

# Dylan Jayatilaka

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

133 papers	12,706 citations	43 h-index	112 g-index
155 ext. papers	15,166 ext. citations	3.3 avg, IF	6.94 L-index

#	Paper	IF	Citations
133	X-ray constrained wavefunctions based on Hirshfeld atoms. II. Reproducibility of electron densities in crystals of oxalic acid dihydrate. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , <b>2022</b> , 78, 397-415	1.8	3
132	X-ray constrained wavefunctions based on Hirshfeld atoms. I. Method and review. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , <b>2022</b> , 78, 312-332	1.8	3
131	The advanced treatment of hydrogen bonding in quantum crystallography. <i>Journal of Applied Crystallography</i> , <b>2021</b> , 54, 718-729	3.8	3
130	CRYSTAL: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. <i>Journal of Applied Crystallography</i> , <b>2021</b> , 54, 1006-1011	3.8	344
129	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 3407-3419	4.8	6
128	HgH meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2021</b> , 77, 54-66	1.7	4
127	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. <i>Structure and Bonding</i> , <b>2020</b> , 65-144	0.9	13
126	Roby-Gould bond indices as a tool for understanding chemical bonding from a mathematical and quantum mechanical perspective. <i>Results in Chemistry</i> , <b>2020</b> , 2, 100053	2.1	0
125	Hydrogen atoms in bridging positions from quantum crystallographic refinements: influence of hydrogen atom displacement parameters on geometry and electron density. <i>CrystEngComm</i> , <b>2020</b> , 22, 4778-4789	3.3	17
124	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1209, 127934	3.4	14
123	fragHAR: towards quantum-crystallographic X-ray structure refinement for polypeptides and proteins. <i>IUCrJ</i> , <b>2020</b> , 7, 158-165	4.7	7
122	On the accuracy and precision of X-ray and neutron diffraction results as a function of resolution and the electron density model. <i>IUCrJ</i> , <b>2020</b> , 7, 920-933	4.7	12
121	Accurate crystal structures and chemical properties from NoSpherA2. <i>Chemical Science</i> , <b>2020</b> , 12, 1675-1692	5.2	41
120	Comment on "Inter/Intramolecular Bonds in TH (T = C/Si/Ge): H as Tetrel Bond Acceptor and the Uniqueness of Carbon Bonds". <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 9242-9243	2.8	1
119	Reversible hydrogen storage properties of defect-engineered C4N nanosheets under ambient conditions. <i>Carbon</i> , <b>2019</b> , 152, 344-353	10.4	37
118	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 16936-16940	3.6	3
117	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 16780-16784	16.4	13

116	Relativistic quantum crystallography of diphenyl- and dicyanomercurey. Theoretical structure factors and Hirshfeld atom refinement. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2019</b> , 75, 705-717	1.7	16
115	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Host-Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 3965-3976	16.4	23
114	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. <i>Applied Surface Science</i> , <b>2019</b> , 471, 887-892	6.7	23
113	A Variety of Bond Analysis Methods, One Answer? An Investigation of the Element-Oxygen Bond of Hydroxides H XOH. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 6248-6261	4.8	24
112	Quantum Crystallography: Current Developments and Future Perspectives. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 10881-10905	4.8	77
111	Linear MgCp* vs Bent CaCp*: London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic C-H...Ca Interactions. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 4906-4920	5.1	9
110	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 1614-1623	6.4	101
109	Predicting the primary fragments in mass spectrometry using ab initio Robyould bond indices. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25603	2.1	9
108	Probing the accuracy and precision of Hirshfeld atom refinement with interfaced with. <i>IUCrJ</i> , <b>2018</b> , 5, 32-44	4.7	60
107	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25460	2.1	8
106	Covalency and Ionicity Do Not Oppose Each Other-Relationship Between Si-O Bond Character and Basicity of Siloxanes. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 15275-15286	4.8	28
105	Is it Reasonable to Obtain Information on the Polarizability and Hyperpolarizability Only from the Electron Density?. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 295	1.2	1
104	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. <i>IUCrJ</i> , <b>2018</b> , 5, 635-646	4.7	16
103	Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis. <i>Australian Journal of Chemistry</i> , <b>2018</b> , 71, 227	1.2	7
102	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasi-isotropic Crystal Packing. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 8588-8592	3.6	28
101	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasi-isotropic Crystal Packing. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 8468-8472	16.4	80
100	Predicting the Position of the Hydrogen Atom in the Short Intramolecular Hydrogen Bond of the Hydrogen Maleate Anion from Geometric Correlations. <i>Crystal Growth and Design</i> , <b>2017</b> , 17, 3812-3825	3.5	16
99	Intermolecular interactions in molecular crystals: what's in a name?. <i>Faraday Discussions</i> , <b>2017</b> , 203, 93-113	13.2	76

98	Validation of X-ray Wavefunction Refinement. <i>ChemPhysChem</i> , <b>2017</b> , 18, 3334-3351	3.2	34
97	model energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. <i>IUCrJ</i> , <b>2017</b> , 4, 575-587	4.7	492
96	Quantitative approaches to crystal engineering: applications to mechanical properties. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2017</b> , 73, C849-C849	1.7	2
95	Importance of Relativistic Effects and Electron Correlation in Structure Factors and Electron Density of Diphenyl Mercury and Triphenyl Bismuth. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 6650-69	2.8	45
94	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. <i>Science Advances</i> , <b>2016</b> , 2, e1600192	14.3	147
93	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 104101	3.9	38
92	High Throughput Profiling of Molecular Shapes in Crystals. <i>Scientific Reports</i> , <b>2016</b> , 6, 22204	4.9	20
91	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1053, 106-111	2	13
90	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartree-Fock level of theory. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1065, 27-41	2	10
89	S···O chalcogen bonding in sulfa drugs: insights from multipole charge density and X-ray wavefunction of acetazolamide. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 25411-20	3.6	52
88	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. <i>Chemical Communications</i> , <b>2015</b> , 51, 3735-8	5.8	339
87	Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). <i>New Journal of Chemistry</i> , <b>2015</b> , 39, 1628-1633	3.6	10
86	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. <i>Chemical Physics</i> , <b>2014</b> , 438, 37-47	2.3	12
85	Hirshfeld atom refinement for modelling strong hydrogen bonds. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2014</b> , 70, 483-98	1.7	47
84	Hirshfeld atom refinement. <i>IUCrJ</i> , <b>2014</b> , 1, 361-79	4.7	140
83	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 4249-55	6.4	258
82	Glycyl-L-alanine: a multi-temperature neutron study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2014</b> , 70, 949-52	0.8	3
81	Modeling electron density distributions from X-ray diffraction to derive optical properties: constrained wavefunction versus multipole refinement. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 064108	3.9	25

80	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. <i>Chemical Physics Letters</i> , <b>2013</b> , 580, 152-159	2.5	4
79	How does overcoordination create ion selectivity?. <i>Biophysical Chemistry</i> , <b>2013</b> , 172, 37-42	3.5	6
78	A comparison of electron density from Hirshfeld-atom refinement, X-ray wavefunction refinement and multipole refinement on three urea derivatives. <i>CrystEngComm</i> , <b>2013</b> , 15, 2084	3.3	26
77	An entropic mechanism of generating selective ion binding in macromolecules. <i>PLoS Computational Biology</i> , <b>2013</b> , 9, e1002914	5	9
76	Can Experimental Electron-Density Studies be Used as a Tool to Predict Biologically Relevant Properties of Low-Molecular Weight Enzyme Ligands?. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2013</b> , 639, 1905-1921	1.3	9
75	X-ray wavefunction refinement Introduction, examples, validation. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2013</b> , 69, s589-s589		
74	Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. <i>Crystal Growth and Design</i> , <b>2012</b> , 12, 2277-2287	3.5	10
73	Contributions of the electronic spin and orbital current to the CoCl <sub>4</sub> (2-) magnetic field probed in polarised neutron diffraction experiments. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 064107	3.9	3
72	Reliable Measurements of Dipole Moments from Single-Crystal Diffraction Data and Assessment of an In-Crystal Enhancement. <i>Structure and Bonding</i> , <b>2012</b> , 27-45	0.9	15
71	Die Bedeutung ionischer Bindungsanteile in Schwefeldioxid Bindungsordnungen aus Röntgenbeugungsdaten. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 6880-6884	3.6	20
70	The significance of ionic bonding in sulfur dioxide: bond orders from X-ray diffraction data. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 6776-9	16.4	83
69	Crystal-field effects in L-homoserine: multipoles versus quantum chemistry. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2012</b> , 68, 435-442		31
68	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) amino] copper (II) complex. <i>Chemical Physics</i> , <b>2012</b> , 395, 44-53	2.3	12
67	Structural investigation of MscL gating using experimental data and coarse grained MD simulations. <i>PLoS Computational Biology</i> , <b>2012</b> , 8, e1002683	5	37
66	ExiFRET: flexible tool for understanding FRET in complex geometries. <i>Journal of Biomedical Optics</i> , <b>2012</b> , 17, 011005	3.5	14
65	Mapping the importance of four factors in creating monovalent ion selectivity in biological molecules. <i>Biophysical Journal</i> , <b>2011</b> , 100, 60-9	2.9	16
64	Reactivity differences between $\alpha$ -unsaturated carbonyls and hydrazones investigated by experimental and theoretical electron density and electron localizability analyses. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 12715-32	2.8	21
63	Intermolecular interactions and electrostatic properties of the hydroquinone apohost: implications for supramolecular chemistry. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 12962-72	2.8	20

62	Using Wavefunctions to Get More Information Out of Diffraction Experiments <b>2011</b> , 213-257		1
61	Visualisation and characterisation of voids in crystalline materials. <i>CrystEngComm</i> , <b>2011</b> , 13, 1804-1813	3.3	271
60	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. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 129, 181-197	1.9	10
59	Testing the use of molecular dynamics to simulate fluorophore motions and FRET. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 11045-54	3.6	18
58	Picture change error correction of radon atom electron density. <i>Journal of Chemical Physics</i> , <b>2010</b> , 133, 174125	3.9	13
57	Determination of Fluorophore Orientation and Energy Transfer from MD Simulations. <i>Biophysical Journal</i> , <b>2010</b> , 98, 582a	2.9	
56	Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. <i>CrystEngComm</i> , <b>2010</b> , 12, 2419	3.3	10
55	The electron localizability indicator from X-ray diffraction data--a first application to a series of epoxide derivatives. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 12818-21	4.8	27
54	X-ray constrained unrestricted Hartree-Fock and Douglas-Kroll-Hess wavefunctions. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2010</b> , 66, 78-92		39
53	Hirshfeld surface analysis. <i>CrystEngComm</i> , <b>2009</b> , 11, 19-32	3.3	3999
52	Refractive indices for molecular crystals from the response of X-ray constrained Hartree-Fock wavefunctions. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 7209-18	3.6	37
51	Simulation of structure, orientation, and energy transfer between AlexaFluor molecules attached to MscL. <i>Biophysical Journal</i> , <b>2008</b> , 95, 2711-21	2.9	35
50	Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. <i>CrystEngComm</i> , <b>2008</b> ,	3.3	83
49	A definition for the covalent and ionic bond index in a molecule. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 119, 275-290	1.9	25
48	X-ray structure refinement using aspherical atomic density functions obtained from quantum-mechanical calculations. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2008</b> , 64, 383-93		124
47	The predominant role of coordination number in potassium channel selectivity. <i>Biophysical Journal</i> , <b>2007</b> , 93, 2635-43	2.9	93
46	The use of dipole lattice sums to estimate electric fields and dipole moment enhancement in molecular crystals. <i>Chemical Physics Letters</i> , <b>2007</b> , 443, 87-91	2.5	37
45	Are intramolecular dynamic electron correlation effects detectable in X-ray diffraction experiments on molecular crystals?. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2007</b> , 63, 135-45		11



44	Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. <i>Chemical Communications</i> , <b>2007</b> , 3814-6	5.8	2014
43	Comparing entire crystal structures: structural genetic fingerprinting. <i>CrystEngComm</i> , <b>2007</b> , 9, 648	3.3	378
42	Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 174505	3.9	42
41	Determination of the orientational distribution and orientation factor for transfer between membrane-bound fluorophores using a confocal microscope. <i>Biophysical Journal</i> , <b>2006</b> , 91, 1032-45	2.9	44
40	Si-O bonded interactions in silicate crystals and molecules: a comparison. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 12678-83	2.8	13
39	Bond length and local energy density property connections for non-transition-metal oxide-bonded interactions. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 12259-66	2.8	31
38	A flexible approach to the calculation of resonance energy transfer efficiency between multiple donors and acceptors in complex geometries. <i>Biophysical Journal</i> , <b>2005</b> , 89, 3822-36	2.9	76
37	Electron localization functions obtained from X-ray constrained Hartree-Fock wavefunctions for molecular crystals of ammonia, urea and alloxan. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2004</b> , 60, 111-9		37
36	Tonto: A Fortran Based Object-Oriented System for Quantum Chemistry and Crystallography. <i>Lecture Notes in Computer Science</i> , <b>2003</b> , 142-151	0.9	78
35	Wave functions derived from experiment. V. Investigation of electron densities, electrostatic potentials, and electron localization functions for noncentrosymmetric crystals. <i>Journal of Computational Chemistry</i> , <b>2003</b> , 24, 470-83	3.5	49
34	A complement to Some fundamental problems with zero flux partitioning of electron densities. <i>Theoretical Chemistry Accounts</i> , <b>2002</b> , 107, 383-384	1.9	9
33	Wavefunctions derived from experiment. III. Topological analysis of crystal fragments. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2002</b> , 58, 232-43		40
32	Wavefunctions derived from experiment. IV. Investigation of the crystal environment of ammonia. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2002</b> , 58, 244-51		44
31	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. <i>Chemical Physics Letters</i> , <b>2002</b> , 352, 245-251	2.5	16
30	Some fundamental problems with zero flux partitioning of electron densities. <i>Theoretical Chemistry Accounts</i> , <b>2001</b> , 105, 213-218	1.9	40
29	Wavefunctions derived from experiment. I. Motivation and theory. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2001</b> , 57, 76-86		135
28	Wavefunctions derived from experiment. II. A wavefunction for oxalic acid dihydrate. <i>Acta Crystallographica Section A: Foundations and Advances</i> , <b>2001</b> , 57, 87-100		70
27	A theoretical study of the polarized neutron scattering from Cs <sub>3</sub> CoCl <sub>5</sub> . <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 2687-2697	3.9	6

26	Concerning the magnetisation density in magnetic neutron scattering experiments <b>2000</b> , 245-251		
25	Electron spin resonance g tensors from general Hartree-Fock calculations. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 7587-7594	3.9	72
24	Wave Function for Beryllium from X-Ray Diffraction Data. <i>Physical Review Letters</i> , <b>1998</b> , 80, 798-801	7.4	112
23	A challenge for density functional theory: the XONO and XNO <sub>2</sub> (X=F, Cl, and Br) molecules. <i>Theoretical Chemistry Accounts</i> , <b>1997</b> , 97, 185-194	1.9	23
22	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. <i>Australian Journal of Chemistry</i> , <b>1997</b> , 50, 505	1.2	10
21	Spatial symmetry and equivalence with unrestricted Hartree-Fock wavefunctions: application to the prediction of spin densities. <i>Molecular Physics</i> , <b>1997</b> , 92, 471-476	1.7	5
20	Ab initio study of the cyclic isomers of N <sub>2</sub> S <sub>4</sub> . <i>Chemical Physics</i> , <b>1995</b> , 198, 169-181	2.3	4
19	An ab initio calculation of magnetic structure factors for Cs <sub>3</sub> CoCl <sub>5</sub> including spin-orbit and finite magnetic field effects. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 4562-4571	3.9	13
18	Open-shell restricted Hartree-Fock perturbation theory: Some considerations and comparisons. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 7400-7409	3.9	89
17	Fourier transforms of property densities with Gaussian functions. <i>Chemical Physics Letters</i> , <b>1994</b> , 230, 228-230	2.5	21
16	Open-shell coupled-cluster theory. <i>Journal of Chemical Physics</i> , <b>1993</b> , 98, 9734-9747	3.9	158
15	An open-shell restricted Hartree-Fock perturbation theory based on symmetric spin orbitals. <i>Chemical Physics Letters</i> , <b>1993</b> , 201, 1-10	2.5	136
14	Analytic SCF third and fourth derivatives with model potentials. <i>Chemical Physics Letters</i> , <b>1993</b> , 212, 18-26	2.5	2
13	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. <i>Journal of Chemical Physics</i> , <b>1992</b> , 97, 4233-4254	3.9	139
12	Higher analytic derivatives. <i>Molecular Physics</i> , <b>1992</b> , 75, 271-291	1.7	29
11	Implications of unitary invariance for gradient theory. <i>International Journal of Quantum Chemistry</i> , <b>1992</b> , 42, 445-458	2.1	5
10	The form of spin orbitals for open-shell restricted Hartree-Fock reference functions. <i>Chemical Physics Letters</i> , <b>1992</b> , 199, 211-219	2.5	41
9	Spin contamination in single-determinant wavefunctions. <i>Chemical Physics Letters</i> , <b>1991</b> , 183, 423-431	2.5	76



8	Higher analytic derivatives. I. A new implementation for the third derivative of the SCF energy. <i>International Journal of Quantum Chemistry</i> , <b>1991</b> , 40, 179-199	2.1	43
7	Anharmonic vibrational properties of CH <sub>2</sub> F <sub>2</sub> : A comparison of theory and experiment. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 8323-8336	3.9	110
6	Higher analytic derivatives. II. The fourth derivative of self-consistent-field energy. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 7409-7417	3.9	53
5	Ab initio prediction of fundamental, overtone and combination band infrared intensities. <i>Chemical Physics Letters</i> , <b>1990</b> , 169, 127-137	2.5	47
4	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. <i>Chemical Physics Letters</i> , <b>1990</b> , 172, 62-68	2.5	193
3	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>1990</b> , 93, 4965-4981	3.9	94
2	Anharmonic corrections to vibrational transition intensities. <i>The Journal of Physical Chemistry</i> , <b>1990</b> , 94, 5608-5616		119
1	Analytic second derivatives with model potentials at SCF and MP2 levels. <i>Chemical Physics Letters</i> , <b>1989</b> , 163, 151-156	2.5	10