

# Ralf Ludwig

## List of Publications by Year in descending order

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310  
papers

17,170  
citations

13068

68  
h-index

19690

117  
g-index

369  
all docs

369  
docs citations

369  
times ranked

12374  
citing authors

#	ARTICLE	IF	CITATIONS
1	Water: From Clusters to the Bulk. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1808-1827.	7.2	1,134
2	Efficient Dehydrogenation of Formic Acid Using an Iron Catalyst. <i>Science</i> , 2011, 333, 1733-1736.	6.0	728
3	Selective Catalytic Hydrogenations of Nitriles, Ketones, and Aldehydes by Well-Defined Manganese Pincer Complexes. <i>Journal of the American Chemical Society</i> , 2016, 138, 8809-8814.	6.6	485
4	Anti-inflammatory activity of IgG1 mediated by Fc galactosylation and association of Fc $\gamma$ RIIB and dectin-1. <i>Nature Medicine</i> , 2012, 18, 1401-1406.	15.2	405
5	Strong, Localized, and Directional Hydrogen Bonds Fluidize Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 8731-8734.	7.2	386
6	Molecular Dynamic Simulations of Ionic Liquids: A Reliable Description of Structure, Thermodynamics and Dynamics. <i>ChemPhysChem</i> , 2007, 8, 2464-2470.	1.0	355
7	Iron-Catalyzed Hydrogen Production from Formic Acid. <i>Journal of the American Chemical Society</i> , 2010, 132, 8924-8934.	6.6	326
8	Hydrogen Bonding in Protic Ionic Liquids: Reminiscent of Water. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 3184-3186.	7.2	308
9	Ion-Pair Formation in the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(triflyl)imide as a Function of Temperature and Concentration. <i>ChemPhysChem</i> , 2006, 7, 1944-1949.	1.0	304
10	The Association of Water in Ionic Liquids: A Reliable Measure of Polarity. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3697-3702.	7.2	272
11	The influence of hydrogen bonding on the physical properties of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14064.	1.3	270
12	Spectroscopic Evidence for an Enhanced Anion $\cdots$ Cation Interaction from Hydrogen Bonding in Pure Imidazolium Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 449-453.	7.2	250
13	Calixarenes in analytical and separation chemistry. <i>Fresenius' Journal of Analytical Chemistry</i> , 2000, 367, 103-128.	1.5	249
14	The Cation $\cdots$ Anion Interaction in Ionic Liquids Probed by Far $\cdots$ Infrared Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 3830-3834.	7.2	249
15	The potential role of hydrogen bonding in aprotic and protic ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8790.	1.3	218
16	Probing molecular interaction in ionic liquids by low frequency spectroscopy: Coulomb energy, hydrogen bonding and dispersion forces. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21903-21929.	1.3	204
17	Imidazolium Salt Ion Pairs in Solution. <i>Chemistry - A European Journal</i> , 2015, 21, 8324-8335.	1.7	158
18	A Stable Manganese Pincer Catalyst for the Selective Dehydrogenation of Methanol. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 559-562.	7.2	158

#	ARTICLE	IF	CITATIONS
19	Analyzing the interaction energies between cation and anion in ionic liquids: The subtle balance between Coulomb forces and hydrogen bonding. <i>Journal of Molecular Liquids</i> , 2014, 192, 94-102.	2.3	148
20	On the Validity of Stokes-Einstein and Stokes-Einstein-Debye Relations in Ionic Liquids and Ionic-Liquid Mixtures. <i>ChemPhysChem</i> , 2008, 9, 1851-1858.	1.0	142
21	Experimental and theoretical determination of the temperature dependence of deuteron and oxygen quadrupole coupling constants of liquid water. <i>Journal of Chemical Physics</i> , 1995, 103, 6941-6950.	1.2	132
22	PI3K $\beta$ Plays a Critical Role in Neutrophil Activation by Immune Complexes. <i>Science Signaling</i> , 2011, 4, ra23.	1.6	130
23	Do We Understand the Volatility of Ionic Liquids?. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 6582-6584.	7.2	124
24	Ionic Liquids: Dissecting the Enthalpies of Vaporization. <i>ChemPhysChem</i> , 2008, 9, 549-555.	1.0	123
25	Base-free hydrogen generation from methanol using a bi-catalytic system. <i>Chemical Communications</i> , 2014, 50, 707-709.	2.2	122
26	Spectroscopic Evidence for Clusters of Like-Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. <i>ChemPhysChem</i> , 2016, 17, 458-462.	1.0	115
27	The Influence of Hydrogen-Bond Defects on the Properties of Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6661-6665.	7.2	114
28	The Structure of Liquid Methanol. <i>ChemPhysChem</i> , 2005, 6, 1369-1375.	1.0	111
29	Quantum Cluster Equilibrium Theory of Liquids: A Temperature Dependence of Hydrogen Bonding in Liquid N-Methylacetamide Studied by IR Spectra. <i>Journal of Physical Chemistry B</i> , 1998, 102, 9312-9318.	1.2	110
30	ortho-Metalation of Iron(0) Tribenzylphosphine Complexes: Homogeneous Catalysts for the Generation of Hydrogen from Formic Acid. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8993-8996.	7.2	109
31	The Importance of Hydrogen Bonds for the Structure of Ionic Liquids: Single-Crystal X-ray Diffraction and Transmission and Attenuated Total Reflection Spectroscopy in the Terahertz Region. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 10221-10224.	7.2	106
32	Photocatalytic Hydrogen Generation from Water with Iron Carbonyl Phosphine Complexes: Improved Water Reduction Catalysts and Mechanistic Insights. <i>Chemistry - A European Journal</i> , 2011, 17, 6425-6436.	1.7	105
33	Temperature Dependence of the Solubility of Carbon Dioxide in Imidazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12727-12735.	1.2	104
34	IR and NMR Properties of Ionic Liquids: Do They Tell Us the Same Thing?. <i>ChemPhysChem</i> , 2007, 8, 2265-2269.	1.0	103
35	Hydrogen bonding in ionic liquids probed by linear and nonlinear vibrational spectroscopy. <i>New Journal of Physics</i> , 2012, 14, 105026.	1.2	102
36	Cation-cation clusters in ionic liquids: Cooperative hydrogen bonding overcomes like-charge repulsion. <i>Scientific Reports</i> , 2015, 5, 17505.	1.6	102

#	ARTICLE	IF	CITATIONS
37	Dissecting Anion-Cation Interaction Energies in Protic Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2368-2372.	7.2	100
38	Theoretical study of hydrogen bonding in liquid and gaseous N-methylformamide. <i>Journal of Chemical Physics</i> , 1997, 107, 499-507.	1.2	99
39	The ability of different forms of heparins to suppress P-selectin function in vitro correlates to their inhibitory capacity on bloodborne metastasis in vivo. <i>Thrombosis and Haemostasis</i> , 2006, 95, 535-540.	1.8	98
40	On the Tautomerism of Secondary Phosphane Oxides. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 2733-2741.	1.2	98
41	Low-Frequency Vibrational Modes of Protic Molten Salts and Ionic Liquids: Detecting and Quantifying Hydrogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 6236-6240.	7.2	97
42	NMR relaxation studies in water-alcohol mixtures: the water-rich region. <i>Chemical Physics</i> , 1995, 195, 329-337.	0.9	93
43	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. <i>Materials Research Bulletin</i> , 2017, 92, 113-122.	2.7	92
44	Therapeutic Use of Heparin beyond Anticoagulation. <i>Current Drug Discovery Technologies</i> , 2009, 6, 281-289.	0.6	90
45	Ion Speciation of Protic Ionic Liquids in Water: Transition from Contact to Solvent-Separated Ion Pairs. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2990-2994.	7.2	89
46	Death and Rebirth: Photocatalytic Hydrogen Production by a Self-Organizing Copper-Iron System. <i>ACS Catalysis</i> , 2014, 4, 1845-1849.	5.5	89
47	Calculation of Clathrate-Like Water Clusters Including H <sub>2</sub> O-Buckminsterfullerene. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 811-815.	7.2	87
48	Experimental and theoretical studies of hydrogen bonding in neat, liquid formamide. <i>Journal of Chemical Physics</i> , 1995, 102, 5118-5125.	1.2	85
49	The effect of hydrogen bonding on the thermodynamic and spectroscopic properties of molecular clusters and liquids. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5481-5487.	1.3	83
50	Volatile Times for the Very First Ionic Liquid: Understanding the Vapor Pressures and Enthalpies of Vaporization of Ethylammonium Nitrate. <i>Chemistry - A European Journal</i> , 2014, 20, 11640-11645.	1.7	83
51	A Molecularly Defined Iron-Catalyst for the Selective Hydrogenation of $\alpha,\beta$ -Unsaturated Aldehydes. <i>Chemistry - A European Journal</i> , 2013, 19, 7701-7707.	1.7	81
52	When Like Charged Ions Attract in Ionic Liquids: Controlling the Formation of Cationic Clusters by the Interaction Strength of the Counterions. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 496-500.	7.2	81
53	Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters. <i>Journal of Molecular Liquids</i> , 2018, 271, 51-64.	2.3	80
54	Selective Earth-Abundant System for CO <sub>2</sub> Reduction: Comparing Photo- and Electrocatalytic Processes. <i>ACS Catalysis</i> , 2019, 9, 2091-2100.	5.5	80

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55	Pressure and Salt Effects in Simulated Water: Two Sides of the Same Coin?. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 8907-8911.	7.2	79
56	Specific Ion Effects on Water Structure and Dynamics beyond the First Hydration Shell. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 352-353.	7.2	78
57	Controlling the Subtle Energy Balance in Protic Ionic Liquids: Dispersion Forces Compete with Hydrogen Bonds. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2792-2795.	7.2	78
58	New Insight into the Transport Mechanism of Hydrated Hydroxide Ions in Water. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 258-260.	7.2	77
59	Kinetics and mechanism of antibacterial activity and cytotoxicity of Ag-RGO nanocomposite. <i>Colloids and Surfaces B: Biointerfaces</i> , 2017, 159, 366-374.	2.5	77
60	Comment on "New Interpretation of the CH Stretching Vibrations in Imidazolium-Based Ionic Liquids". <i>Journal of Physical Chemistry A</i> , 2010, 114, 685-686.	1.1	76
61	Copper-Based Photosensitisers in Water Reduction: A More Efficient In Situ Formed System and Improved Mechanistic Understanding. <i>Chemistry - A European Journal</i> , 2016, 22, 1233-1238.	1.7	76
62	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 305, 112829.	2.3	76
63	Quantum cluster equilibrium theory of liquids: Freezing of QCE/3-21G water to tetrakaidecahedral "Bucky-ice". <i>Journal of Chemical Physics</i> , 1999, 110, 508-515.	1.2	75
64	Quantum cluster equilibrium theory of liquids: molecular clusters and thermodynamics of liquid ethanol. <i>Molecular Physics</i> , 1999, 97, 465-477.	0.8	75
65	Hydrogen bonding in a mixture of protic ionic liquids: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8431-8440.	1.3	74
66	Thermodynamic properties of ionic liquids—a cluster approach. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4333.	1.3	73
67	Formation of Water Clusters in a Hydrophobic Solvent. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 4904-4908.	7.2	71
68	Combined THz, FIR and Raman Spectroscopy Studies of Imidazolium-Based Ionic Liquids Covering the Frequency Range 2–300 cm <sup>-1</sup> . <i>ChemPhysChem</i> , 2010, 11, 349-353.	1.0	71
69	Molecular reorientation in ionic liquids: A comparative dielectric and magnetic relaxation study. <i>Chemical Physics Letters</i> , 2007, 439, 323-326.	1.2	65
70	Structure of Liquid N-Methylacetamide: Temperature Dependence of NMR Chemical Shifts and Quadrupole Coupling Constants. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8861-8870.	1.1	64
71	Spectroscopic evidence of "jumping and pecking" of cholinium and H-bond enhanced cation-cation interaction in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30978-30982.	1.3	64
72	An Elemental Mercury Diffusion Coefficient for Natural Waters Determined by Molecular Dynamics Simulation. <i>Environmental Science &amp; Technology</i> , 2009, 43, 3183-3186.	4.6	62

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73	Estimating Enthalpies of Vaporization of Imidazolium-Based Ionic Liquids from Far-Infrared Measurements. <i>ChemPhysChem</i> , 2010, 11, 1623-1626.	1.0	61
74	Insights into the Mechanism of Photocatalytic Water Reduction by DFT-Supported In Situ EPR/Raman Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10246-10250.	7.2	59
75	Equilibrium of Contact and Solvent-Separated Ion Pairs in Mixtures of Protic Ionic Liquids and Molecular Solvents Controlled by Polarity. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 12439-12442.	7.2	59
76	Iron-catalyzed photoreduction of carbon dioxide to synthesis gas. <i>Catalysis Science and Technology</i> , 2016, 6, 3623-3630.	2.1	58
77	Structure-Property Relationships in Ionic Liquids: A Study of the Anion Dependence in Vaporization Enthalpies of Imidazolium-Based Ionic Liquids. <i>ChemPhysChem</i> , 2012, 13, 1868-1876.	1.0	56
78	Mechanistic Study on the Addition of CO <sub>2</sub> to Epoxides Catalyzed by Ammonium and Phosphonium Salts: A Combined Spectroscopic and Kinetic Approach. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 10778-10788.	3.2	56
79	Water: From Clusters to the Bulk. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1808-1827.	7.2	56
80	Cooperative hydrogen bonding in amides and peptides. <i>Journal of Molecular Liquids</i> , 2000, 84, 65-75.	2.3	55
81	The Anion Dependence of the Interaction Strength between Ions in Imidazolium-Based Ionic Liquids Probed by Far-Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9507-9511.	1.2	54
82	Base-Free Non-Noble-Metal-Catalyzed Hydrogen Generation from Formic Acid: Scope and Mechanistic Insights. <i>Chemistry - A European Journal</i> , 2014, 20, 13589-13602.	1.7	53
83	Highly active and selective photochemical reduction of CO <sub>2</sub> to CO using molecular-defined cyclopentadienone iron complexes. <i>Chemical Communications</i> , 2016, 52, 8393-8396.	2.2	53
84	Temperature dependence of hydrogen bonding in alcohols. <i>Journal of Molecular Liquids</i> , 2000, 85, 105-125.	2.3	52
85	Exploring Between the Extremes: Conversion-Dependent Kinetics of Phosphite-Modified Hydroformylation Catalysis. <i>Chemistry - A European Journal</i> , 2012, 18, 8780-8794.	1.7	52
86	What Far-Infrared Spectra Can Contribute to the Development of Force Fields for Ionic Liquids Used in Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2009, 10, 1181-1186.	1.0	51
87	Microheterogeneities in Ionic-Liquid-Methanol Solutions Studied by FTIR Spectroscopy, DFT Calculations and Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2012, 13, 1708-1717.	1.0	51
88	Spectroscopic Evidence for an Attractive Cation-Cation Interaction in Hydroxy-Functionalized Ionic Liquids: A Hydrogen-Bonded Chain-Like Trimer. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15364-15368.	7.2	51
89	Cationic clustering influences the phase behaviour of ionic liquids. <i>Scientific Reports</i> , 2018, 8, 14753.	1.6	51
90	Non-Ideal Mixing Behaviour of Hydrogen Bonding in Mixtures of Protic Ionic Liquids. <i>ChemPhysChem</i> , 2015, 16, 299-304.	1.0	50

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91	Dispersion and Hydrogen Bonding Rule: Why the Vaporization Enthalpies of Aprotic Ionic Liquids Are Significantly Larger than those of Protic Ionic liquids. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11682-11686.	7.2	50
92	NMR relaxation in ethanol and propanol and in their binary mixtures with carbon tetrachloride. <i>Molecular Physics</i> , 1994, 82, 313-323.	0.8	49
93	Temperature dependence of hydrogen bonding in neat, liquid formamide. <i>Journal of Chemical Physics</i> , 1995, 103, 3636-3642.	1.2	49
94	A Comparative In-situ HPFTIR Spectroscopic Study of Bi- and Monodentate Phosphite-Modified Hydroformylation. <i>ChemCatChem</i> , 2010, 2, 287-295.	1.8	48
95	Molecular Dynamics in Lower Alcohols. <i>Zeitschrift Fur Physikalische Chemie</i> , 1995, 189, 19-27.	1.4	47
96	A Simple Geometrical Explanation for the Occurrence of Specific Large Aggregated Ions in Some Protic Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15419-15422.	1.2	47
97	Structural Motifs in Cold Ternary Ion Complexes of Hydroxyl-Functionalized Ionic Liquids: Isolating the Role of Cation-Cation Interactions. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2979-2984.	2.1	47
98	Molecular Reorientation in Liquid Methanol. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1991, 46, 89-94.	0.7	46
99	Structure and Dynamics of Water Confined in Dimethyl Sulfoxide. <i>ChemPhysChem</i> , 2006, 7, 266-272.	1.0	46
100	The effect of dispersion forces on the interaction energies and far infrared spectra of protic ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13790-13793.	1.3	46
101	tert-Butylphosphonic Acid: From the Bulk to the Gas Phase. <i>Chemistry - A European Journal</i> , 2003, 9, 837-849.	1.7	45
102	Hexamers: From Covalently Bound Organic Structures to Hydrogen Bonded Water Clusters. <i>ChemPhysChem</i> , 2000, 1, 53-56.	1.0	44
103	Management of cutaneous type IV hypersensitivity reactions induced by heparin. <i>Thrombosis and Haemostasis</i> , 2006, 96, 611-617.	1.8	44
104	Transport properties of graphene quantum dots in glycerol and distilled water. <i>Journal of Molecular Liquids</i> , 2017, 241, 831-838.	2.3	44
105	Temperature Dependence of the Deuteron and Oxygen Quadrupole Coupling Constants of Water in the System Water/Dimethyl Sulfoxide. <i>The Journal of Physical Chemistry</i> , 1994, 98, 6684-6687.	2.9	43
106	Quantum cluster equilibrium theory of liquids: temperature dependent chemical shifts, quadrupole coupling constants and vibrational frequencies in liquid ethanol. <i>Molecular Physics</i> , 1999, 97, 479-486.	0.8	43
107	Revisiting imidazolium based ionic liquids: Effect of the conformation bias of the [NTf <sub>2</sub> ] anion studied by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 193828.	1.2	42
108	Collective contributions to the dielectric relaxation of hydrogen-bonded liquids. <i>Journal of Chemical Physics</i> , 2004, 120, 11692-11697.	1.2	41

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109	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constants—Comparison with Salt Bridges and Molecular Systems. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17863-17871.	7.2	41
110	In Spite of the Chemist's Belief: Carbonic Acid Is Surprisingly Stable. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 1421-1423.	7.2	40
111	Raman spectroscopic investigation of small matrix-isolated lithium clusters. <i>Journal of Chemical Physics</i> , 2003, 118, 6957-6963.	1.2	40
112	Ion Pairing in Protic Ionic Liquids Probed by Far-Infrared Spectroscopy: Effects of Solvent Polarity and Temperature. <i>ChemPhysChem</i> , 2014, 15, 2604-2609.	1.0	40
113	Predicting the Ionic Product of Water. <i>Scientific Reports</i> , 2017, 7, 10244.	1.6	40
114	The Double-Faced Nature of Hydrogen Bonding in Hydroxy-Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12887-12892.	7.2	40
115	The Importance of Tetrahedrally Coordinated Molecules for the Explanation of Liquid Water Properties. <i>ChemPhysChem</i> , 2007, 8, 938-943.	1.0	39
116	Hydrogen bonding in a sterically hindered alcohol. <i>Journal of Molecular Liquids</i> , 2002, 98-99, 163-171.	2.3	38
117	How Does Water Bind to Metal Surfaces: Hydrogen Atoms Up or Hydrogen Atoms Down?. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3458-3460.	7.2	38
118	A Stable Manganese Pincer Catalyst for the Selective Dehydrogenation of Methanol. <i>Angewandte Chemie</i> , 2017, 129, 574-577.	1.6	37
119	Improving antibacterial activity of phosphomolybdic acid using graphene. <i>Materials Chemistry and Physics</i> , 2017, 188, 58-67.	2.0	37
120	Synthesis of .alpha.,.alpha.,.beta.,.beta.-Tetrasubstituted .beta.-Lactones from Ketones, Ethyl .alpha.-Bromoisobutyrate, and Indium or Zinc. Factors Influencing the .beta.-Lactone Formation in the Electrochemical and the Classical Procedure of the Reformatsky Reaction. <i>Journal of Organic Chemistry</i> , 1994, 59, 3161-3164.	1.7	36
121	Characterization of Doubly Ionic Hydrogen Bonds in Protic Ionic Liquids by NMR Deuteron Quadrupole Coupling Constants: Differences to H-bonds in Amides, Peptides, and Proteins. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14310-14314.	7.2	35
122	Hydronium Ion Complex of 18-Crown-6: Theory Confirms Three "Normal"-Linear Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11463-11468.	1.1	34
123	Limiting diffusion coefficients of ionic liquids in water and methanol: a combined experimental and molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3268.	1.3	34
124	Comparison of Force Fields on the Basis of Various Model Approaches—How To Design the Best Model for the [C <sub>n</sub> MIM] <sub>2</sub> Family of Ionic Liquids. <i>ChemPhysChem</i> , 2013, 14, 3368-3374.	1.0	34
125	Site Selective Synthesis of Pentaarylpyridines via Multiple Suzuki-Miyaura Cross-Coupling Reactions. <i>Advanced Synthesis and Catalysis</i> , 2014, 356, 1987-2008.	2.1	34
126	Novel acridine-based thiosemicarbazones as "turn-on" chemosensors for selective recognition of fluoride anion: a spectroscopic and theoretical study. <i>Royal Society Open Science</i> , 2018, 5, 180646.	1.1	34



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127	First row transition metals decorated boron phosphide nanoclusters as nonlinear optical materials with high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study. <i>Optics and Laser Technology</i> , 2021, 134, 106570.	2.2	34
128	Quantum cluster equilibrium theory of liquids part I: Molecular clusters and thermodynamics of liquid ammonia. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1998, 102, 197-204.	0.9	33
129	From Intramolecularly [4 + 1]- and [4 + 2]-Coordinated Tri- and Tetraorganosilanes to Hypercoordinated Benzoxasilaphospholes. <i>Organometallics</i> , 2001, 20, 4654-4663.	1.1	33
130	Model-free multivariate curve resolution combined with model-based kinetics: algorithm and applications. <i>Journal of Chemometrics</i> , 2012, 26, 538-548.	0.7	33
131	Light to Hydrogen: Photocatalytic Hydrogen Generation from Water with Molecularly-Defined Iron Complexes. <i>Inorganics</i> , 2017, 5, 14.	1.2	33
132	Effective $\alpha$ - $\beta$ quadrupole moments for the calibrated computation of quadrupole coupling parameters at different levels of theory. <i>Journal of Chemical Physics</i> , 1996, 105, 8223-8230.	1.2	32
133	Isotopic Quantum Effects in Liquid Methanol. <i>ChemPhysChem</i> , 2005, 6, 1376-1380.	1.0	32
134	Small Magnesium Clusters: Between van der Waals and Valence Bonds. <i>Inorganic Chemistry</i> , 2010, 49, 3851-3856.	1.9	31
135	An Operando FTIR Spectroscopic and Kinetic Study of Carbon Monoxide Pressure Influence on Rhodium-Catalyzed Olefin Hydroformylation. <i>Chemistry - A European Journal</i> , 2014, 20, 11921-11931.	1.7	31
136	Preparation and Crystal Structure of Tetraphenylphosphonium Triiodotetrabromide [PPh <sub>4</sub> ][I <sub>3</sub> Br <sub>4</sub> ]. <i>Inorganic Chemistry</i> , 2001, 40, 25-28.	1.9	30
137	Investigation into the Equilibrium of Iridium Catalysts for the Hydroformylation of Olefins by Combining In Situ High-Pressure FTIR and NMR Spectroscopy. <i>ACS Catalysis</i> , 2014, 4, 2097-2108.	5.5	30
138	Quantum cluster equilibrium theory of liquids part II: Temperature dependent chemical shifts, quadrupole coupling constants and vibrational frequencies in liquid ammonia. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1998, 102, 205-212.	0.9	29
139	Correlations between structural, NMR and IR spectroscopic properties of N-methylacetamide. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S127-S134.	1.1	29
140	The Effect of Neutral Ion Aggregate Formation on the Electrical Conductivity of an Ionic Liquid and its Mixtures with Chloroform. <i>ChemPhysChem</i> , 2012, 13, 1748-1752.	1.0	29
141	A simple guiding principle for the temperature dependence of the solubility of light gases in imidazolium-based ionic liquids derived from molecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1770-1780.	1.3	29
142	Controlling the kinetic and thermodynamic stability of cationic clusters by the addition of molecules or counterions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18854-18862.	1.3	29
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