Interactions. Inorganic Chemistry, 2018, 57, 4906-4920.	4.0	17
25	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. Journal of Chemical Theory and Computation, 2018, 14, 1614-1623.	5.3	164
26	Predicting the primary fragments in mass spectrometry using ab initio Robyâ€“Gould bond indices. International Journal of Quantum Chemistry, 2018, 118, e25603.	2.0	12
27	Probing the accuracy and precision of Hirshfeld atom refinement with HARt interfaced with Olex2. IUCrJ, 2018, 5, 32-44.	2.2	74
28	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. International Journal of Quantum Chemistry, 2018, 118, e25460.	2.0	11
29	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. IUCrJ, 2018, 5, 635-646.	2.2	25
30	Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis. Australian Journal of Chemistry, 2018, 71, 227.	0.9	8
31	Covalency and Ionicity Do Not Oppose Each Otherâ€”Relationship Between Siâ^'O Bond Character and Basicity of Siloxanes. Chemistry - A European Journal, 2018, 24, 15275-15286.	3.3	40
32	Is it Reasonable to Obtain Information on the Polarizability and Hyperpolarizability Only from the Electron Density?. Australian Journal of Chemistry, 2018, 71, 295.	0.9	4
33	Quantum crystallography towards 'quantitative crystal engineering'. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e78-e78.	0.1	0
34	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€isotropic Crystal Packing. Angewandte Chemie, 2017, 129, 8588-8592.	2.0	29
35	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€isotropic Crystal Packing. Angewandte Chemie - International Edition, 2017, 56, 8468-8472.	13.8	104
36	Predicting the Position of the Hydrogen Atom in the Short Intramolecular Hydrogen Bond of the Hydrogen Maleate Anion from Geometric Correlations. Crystal Growth and Design, 2017, 17, 3812-3825.	3.0	18

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37	Intermolecular interactions in molecular crystals: whatâ€™s in a name?. Faraday Discussions, 2017, 203, 93-112.	3.2	121
38	Validation of Xâ€ray Wavefunction Refinement. ChemPhysChem, 2017, 18, 3334-3351.	2.1	49
39	CrystalExplorermodel energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. IUCrJ, 2017, 4, 575-587.	2.2	848
40	Quantum mechanical synthon interaction energies. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C682-C682.	0.1	0
41	Quantitative approaches to crystal engineering: applications to mechanical properties. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C849-C849.	0.1	2
42	Precision and accuracy of single-crystal X-ray results. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1388-C1388.	0.1	0
43	Waverfunction refinement-derived spin density of two cAAC-SiCl₃ polymorphs. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C571-C571.	0.1	0
44	Introducing iterative X-ray wavefunction refinement. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C702-C702.	0.1	0
45	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. Science Advances, 2016, 2, e1600192.	10.3	211
46	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. Journal of Chemical Physics, 2016, 145, 104101.	3.0	50
47	High Throughput Profiling of Molecular Shapes in Crystals. Scientific Reports, 2016, 6, 22204.	3.3	26
48	Importance of Relativistic Effects and Electron Correlation in Structure Factors and Electron Density of Diphenyl Mercury and Triphenyl Bismuth. Journal of Physical Chemistry A, 2016, 120, 6650-6669.	2.5	57
49	Hydrogen maleate salts: precise and accurate determination of the hydrogen atom position in short hydrogen bonds using X-ray diffraction at extremely low temperatures. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s89-s89.	0.1	0
50	Hirshfeld atom refinement for determining hydrogen positions in routine X-ray experiments. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s107-s107.	0.1	0
51	A technique for the comparison and analysis of decorated molecular surfaces. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s474-s475.	0.1	0
52	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. Computational and Theoretical Chemistry, 2015, 1053, 106-111.	2.5	15
53	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartreeâ€“Fock level of theory. Computational and Theoretical Chemistry, 2015, 1065, 27-41.	2.5	10
54	Sâ‹¯O chalcogen bonding in sulfa drugs: insights from multipole charge density and X-ray wavefunction of acetazolamide. Physical Chemistry Chemical Physics, 2015, 17, 25411-25420.	2.8	74

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55	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. Chemical Communications, 2015, 51, 3735-3738.	4.1	515
56	Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). New Journal of Chemistry, 2015, 39, 1628-1633.	2.8	10
57	Hirshfeld atom refinement for modelling strong hydrogen bonds. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 483-498.	0.1	59
58	Hirshfeld atom refinement. IUCrJ, 2014, 1, 361-379.	2.2	200
59	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. Journal of Physical Chemistry Letters, 2014, 5, 4249-4255.	4.6	380
60	Glycyl-<scp>L</scp>-alanine: a multi-temperature neutron study. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 949-952.	0.5	3
61	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. Chemical Physics, 2014, 438, 37-47.	1.9	14
62	Applications of X-ray Wavefunction Refinement. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1343-C1343.	0.1	0
63	Modeling electron density distributions from X-ray diffraction to derive optical properties: Constrained wavefunction versus multipole refinement. Journal of Chemical Physics, 2013, 139, 064108.	3.0	30
64	The quasirelativistic contact interaction and effective electron and spin densities at the nucleus: A model based on weighting the electron density with the finite Gaussian nucleus model. Chemical Physics Letters, 2013, 580, 152-159.	2.6	4
65	How does overcoordination create ion selectivity?. Biophysical Chemistry, 2013, 172, 37-42.	2.8	6
66	A comparison of electron density from Hirshfeld-atom refinement, X-ray wavefunction refinement and multipole refinement on three urea derivatives. CrystEngComm, 2013, 15, 2084.	2.6	28
67	An Entropic Mechanism of Generating Selective Ion Binding in Macromolecules. PLoS Computational Biology, 2013, 9, e1002914.	3.2	12
68	Can Experimental Electronâ€Ðensity Studies be Used as a Tool to Predict Biologically Relevant Properties of Lowâ€Molecular Weight Enzyme Ligands?. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1905-1921.	1.2	11
69	X-ray wavefunction refinement â€“ introduction, examples, validation. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s589-s589.	0.3	0
70	Structural Investigation of MscL Gating Using Experimental Data and Coarse Grained MD Simulations. PLoS Computational Biology, 2012, 8, e1002683.	3.2	50
71	ExiFRET: flexible tool for understanding FRET in complex geometries. Journal of Biomedical Optics, 2012, 17, 011005.	2.6	17
72	Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. Crystal Growth and Design, 2012, 12, 2277-2287.	3.0	10

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73	A Model of the Open Pore MscL Based on Experimental Data and Restrained Coarse Grained Simulations. Biophysical Journal, 2012, 102, 121a-122a.	0.5	1
74	Contributions of the electronic spin and orbital current to the ${m CoCl}_4^{2-}$ CoCl 42â^' magnetic field probed in polarised neutron diffraction experiments. Journal of Chemical Physics, 2012, 137, 064107.	3.0	3
75	Reliable Measurements of Dipole Moments from Single-Crystal Diffraction Data and Assessment of an In-Crystal Enhancement. Structure and Bonding, 2012, , 27-45.	1.0	18
76	The Significance of Ionic Bonding in Sulfur Dioxide: Bond Orders from Xâ€ray Diffraction Data. Angewandte Chemie - International Edition, 2012, 51, 6776-6779.	13.8	99
77	Crystal-field effects in<scp>L</scp>-homoserine: multipolesversusquantum chemistry. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 435-442.	0.3	36
78	Study of the picture change error at the 2nd order Douglas Kroll Hess level of theory. Electron and spin density and structure factors of the Bis[bis(methoxycarbimido) aminato] copper (II) complex. Chemical Physics, 2012, 395, 44-53.	1.9	14
79	Testing the use of molecular dynamics to simulate fluorophore motions and FRET. Physical Chemistry Chemical Physics, 2011, 13, 11045.	2.8	20
80	Mapping the Importance of 4 factors in Creating Monovalent Ion Selectivity in Biological Molecules. Biophysical Journal, 2011, 100, 578a.	0.5	0
81	Mapping the Importance of Four Factors in Creating Monovalent Ion Selectivity in Biological Molecules. Biophysical Journal, 2011, 100, 60-69.	0.5	19
82	Reactivity Differences between Î±,Î²-Unsaturated Carbonyls and Hydrazones Investigated by Experimental and Theoretical Electron Density and Electron Localizability Analyses. Journal of Physical Chemistry A, 2011, 115, 12715-12732.	2.5	25
83	Intermolecular Interactions and Electrostatic Properties of the Î²-Hydroquinone Apohost: Implications for Supramolecular Chemistry. Journal of Physical Chemistry A, 2011, 115, 12962-12972.	2.5	21
84	Using Wavefunctions to Get More Information Out of Diffraction Experiments. , 2011, , 213-257.		1
85	Visualisation and characterisation of voids in crystalline materials. CrystEngComm, 2011, 13, 1804-1813.	2.6	397
86	Picture change error correction in the radial distributions of canonical orbital densities and total electron density of radon atom: the effect of the size of nucleus and the basis set limit. Theoretical Chemistry Accounts, 2011, 129, 181-197.	1.4	11
87	The Electron Localizability Indicator from Xâ€Ray Diffraction Dataâ€"A First Application to a Series of Epoxide Derivatives. Chemistry - A European Journal, 2010, 16, 12818-12821.	3.3	31
88	X-ray constrained unrestricted Hartreeâ€"Fock and Douglasâ€"Krollâ€"Hess wavefunctions. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 78-92.	0.3	44
89	Picture change error correction of radon atom electron density. Journal of Chemical Physics, 2010, 133, 174125.	3.0	14
90	Determination of Fluorophore Orientation and Energy Transfer from MD Simulations. Biophysical Journal, 2010, 98, 582a.	0.5	0

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91	Interpreting FRET in Complex Geometries. Biophysical Journal, 2010, 98, 584a.	0.5	0
92	Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. CrystEngComm, 2010, 12, 2419.	2.6	12
93	Hirshfeld surface analysis. CrystEngComm, 2009, 11, 19-32.	2.6	5,526
94	Refractive indices for molecular crystals from the response of X-ray constrained Hartreeâ€“Fock wavefunctions. Physical Chemistry Chemical Physics, 2009, 11, 7209.	2.8	41
95	Mapping the Common Origins of Ion Selectivity in Biological Molecules. Biophysical Journal, 2009, 96, 660a-661a.	0.5	0
96	A definition for the covalent and ionic bond index in a molecule. Theoretical Chemistry Accounts, 2008, 119, 275-290.	1.4	30
97	X-ray structure refinement using aspherical atomic density functions obtained from quantum-mechanical calculations. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 383-393.	0.3	172
98	Simulation of Structure, Orientation, and Energy Transfer between AlexaFluor Molecules Attached to MscL. Biophysical Journal, 2008, 95, 2711-2721.	0.5	39
99	Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. CrystEngComm, 2008, , .	2.6	133
100	Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. Chemical Communications, 2007, , 3814.	4.1	2,589
101	Comparing entire crystal structures: structural genetic fingerprinting. CrystEngComm, 2007, 9, 648.	2.6	486
102	The Predominant Role of Coordination Number in Potassium Channel Selectivity. Biophysical Journal, 2007, 93, 2635-2643.	0.5	101
103	The use of dipole lattice sums to estimate electric fields and dipole moment enhancement in molecular crystals. Chemical Physics Letters, 2007, 443, 87-91.	2.6	42
104	Are intramolecular dynamic electron correlation effects detectable in X-ray diffraction experiments on molecular crystals?. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, 135-145.	0.3	13
105	Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. Journal of Chemical Physics, 2006, 125, 174505.	3.0	48
106	Determination of the Orientational Distribution and Orientation Factor for Transfer between Membrane-Bound Fluorophores using a Confocal Microscope. Biophysical Journal, 2006, 91, 1032-1045.	0.5	50
107	Siâ‹¯O Bonded Interactions in Silicate Crystals and Molecules:Â A Comparison. Journal of Physical Chemistry A, 2006, 110, 12678-12683.	2.5	14
108	Bond Length and Local Energy Density Property Connections for Non-Transition-Metal Oxide-Bonded Interactions. Journal of Physical Chemistry A, 2006, 110, 12259-12266.	2.5	33

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109	A Flexible Approach to the Calculation of Resonance Energy Transfer Efficiency between Multiple Donors and Acceptors in Complex Geometries. Biophysical Journal, 2005, 89, 3822-3836.	0.5	83
110	Electron localization functions obtained from X-ray constrained Hartreeâ€“Fock wavefunctions for molecular crystals of ammonia, urea and alloxanWork presented at the Microsymposium on Quantum Crystallography, XIX IUCr Congress, Geneva, Switzerland, August 2002.. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 111-119.	0.3	46
111	Wave functions derived from experiment. V. Investigation of electron densities, electrostatic potentials, and electron localization functions for noncentrosymmetric crystals. Journal of Computational Chemistry, 2003, 24, 470-483.	3.3	59
112	Tonto: A Fortran Based Object-Oriented System for Quantum Chemistry and Crystallography. Lecture Notes in Computer Science, 2003, , 142-151.	1.3	119
113	A complement to "Some fundamental problems with zero flux partitioning of electron densities". Theoretical Chemistry Accounts, 2002, 107, 383-384.	1.4	11
114	Wavefunctions derived from experiment. III. Topological analysis of crystal fragments. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 232-243.	0.3	51
115	Wavefunctions derived from experiment. IV. Investigation of the crystal environment of ammonia. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 244-251.	0.3	55
116	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. Chemical Physics Letters, 2002, 352, 245-251.	2.6	17
117	A theoretical study of the polarized neutron scattering from Cs3CoCl5. Journal of Chemical Physics, 2001, 114, 2687-2697.	3.0	6
118	Some fundamental problems with zero flux partitioning of electron densities. Theoretical Chemistry Accounts, 2001, 105, 213-218.	1.4	46
119	Wavefunctions derived from experiment. I. Motivation and theory. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 76-86.	0.3	178
120	Wavefunctions derived from experiment. II. A wavefunction for oxalic acid dihydrate. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 87-100.	0.3	89
121	Electron spin resonance g tensors from general Hartreeâ€“Fock calculations. Journal of Chemical Physics, 1998, 108, 7587-7594.	3.0	77
122	Wave Function for Beryllium from X-Ray Diffraction Data. Physical Review Letters, 1998, 80, 798-801.	7.8	131
123	A challenge for density functional theory: the XONO and XNO 2 (X=F, Cl, and Br) molecules. Theoretical Chemistry Accounts, 1997, 97, 185-194.	1.4	24
124	Cyclopropa-Fused Quinones. The Generation and Trapping of Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione and 1H-Cyclopropa[b]naphthalene-2,7-dione. Australian Journal of Chemistry, 1997, 50, 505.	0.9	12
125	Spatial symmetry and equivalence with unrestricted Hartree-Fock wavefunctions: application to the prediction of spin densities. Molecular Physics, 1997, 92, 471-476.	1.7	6
126	Ab initio study of the cyclic isomers of N2S4. Chemical Physics, 1995, 198, 169-181.	1.9	4

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127	An ab initio calculation of magnetic structure factors for Cs3CoCl5 including spinâ€“orbit and finite magnetic field effects. Journal of Chemical Physics, 1995, 103, 4562-4571.	3.0	13
128	Openâ€shell restricted Hartreeâ€“Fock perturbation theory: Some considerations and comparisons. Journal of Chemical Physics, 1994, 100, 7400-7409.	3.0	92
129	Fourier transforms of property densities with Gaussian functions. Chemical Physics Letters, 1994, 230, 228-230.	2.6	23
130	An open-shell restricted Hartreeâ€”Fock perturbation theory based on symmetric spin orbitals. Chemical Physics Letters, 1993, 201, 1-10.	2.6	150
131	Analytic SCF third and fourth derivatives with model potentials. Chemical Physics Letters, 1993, 212, 18-26.	2.6	2
132	Openâ€shell coupledâ€cluster theory. Journal of Chemical Physics, 1993, 98, 9734-9747.	3.0	182
133	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. Journal of Chemical Physics, 1992, 97, 4233-4254.	3.0	150
134	Higher analytic derivatives. Molecular Physics, 1992, 75, 271-291.	1.7	31
135	Implications of unitary invariance for gradient theory. International Journal of Quantum Chemistry, 1992, 42, 445-458.	2.0	6
136	The form of spin orbitals for open-shell restricted Hartreeâ€”Fock reference functions. Chemical Physics Letters, 1992, 199, 211-219.	2.6	44
137	Higher analytic derivatives. II. The fourth derivative of selfâ€consistentâ€field energy. Journal of Chemical Physics, 1991, 95, 7409-7417.	3.0	55
138	Spin contamination in single-determinant wavefunctions. Chemical Physics Letters, 1991, 183, 423-431.	2.6	91
139	Higher analytic derivatives. I. A new implementation for the third derivative of theSCF energy. International Journal of Quantum Chemistry, 1991, 40, 179-199.	2.0	43
140	Anharmonic vibrational properties of CH2F2: A comparison of theory and experiment. Journal of Chemical Physics, 1991, 95, 8323-8336.	3.0	115
141	Ab initio prediction of fundamental, overtone and combination band infrared intensities. Chemical Physics Letters, 1990, 169, 127-137.	2.6	49
142	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. Chemical Physics Letters, 1990, 172, 62-68.	2.6	221
143	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. Journal of Chemical Physics, 1990, 93, 4965-4981.	3.0	101
144	Anharmonic corrections to vibrational transition intensities. The Journal of Physical Chemistry, 1990, 94, 5608-5616.	2.9	132

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145	Analytic second derivatives with model potentials at SCF and MP2 levels. Chemical Physics Letters, 1989, 163, 151-156.	2.6	11