

List of Publications by Citations

Source: <https://exaly.com/author-pdf/7584356/jeremy-g-frey-publications-by-citations.pdf>
Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

145 papers	2,180 citations	24 h-index	40 g-index
176 ext. papers	2,454 ext. citations	5 avg, IF	4.68 L-index

#	Paper	IF	Citations
145	Anion-directed assembly: the first fluoride-directed double helix. <i>Chemical Communications</i> , 2003 , 568-958	5.8	141
144	Infrared predissociation spectra of water dimer in a supersonic molecular beam. <i>Chemical Physics Letters</i> , 1984 , 106, 373-376	2.5	138
143	Interferometric measurements of the dipole polarizability of molecules between 300 K and 1100 K. <i>Molecular Physics</i> , 1990 , 69, 803-817	1.7	98
142	Towards predictable transmembrane transport: QSAR analysis of anion binding and transport. <i>Chemical Science</i> , 2013 , 4, 3036	9.4	89
141	Are Distributed Ledger Technologies the panacea for food traceability?. <i>Global Food Security</i> , 2019 , 20, 145-149	8.3	82
140	Enzyme accessibility and solid supports: which molecular weight enzymes can be used on solid supports? An investigation using confocal Raman microscopy. <i>Chemistry - A European Journal</i> , 2002 , 8, 3769-72	4.8	68
139	Synthesis of guanidinium-derived receptor libraries and screening for selective peptide receptors in water. <i>Chemistry - A European Journal</i> , 2002 , 8, 1300-9	4.8	58
138	Tagging in combinatorial chemistry: the use of coloured and fluorescent beads. <i>Chemical Communications</i> , 1997 , 735-736	5.8	56
137	Second harmonic generation from the air/water interface of an aqueous solution of the dipeptide Boc-Trp-Trp. <i>Chemical Physics Letters</i> , 1994 , 230, 260-264	2.5	48
136	Soft-x-ray wavelength shift induced by ionization effects in a capillary. <i>Optics Letters</i> , 2006 , 31, 374-6	3	46
135	Ptychographic coherent diffractive imaging with orthogonal probe relaxation. <i>Optics Express</i> , 2016 , 24, 8360-9	3.3	43
134	Bringing chemical data onto the Semantic Web. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 939-52	6.1	42
133	QSAR analysis of substituent effects on tambjamine anion transporters. <i>Chemical Science</i> , 2016 , 7, 1600-1608	4.08	36
132	The semantic smart laboratory: a system for supporting the chemical eScientist. <i>Organic and Biomolecular Chemistry</i> , 2004 , 2, 3284-93	3.9	35
131	The temperature dependence of surface second-harmonic generation from the air-water interface. <i>Molecular Physics</i> , 2001 , 99, 677-687	1.7	34
130	An e-science environment for service crystallography--from submission to dissemination. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 1006-16	6.1	33
129	Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences. <i>Chemical Society Reviews</i> , 2013 , 42, 8157-75	58.5	32

128	Chemical information matters: an e-Research perspective on information and data sharing in the chemical sciences. <i>Chemical Society Reviews</i> , 2013 , 42, 6754-76	58.5	31
127	Electronic lab notebooks: can they replace paper?. <i>Journal of Cheminformatics</i> , 2017 , 9, 31	8.6	29
126	The calculation of the ground state energy of weakly bound van der waals trimers using the method of hyperspherical harmonics I. The BornOppenheimer and adiabatic approximations. <i>Chemical Physics</i> , 1985 , 99, 415-426	2.3	29
125	Data Science Professional Uncovered: How the EDISON Project will Contribute to a Widely Accepted Profile for Data Scientists 2015 ,		27
124	Site distribution in resin beads as determined by confocal Raman spectroscopy. <i>Chemistry - A European Journal</i> , 2001 , 7, 3880-3	4.8	25
123	Second harmonic generation by p-nitrophenol at water/air and water/heptane interfaces. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992 , 88, 2027		25
122	Isomerization of cis-stilbene in rare-gas clusters: direct measurements of trans-stilbene formation rates on a picosecond time scale. <i>Journal of the Optical Society of America B: Optical Physics</i> , 1990 , 7, 1540-1547	1.7	25
121	Rayleigh Scattering of Laser and Synchrotron Radiation from Pulsed Free Jets of Ar and (N ₂ O) _n Clusters. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 6457-6463	2.8	24
120	Which sites react first? Functional site distribution and kinetics on solid supports investigated using confocal Raman and fluorescence microscopy. <i>ACS Combinatorial Science</i> , 2003 , 5, 28-32		23
119	Surface second harmonic generation studies of the dodecane/water interface: the equilibrium and kinetic behaviour of p-nitrophenol and tri-n-butyl phosphate. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 3235-3245	3.6	22
118	Investigation of transport across an immiscible liquid/liquid interface. Electrochemical and second harmonic generation studies. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996 , 92, 1369		22
117	First steps towards semantic descriptions of electronic laboratory notebook records. <i>Journal of Cheminformatics</i> , 2013 , 5, 52	8.6	21
116	Photodissociation of CS ₂ at 193 nm investigated by polarised photofragment translational spectroscopy. <i>Chemical Physics</i> , 1996 , 202, 397-406	2.3	21
115	Energy dependence of the inelastic process Ba(6s6p1P1)+Ar,He-Ba(6s6p3P1,2)+Ar,He. <i>Journal of Chemical Physics</i> , 1990 , 93, 5354-5355	3.9	21
114	LabTrove: a lightweight, web based, laboratory "blog" as a route towards a marked up record of work in a bioscience research laboratory. <i>PLoS ONE</i> , 2013 , 8, e67460	3.7	20
113	Cheminformatics and the Semantic Web: adding value with linked data and enhanced provenance. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013 , 3, 465-481	7.9	19
112	The value of the Semantic Web in the laboratory. <i>Drug Discovery Today</i> , 2009 , 14, 552-61	8.8	19
111	The Semantic Grid and chemistry: Experiences with CombeChem. <i>Web Semantics</i> , 2006 , 4, 84-101	2.9	19

110	266 nm Photolysis of HOCl and DOCl: laser-excitation fluorescence detection of OH and OD. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993 , 89, 1623		19
109	Photolysis of HOCl at 248 nm in a supersonic molecular beam: laser-induced fluorescence spectra of OH. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1990 , 86, 3831		19
108	The calculation of the ground state energy of weakly bound van der waals trimers using the method of hyperspherical harmonics.. <i>Chemical Physics</i> , 1985 , 99, 427-435	2.3	19
107	Wide-field broadband extreme ultraviolet transmission ptychography using a high-harmonic source. <i>Optics Letters</i> , 2016 , 41, 1317-20	3	19
106	Experiences with a researcher-centric ELN. <i>Chemical Science</i> , 2015 , 6, 1614-1629	9.4	18
105	An accurate calculation of the ground state energy of the helium atom and the hydrogen negative ion using hyperspherical coordinates. <i>Chemical Physics</i> , 1987 , 111, 33-36	2.3	18
104	Dark Lab or Smart Lab: The Challenges for 21st Century Laboratory Software. <i>Organic Process Research and Development</i> , 2004 , 8, 1024-1035	3.9	17
103	Grid computing and biomolecular simulation. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005 , 363, 2017-35	3	16
102	Enantioselective binding of dipeptides using acyclic receptors. <i>Chemical Communications</i> , 2001 , 1358-1359	5.8	15
101	Raman spectra of NOCl and Cl ₂ photodissociation dynamics. <i>Molecular Physics</i> , 1989 , 67, 465-472	1.7	15
100	Efficient high-harmonic generation from a stable and compact ultrafast Yb-fiber laser producing 100fs, 350fs pulses based on bendable photonic crystal fiber. <i>Applied Physics B: Lasers and Optics</i> , 2017 , 123, 43	1.9	13
99	A new wave of innovation in Semantic web tools for drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2019 , 14, 433-444	6.2	13
98	Reflection second harmonic generation on a z-cut congruent lithium niobate crystal. <i>Physical Review B</i> , 2006 , 74,	3.3	13
97	Ultraviolet photolysis of HOCl: REMPI measurement of the relative population of chlorine atom (2P) spin-orbit states. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994 , 90, 17-21		13
96	The 248 nm photodissociation of DOCl: laser excitation fluorescence spectra of OD. <i>Chemical Physics Letters</i> , 1991 , 185, 101-104	2.5	13
95	The analysis of anisotropic photodissociation time-of-flight data obtained from a rotating source machine. <i>Molecular Physics</i> , 1992 , 75, 1419-1434	1.7	13
94	Curation of Laboratory Experimental Data as Part of the Overall Data Lifecycle. <i>International Journal of Digital Curation</i> , 2008 , 3, 44-62	0.9	13
93	Making tea 2004 ,		12

92	Synthesis, structure, and magnetism of a new type of π -molecular complex containing binuclear copper(II) complexes and benzene: bis[2,2-dimethyl-7-(phenylimino)-3,5,7-octanetrionato]dicopper(II)-benzene and bis[2,2-dimethyl-7-[(4-nitrophenyl)imino]-3,5,7-octanetrionato]dicopper(II)-bis(benzene). <i>Inorganic Chemistry</i> , 2013 , 52, 1237-1244	5.1	12
91	Quantitative and correlative extreme ultraviolet coherent imaging of mouse hippocampal neurons at high resolution. <i>Science Advances</i> , 2020 , 6, eaaz3025	14.3	11
90	Mass transfer enhancement produced by laser induced cavitation. <i>Electrochemistry Communications</i> , 2006 , 8, 1603-1609	5.1	11
89	Modal effects on pump-pulse propagation in an Ar-filled capillary. <i>Optics Express</i> , 2010 , 18, 13279-84	3.3	10
88	Resin bead micro-UV-visible absorption spectroscopy. <i>Analytical Chemistry</i> , 2005 , 77, 2247-51	7.8	10
87	Interfacial second harmonic generation in the limit of weak orientational order: determining interfacial refractive index. <i>Chemical Physics Letters</i> , 2000 , 323, 454-459	2.5	10
86	Raman emission from the photolysis of NOCl at 266 nm. <i>Molecular Physics</i> , 1990 , 69, 943-945	1.7	10
85	High-energy laser-pulse self-compression in short gas-filled fibers. <i>Physical Review A</i> , 2014 , 89,	2.6	9
84	Web-based services for drug design and discovery. <i>Expert Opinion on Drug Discovery</i> , 2011 , 6, 885-95	6.2	9
83	Direct measurement of the complex refractive index in the extreme ultraviolet spectral region using diffraction from a nanosphere array. <i>Applied Physics Letters</i> , 2008 , 93, 231103	3.4	9
82	The water-like film on water. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008 , 5, 1184-1186		9
81	Second harmonic ellipsometry. <i>Measurement Science and Technology</i> , 2003 , 14, 508-515	2	9
80	ECSES Examining crystal structures using 'e-science': a demonstrator employing web and grid services to enhance user participation in crystallographic experiments. <i>Journal of Applied Crystallography</i> , 2005 , 38, 819-826	3.8	9
79	Three-particle hyperspherical coordinates: permutation-inversion symmetry properties. <i>Molecular Physics</i> , 1990 , 70, 145-159	1.7	9
78	Ultra-broadband support determination for extreme ultraviolet coherent diffractive imaging from a high harmonic source. <i>Journal of Optics (United Kingdom)</i> , 2013 , 15, 094009	1.7	8
77	ChemTrove: enabling a generic ELN to support chemistry through the use of transferable plug-ins and online data sources. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 501-9	6.1	8
76	Creating context for the experiment record. User-defined metadata: investigations into metadata usage in the LabTrove ELN. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3268-83	6.1	8
75	Bright extreme-ultraviolet high-order-harmonic radiation from optimized pulse compression in short hollow waveguides. <i>Physical Review A</i> , 2013 , 87,	2.6	8

74	A Semantic eScience Platform for Chemistry 2010 ,		8
73			8
72	Prediction of properties from simulations: a re-examination with modern statistical methods. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 1791-803	6.1	8
71	A computer-aided drug discovery system for chemistry teaching. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 960-70	6.1	8
70	Combinatorial Chemistry and the Grid945-962		8
69	Non-adiabatic corrections for coupled oscillators using Rayleigh-Schrödinger perturbation theory. <i>Molecular Physics</i> , 1988 , 64, 191-206	1.7	8
68	Improved understanding of aqueous solubility modeling through topological data analysis. <i>Journal of Cheminformatics</i> , 2018 , 10, 54	8.6	8
67	Spatially resolved soft X-ray spectrometry from single-image diffraction. <i>Nature Physics</i> , 2007 , 3, 176-179	6.2	7
66	Synthesis, Conformational Studies and Binding Properties of Acyclic Receptors for N-Protected Amino Acids and Dipeptides. <i>European Journal of Organic Chemistry</i> , 2001 , 2001, 4625	3.2	7
65	Ab initio calculations on the ground and low-lying electronic states of the Cl3 radical: emission from Cl3. <i>Chemical Physics Letters</i> , 1992 , 189, 297-302	2.5	7
64	Taking FAIR on the CHIN: The Chemistry Implementation Network. <i>Data Intelligence</i> , 2020 , 2, 131-138	3	7
63	A new topological descriptor for water network structure. <i>Journal of Cheminformatics</i> , 2019 , 11, 48	8.6	6
62	A semantic datagrid for combinatorial chemistry 2005 ,		6
61	Too many tags spoil the metadata: investigating the knowledge management of scientific research with semantic web technologies. <i>Journal of Cheminformatics</i> , 2019 , 11, 23	8.6	5
60	Unexpected finite size effects in interfacial systems: Why bigger is not always better-Increase in uncertainty of surface tension with bulk phase width. <i>Journal of Chemical Physics</i> , 2018 , 148, 214704	3.9	5
59	MyExperimentalScience, extending the workflow Concurrency Computation Practice and Experience, 2013 , 25, 481-496	1.4	5
58	Grid-based dynamic electronic publication: a case study using combined experiment and simulation studies of crown ethers at the air/water interface. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005 , 363, 2075-95	3	5
57	The collision of electronically excited Ba (6s6p 1P1) with CO2 and H2O clusters. <i>Chemical Physics Letters</i> , 1991 , 176, 325-328	2.5	5

56	The adiabatic approach to $e + 2 e^-$ in the hyperspherical coordinates. <i>Molecular Physics</i> , 1986 , 57, 1-6	1.7	5
55	. <i>IEEE Internet of Things Journal</i> , 2020 , 7, 8631-8640	10.7	4
54	Monolayer detection of ion binding at a crown ether-functionalised supramolecular surface via an integrated optical Bragg grating. <i>Analyst, The</i> , 2014 , 139, 2774-82	5	4
53	Digital IUPAC. <i>Chemistry International</i> , 2014 , 36,	1.6	4
52	Adiabatic and diabatic approaches to bound state calculations. <i>Molecular Physics</i> , 1988 , 65, 1313-1320	1.7	4
51	Excited vibrational states near dissociation in weakly bound triatomic systems. <i>Chemical Physics Letters</i> , 1983 , 102, 421-424	2.5	4
50	Collection, Curation, Citation at Source: Publication@Source 10 Years On. <i>International Journal of Digital Curation</i> , 2015 , 10, 1-11	0.9	4
49	Data Curation Issues in the Chemical Sciences. <i>Information Standards Quarterly</i> , 2013 , 25, 4		4
48	Scientific and technical data sharing: a trading perspective. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 989-96	4.2	3
47	Crown ethers at the aqueous solution-air interface: 1. Assignments and surface spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7930-8	3.6	3
46	Spatiotemporal phase-matching in capillary high-harmonic generation. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2012 , 29, 806	1.7	3
45	High-Throughput Structure/Function Screening of Materials and Catalysts with Multiple Spectroscopic Techniques. <i>AIP Conference Proceedings</i> , 2007 ,	0	3
44	Thermal decomposition of 3-ethyl-3-methyloxetan and 3,3-diethyloxetan. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1975 , 71, 2485		3
43	User-Defined Metadata: Using Cues and Changing Perspectives. <i>International Journal of Digital Curation</i> , 2015 , 10, 18-47	0.9	3
42	Lloyd mirror interference lithography with EUV radiation from a high-harmonic source. <i>Applied Physics Express</i> , 2016 , 9, 076701	2.4	3
41	Effects of using structured templates for recalling chemistry experiments. <i>Journal of Cheminformatics</i> , 2016 , 8, 9	8.6	2
40	Usage and applications of Semantic Web techniques and technologies to support chemistry research. <i>Journal of Cheminformatics</i> , 2014 , 6, 18	8.6	2
39	Connecting Chemistry with Global Challenges through Data Standards. <i>Chemistry International</i> , 2017 , 39, 5-8	1.6	2

38	The Evolution of Digital Chemistry at Southampton. <i>Molecular Informatics</i> , 2015 , 34, 585-97	3.8	2
37	Ultra-broadband ptychography with self-consistent coherence estimation from a high harmonic source 2015 ,		2
36	Enhancing research publications using Rich Interactive Narratives. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2013 , 371, 20120090	3	2
35	Gas jet structure influence on high harmonic generation. <i>Optics Express</i> , 2011 , 19, 9801-6	3.3	2
34	The smartLab: Experimental and environmental control and monitoring of the chemistry laboratory 2009 ,		2
33	EUV off-axis focusing using a high harmonic source 2009 ,		2
32	Combining System Introspection with User-Provided Description to Support Configuration and Understanding of Pervasive systems 2008 ,		2
31	Molecular variation of capillary-produced soft x-ray high harmonics. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2008 , 41, 145602	1.3	2
30	Adsorption of rhodamine 6G at the water-air interface. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008 , 5, 1187-1189		2
29	Grid-enabling an existing instrument-based national service		2
28	Probing possible structural models at the air/H ₂ SO ₄ (aq) interface: a second harmonic generation study. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 2415	3.6	2
27	Statistical analysis of second harmonic generation experiments: a phenomenological model. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2005 , 75, 45-54	3.8	2
26	Analysis of time-of-flight data constraints and error bars. <i>Molecular Physics</i> , 1993 , 79, 1287-1303	1.7	2
25	Photolysis of HOBr and DOBr at 266 nm: OH and OD product-state distributions. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994 , 90, 817		2
24	Canine mammary cancer diagnosis from quantitative properties of nonlinear optical images. <i>Biomedical Optics Express</i> , 2020 , 11, 6413-6427	3.5	2
23	Surface reconstruction amendment to the intrinsic sampling method. <i>Journal of Chemical Physics</i> , 2018 , 149, 234705	3.9	2
22	A trust framework for digital food systems. <i>Nature Food</i> , 2021 , 2, 543-545	14.4	2
21	. <i>IEEE Sensors Journal</i> , 2019 , 19, 2984-2990	4	1

20	Quantitative Evaluation of Hard X-ray Damage to Biological Samples using EUV Ptychography. <i>Journal of Physics: Conference Series</i> , 2017 , 849, 012034	0.3	1
19	Spatially resolved Ar [*] and Ar ⁺ imaging as a diagnostic for capillary-based high harmonic generation. <i>Journal of Optics</i> , 2009 , 11, 054011		1
18	e-Malaria: the schools Malaria project. <i>Concurrency Computation Practice and Experience</i> , 2008 , 20, 225-238		1
17	The Collaborative Semantic Grid		1
16	Generalized ultrafast dispersion scans of continuum generation induced by sub-50fs chirped pulses in highly nonlinear tapered planar waveguides 2005 , 5714, 200		1
15	Considering the ethical implications of digital collaboration in the Food Sector. <i>Patterns</i> , 2021 , 2, 100335	5.1	1
14	Semantic Technologies in Drug Discovery 2021 , 129-144		1
13	The AI for Scientific Discovery Network. <i>Patterns</i> , 2021 , 2, 100162	5.1	1
12	A further structural examination of PVC gels. <i>Materials Letters</i> , 1991 , 11, 105-108	3.3	0
11	Canine mammary cancer tumour behaviour and patient survival time are associated with collagen fibre characteristics. <i>Scientific Reports</i> , 2021 , 11, 5668	4.9	0
10	Data management matters		0
9	Artificial Intelligence and Chemistry. <i>Chemistry International</i> , 2022 , 44, 6-9	1.6	0
8	Artificial intelligence and ethics within the food sector: Developing a common language for technology adoption across the supply chain. <i>Trends in Food Science and Technology</i> , 2022 , 125, 33-42	15.3	0
7	Temporal Coherence Effects on Coherent Diffractive Imaging of a Binary Sample by a High Harmonic Source. <i>EPJ Web of Conferences</i> , 2013 , 41, 12015	0.3	
6	Crown ethers at the aqueous solution-air interface. Part 2. Electrolyte effects, ethylene oxide hydration and temperature behaviour. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7939-47	3.6	
5	Multiphoton transitions for the harmonic oscillator. <i>Molecular Physics</i> , 2006 , 104, 2523-2525	1.7	
4	Second Harmonic Generation at Liquid/Liquid Interfaces 2005 , 1-23		
3	Calculation of non-adiabatic matrix elements. <i>Molecular Physics</i> , 1990 , 69, 783-785	1.7	

- | | | |
|---|---|-----|
| 2 | Adiabatic and diabatic representations, coordinate and unitary transformations: coupled oscillators. <i>Molecular Physics</i> , 1990 , 71, 659-665 | 1.7 |
| 1 | Wide-field broadband extreme ultraviolet transmission ptychography using a high-harmonic source: publisher's note. <i>Optics Letters</i> , 2016 , 41, 3057 | 3 |