Thomas Loerting

List of Publications by Year
in descending order

177 papers	7,299 citations	57758 44 h-index	66911 78 g-index
194 all docs	194 docs citations	194 times ranked	4924 citing authors

#	Article	IF	Citations
1	Substrate Dependent Charge Transfer Kinetics at the Solid/Liquid Interface of Carbonâ€Based Electrodes with Potential Application for Organic Naâ€Ion Batteries. Israel Journal of Chemistry, 2022, 62, .	2.3	4
2	Wasser: 1 MolekÃ¼l, 2 FlÃ¼ssigkeiten, 23 FestkÃ¶rper. Nachrichten Aus Der Chemie, 2022, 70, 63-67.	0.0	0
3	Oxygen NMR of high-density and low-density amorphous ice. Journal of Chemical Physics, 2022, 156, 084503.	3.0	3
4	Raman spectroscopy study of the slow orderâ€"order transformation of deuterium atoms: Ice XIX decay and ice XV formation. Journal of Chemical Physics, 2022, 156, 154507.	3.0	2
5	Increase of Radiative Forcing through Midinfrared Absorption by Stable CO₂ Dimers?. Journal of Physical Chemistry A, 2022, 126, 2966-2975.	2.5	3
6	Isotope effects on the dynamics of amorphous ices and aqueous phosphoric acid solutions. Physical Chemistry Chemical Physics, 2022, 24, 14846-14856.	2.8	1
7	Structural characterization of ice XIX as the second polymorph related to ice VI. Nature Communications, 2021, 12, 1128.	12.8	45
8	Optical cryomicroscopy and differential scanning calorimetry of buffer solutions containing cryoprotectants. European Journal of Pharmaceutics and Biopharmaceutics, 2021, 163, 127-140.	4.3	10
9	Experimental evidence for glass polymorphism in vitrified water droplets. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	17
10	Near-Infrared Spectra of High-Density Crystalline H₂O Ices II, IV, V, VI, IX, and XII. Journal of Physical Chemistry A, 2021, 125, 1062-1068.	2.5	6
11	Calorimetric Investigation of Hydrogen-Atom Sublattice Transitions in the Ice VI/XV/XIX Trio. Journal of Physical Chemistry B, 2021, 125, 11777-11783.	2.6	6
12	Advances in the study of supercooled water. European Physical Journal E, 2021, 44, 143.	1.6	40
13	The impact of temperature and unwanted impurities on slow compression of ice. Physical Chemistry Chemical Physics, 2021, 24, 35-41.	2.8	2
14	The interplay of VSCF/VCI calculations and matrix-isolation IR spectroscopy â€" Mid infrared spectrum of CH3CH2F and CD3CD2F. Journal of Molecular Spectroscopy, 2020, 367, 111224.	1.2	22
15	Alphaâ€Carbonic Acid Revisited: Carbonic Acid Monomethyl Ester as a Solid and its Conformational Isomerism in the Gas Phase. Chemistry - A European Journal, 2020, 26, 285-305.	3.3	9
16	On the synergy of matrix-isolation infrared spectroscopy and vibrational configuration interaction computations. Theoretical Chemistry Accounts, 2020, 139, 174.	1.4	3
17	Using Excimeric Fluorescence to Study How the Cooling Rate Determines the Behavior of Naphthalenes in Freeze-Concentrated Solutions: Vitrification and Crystallization. Journal of Physical Chemistry B, 2020, 124, 10556-10566.	2.6	5
18	Decomposing anharmonicity and mode-coupling from matrix effects in the IR spectra of matrix-isolated carbon dioxide and methane. Physical Chemistry Chemical Physics, 2020, 22, 17932-17947.	2.8	9

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19	Calorimetric Signature of Deuterated Ice II: Turning an Endotherm to an Exotherm. Journal of Physical Chemistry Letters, 2020, 11, 8268-8274.	4.6	3
20	Open questions on the structures of crystalline water ices. Communications Chemistry, 2020, 3, .	4.5	20
21	Absence of the liquid-liquid phase transition in aqueous ionic liquids. Physical Review E, 2020, 102, 060601.	2.1	5
22	Co-deposition of gas hydrates by pressurized thermal evaporation. Physical Chemistry Chemical Physics, 2020, 22, 4266-4275.	2.8	0
23	Glass transition of LiCl aqueous solutions confined in mesoporous silica. Journal of Chemical Physics, 2019, 151, .	3.0	8
24	Vitrification and increase of basicity in between ice Ih crystals in rapidly frozen dilute NaCl aqueous solutions. Journal of Chemical Physics, 2019, 151, 014503.	3.0	23
25	Distinguishing ice Î²-XV from deep glassy ice VI: Raman spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 15452-15462.	2.8	20
26	Toward Elimination of Discrepancies between Theory and Experiment: Anharmonic Rotationalâ€"Vibrational Spectrum of Water in Solid Noble Gas Matrices. Journal of Physical Chemistry A, 2019, 123, 8234-8242.	2.5	9
27	Structural differences between unannealed and expanded high-density amorphous ice based on isotope substitution neutron diffraction. Molecular Physics, 2019, 117, 3207-3216.	1.7	4
28	Glass polymorphism and liquidâ€"liquid phase transition in aqueous solutions: experiments and computer simulations. Physical Chemistry Chemical Physics, 2019, 21, 23238-23268.	2.8	33
29	Nature of Waterâ€™s Second Glass Transition Elucidated by Doping and Isotope Substitution Experiments. Physical Review X, 2019, 9, .	8.9	15
30	Amorphous and crystalline ices studied by dielectric spectroscopy. Journal of Chemical Physics, 2019, 150, 244501.	3.0	10
31	Macroscopic defects upon decomposition of CO₂ clathrate hydrate crystals. Physical Chemistry Chemical Physics, 2019, 21, 9694-9708.	2.8	8
32	Evidence for high-density liquid water between 0.1 and 0.3 GPa near 150 K. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9191-9196.	7.1	36
33	Nanoscale structure of amorphous solid water: What determines the porosity in ASW?. Proceedings of the International Astronomical Union, 2019, 15, 368-369.	0.0	2
34	Supercooled water: A polymorphic liquid with a cornucopia of behaviors. Journal of Chemical Physics, 2019, 151, 210401.	3.0	9
35	Distribution of Protein Content and Number of Aggregates in Monoclonal Antibody Formulation After Large-Scale Freezing. AAPS PharmSciTech, 2019, 20, 72.	3.3	23
36	Dynamic signatures of the transition from stacking disordered to hexagonal ice: Dielectric and nuclear magnetic resonance studies. Journal of Chemical Physics, 2018, 148, 134502.	3.0	3

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37	On the crystallisation temperature of very high-density amorphous ice. Physical Chemistry Chemical Physics, 2018, 20, 12589-12598.	2.8	7
38	Calorimetric study of water's two glass transitions in the presence of LiCl. Physical Chemistry Chemical Physics, 2018, 20, 6401-6408.	2.8	17
39	Experimental study of the polyamorphism of water. II. The isobaric transitions between HDA and VHDA at intermediate and high pressures. Journal of Chemical Physics, 2018, 148, 124509.	3.0	17
40	Experiments indicating a second hydrogen ordered phase of ice VI. Chemical Science, 2018, 9, 4224-4234.	7.4	35
41	Experimental study of the polyamorphism of water. I. The isobaric transitions from amorphous ices to LDA at 4 MPa. Journal of Chemical Physics, 2018, 148, 124508.	3.0	13
42	Impact of Buffer, Protein Concentration and Sucrose Addition on the Aggregation and Particle Formation during Freezing and Thawing. Pharmaceutical Research, 2018, 35, 101.	3.5	49
43	High-density amorphous ice: nucleation of nanosized low-density amorphous ice. Journal of Physics Condensed Matter, 2018, 30, 034002.	1.8	16
44	Distinct Speciation of Naphthalene Vapor Deposited on Ice Surfaces at 253 or 77 K: Formation of Submicrometer-Sized Crystals or an Amorphous Layer. Journal of Physical Chemistry C, 2018, 122, 11945-11953.	3.1	9
45	Thermodynamic and kinetic isotope effects on the orderâ€“disorder transition of ice XIV to ice XII. Physical Chemistry Chemical Physics, 2018, 20, 21607-21616.	2.8	10
46	Carbonic acid monoethyl ester as a pure solid and its conformational isomerism in the gas-phase. RSC Advances, 2017, 7, 22222-22233.	3.6	11
47	Formation and decomposition of CO2-filled ice. Journal of Chemical Physics, 2017, 147, 134503.	3.0	8
48	Relaxation dynamics and transformation kinetics of deeply supercooled water: Temperature, pressure, doping, and proton/deuteron isotope effects. Journal of Chemical Physics, 2017, 147, 034506.	3.0	23
49	Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins. Scientific Reports, 2017, 7, 11901.	3.3	21
50	Genuine antiplasticizing effect of water on a glass-former drug. Scientific Reports, 2017, 7, 7470.	3.3	17
51	Supercooled and glassy water: Metastable liquid(s), amorphous solid(s), and a no-manâ€™s land. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13336-13344.	7.1	99
52	Diffusive dynamics during the high-to-low density transition in amorphous ice. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8193-8198.	7.1	155
53	Crystallisation of the amorphous ices in the intermediate pressure regime. Scientific Reports, 2017, 7, 3995.	3.3	14
54	Micro-Tomographic Investigation of Ice and Clathrate Formation and Decomposition under Thermodynamic Monitoring. Materials, 2016, 9, 668.	2.9	4

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55	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	47.7	627
56	X-ray and Neutron Scattering of Water. Chemical Reviews, 2016, 116, 7570-7589.	47.7	170
57	Chapter 3 Solids and Fluids at Low Temperatures. , 2016, , 27-54.		0
58	Dynamics anomaly in high-density amorphous ice between 0.7 and 1.1 GPa. Physical Review B, 2016, 93, .	3.2	19
59	Neutron Scattering Analysis of Waterâ€™s Glass Transition and Micropore Collapse in Amorphous Solid Water. Physical Review Letters, 2016, 116, 215501.	7.8	37
60	Doping-enhanced dipolar dynamics in ice V as a precursor of hydrogen ordering in ice XIII. Physical Review B, 2016, 94, .	3.2	16
61	Does the emulsification procedure influence freezing and thawing of aqueous droplets?. Journal of Chemical Physics, 2016, 145, 211923.	3.0	17
62	Ex situ studies of relaxation and crystallization in high-density amorphous ice annealed at 0.1 and 0.2 GPa. Thermochimica Acta, 2016, 636, 11-22.	2.7	5
63	Glass polymorphism in glycerolâ€“water mixtures: I. A computer simulation study. Physical Chemistry Chemical Physics, 2016, 18, 11042-11057.	2.8	26
64	Glass polymorphism in glycerolâ€“water mixtures: II. Experimental studies. Physical Chemistry Chemical Physics, 2016, 18, 11058-11068.	2.8	44
65	<i>Colloquium</i>: Waterâ€™s controversial glass transitions. Reviews of Modern Physics, 2016, 88, .	45.6	146
66	Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091.	4.9	198
67	Vibrational study of anharmonicity, supramolecular structure, and hydrogen bonding in two octanol isomers. Vibrational Spectroscopy, 2015, 79, 59-66.	2.2	9
68	Experimental evidence for two distinct deeply supercooled liquid states of water â€“ Response to â€œComment on â€˜Water's second glass transitionâ€â€™, by G.P. Johari, Thermochim. Acta (2015). Thermochimica Acta, 2015, 617, 200-207.	2.7	8
69	Temperature-induced amorphisation of hexagonal ice. Physical Chemistry Chemical Physics, 2015, 17, 5403-5412.	2.8	14
70	Anomalous Behavior of the Homogeneous Ice Nucleation Rate in â€œNo-Manâ€™s Landâ€. Journal of Physical Chemistry Letters, 2015, 6, 2826-2832.	4.6	102
71	Dynamics enhanced by HCl doping triggers 60% Pauling entropy release at the ice XIIâ€“XIV transition. Nature Communications, 2015, 6, 7349.	12.8	22
72	Shrinking water's no man's land by lifting its low-temperature boundary. Physical Review B, 2015, 91, .	3.2	25

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73	Tomography based numerical simulation of the demagnetizing field in soft magnetic composites. Journal of Applied Physics, 2015, 117, .	2.5	12
74	Multiple Glass Transitions and Freezing Events of Aqueous Citric Acid. Journal of Physical Chemistry A, 2015, 119, 4515-4523.	2.5	22
75	Visualization of Freezing Process in situ upon Cooling and Warming of Aqueous Solutions. Scientific Reports, 2015, 4, 7414.	3.3	32
76	The glass transition in high-density amorphous ice. Journal of Non-Crystalline Solids, 2015, 407, 423-430.	3.1	52
77	Phase separation during freezing upon warming of aqueous solutions. Journal of Chemical Physics, 2014, 141, 18C533.	3.0	7
78	Anomalously large isotope effect in the glass transition of water. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17402-17407.	7.1	57
79	Cordierite under hydrostatic compression: Anomalous elastic behavior as a precursor for a pressure-induced phase transition. American Mineralogist, 2014, 99, 479-493.	1.9	23
80	Simulation of high-density water: Its glass transition for various water models. Journal of Chemical Physics, 2014, 140, 134504.	3.0	5
81	Small-angle neutron scattering study of micropore collapse in amorphous solid water. Physical Chemistry Chemical Physics, 2014, 16, 16013-16020.	2.8	33
82	Pressure-induced transformations in LiClâ€“H₂O at 77 K. Physical Chemistry Chemical Physics, 2014, 16, 18553-18562.	2.8	30
83	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 10989-10997.	3.1	35
84	Ultra-slow dynamics in low density amorphous ice revealed by deuteron NMR: indication of a glass transition. Physical Chemistry Chemical Physics, 2013, 15, 9308.	2.8	14
85	Limits of metastability in amorphous ices:²H-NMR relaxation. Physical Chemistry Chemical Physics, 2013, 15, 576-580.	2.8	13
86	Matrix Isolation Studies of Carbonic Acidâ€"The Vapor Phase above the Î²-Polymorph. Journal of the American Chemical Society, 2013, 135, 7732-7737.	13.7	33
87	Comment on â€œExperimental evidence for excess entropy discontinuities in glass-forming solutionsâ€• [J. Chem. Phys.136, 074515 (2012)]. Journal of Chemical Physics, 2013, 139, 047101.	3.0	1
88	From parallel to single crystallization kinetics in high-density amorphous ice. Physical Review B, 2013, 88, .	3.2	34
89	Waterâ€™s second glass transition. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17720-17725.	7.1	243
90	Solution coating around ice particles of incipient cirrus clouds. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E2439-E2439.	7.1	10

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91	Note: Molecular dynamics studies of high-density amorphous ice: Influence of long-range Coulomb interactions. Journal of Chemical Physics, 2012, 136, 026101.	3.0	3
92	Relaxation Time of High-Density Amorphous Ice. Physical Review Letters, 2012, 108, 225901.	7.8	36
93	Limits of metastability in amorphous ices: the neutron scattering Debyeâ€“Waller factor. Physical Chemistry Chemical Physics, 2012, 14, 16386.	2.8	12
94	Ferroelectric Transition Vanishes in (NH₄)₂SO₄ Precipitated in Small-Sized Aqueous Droplets. Journal of Physical Chemistry C, 2012, 116, 9372-9377.	3.1	5
95	Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water. Scientific Reports, 2012, 2, 390.	3.3	80
96	Formation and Stability of Bulk Carbonic Acid (H₂CO₃) by Protonation of Tropospheric Calcite. ChemPhysChem, 2012, 13, 3087-3091.	2.1	23
97	Local structural order in carbonic acid polymorphs: Raman and FTâ€IR spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 108-115.	2.5	26
98	Clathrate hydrate formation after CO2â€“H2O vapour deposition. Physical Chemistry Chemical Physics, 2011, 13, 19765.	2.8	14
99	Pressure-amorphized cubic structure II clathrate hydrate: crystallization in slow motion. Physical Chemistry Chemical Physics, 2011, 13, 2167-2171.	2.8	17
100	Single freezing and triple melting of micrometre-scaled (NH4)2SO4/H2O droplets. Physical Chemistry Chemical Physics, 2011, 13, 19704.	2.8	6
101	Equilibrated High-Density Amorphous Ice and Its First-Order Transition to the Low-Density Form. Journal of Physical Chemistry B, 2011, 115, 14141-14148.	2.6	116
102	Impact of Substrate, Aging, and Size on the Two Freezing Events of (NH₄)₂SO₄/H₂O Droplets. Journal of Physical Chemistry C, 2011, 115, 10682-10693.	3.1	12
103	How many amorphous ices are there?. Physical Chemistry Chemical Physics, 2011, 13, 8783.	2.8	167
104	Cryoflotation: Densities of Amorphous and Crystalline Ices. Journal of Physical Chemistry B, 2011, 115, 14167-14175.	2.6	54
105	RÃ¼cktitelbild: Spektroskopische Beobachtung von matrixisolierter KohlensÃure, abgeschieden aus der Gasphase (Angew. Chem. 8/2011). Angewandte Chemie, 2011, 123, 1988-1988.	2.0	0
106	Spectroscopic Observation of Matrixâ€Isolated Carbonic Acid Trapped from the Gas Phase. Angewandte Chemie - International Edition, 2011, 50, 1939-1943.	13.8	50
107	Back Cover: Spectroscopic Observation of Matrix-Isolated Carbonic Acid Trapped from the Gas Phase (Angew. Chem. Int. Ed. 8/2011). Angewandte Chemie - International Edition, 2011, 50, 1946-1946.	13.8	2
108	Different freezing behavior of millimeter- and micrometer-scaled (NH₄)₂SO₄/H₂O droplets. Journal of Physics Condensed Matter, 2011, 23, 035103.	1.8	4

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109	Volumetric study consistent with a glass-to-liquid transition in amorphous ices under pressure. Physical Review B, 2011, 83, .	3.2	56
110	Comment on Y. Yoshimura: â€œPressure-induced phase transition of ice in aqueous KOH solutionâ€• High Pressure Research, 2011, 31, 488-490.	1.2	2
111	Structural study of low concentration LiCl aqueous solutions in the liquid, supercooled, and hyperquenched glassy states. Journal of Chemical Physics, 2011, 134, 024515.	3.0	44
112	The many faces of â€œevidenceâ€•for dependent and independent variables in the â€˜Stewart approachâ€™: reply to Lang. Intensive Care Medicine, 2010, 36, 1626-1627.	8.2	0
113	Aqueous Carbonic Acid (H₂CO₃). ChemPhysChem, 2010, 11, 2305-2309.	2.1	53
114	Formation of mixed-phase particles during the freezing of polar stratospheric ice clouds. Nature Chemistry, 2010, 2, 197-201.	13.6	39
115	Reversibility and isotope effect of the calorimetric glass â†’ liquid transition of low-density amorphous ice. Physical Chemistry Chemical Physics, 2010, 12, 708-712.	2.8	72
116	Hexagonal ice transforms at high pressures and compression rates directly into â€œdoubly metastableâ€• ice phases. Journal of Chemical Physics, 2009, 131, 224514.	3.0	11
117	Relaxation effects in low density amorphous ice: Two distinct structural states observed by neutron diffraction. Journal of Chemical Physics, 2009, 130, 204502.	3.0	59
118	High-density amorphous ice: Molecular dynamics simulations of the glass transition at 0.3 GPa. Journal of Chemical Physics, 2009, 131, 114502.	3.0	10
119	Raman Spectroscopic Study of the Phase Transition of Amorphous to Crystalline Î²â€Carbonic Acid. Angewandte Chemie - International Edition, 2009, 48, 2690-2694.	13.8	33
120	Molecular Dynamics Simulations on the Glass-to-liquid Transition in High Density Amorphous Ice. Zeitschrift Fur Physikalische Chemie, 2009, 223, 1047-1062.	2.8	2
121	Structural transitions in amorphous H₂O and D₂O: the effect of temperature. Journal of Physics Condensed Matter, 2008, 20, 494212.	1.8	41
122	Compression-rate dependence of the phase transition from hexagonal ice to ice II and/or ice III. Physical Review B, 2008, 77, .	3.2	24
123	Water polyamorphism: Reversibility and (dis)continuity. Journal of Chemical Physics, 2008, 128, 044510.	3.0	134
124	Fluctuations and Phase Separation in a Quasi-One-Dimensional System. Physical Review Letters, 2007, 98, 186101.	7.8	13
125	Novel Method to Detect the Volumetric Glass â†’ Liquid Transition at High Pressures:Â Glycerol as a Test Case. Journal of Physical Chemistry B, 2007, 111, 8038-8044.	2.6	13
126	Interaction of Hydrogen Chloride with Ice Surfaces:â€‰ The Effects of Grain Size, Surface Roughness, and Surface Disorder. Journal of Physical Chemistry A, 2007, 111, 6274-6284.	2.5	53

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127	Carbonic Acid:â€‰ From Polyamorphism to Polymorphism. Journal of the American Chemical Society, 2007, 129, 13863-13871.	13.7	61
128	Fluctuations and phase separation in Br/Pt(110). Surface Science, 2007, 601, 4386-4389.	1.9	2
129	Chemisorption of hydrogen on the missing-row Pt(110)-(1 Ã— 2) surface. Topics in Catalysis, 2007, 46, 161-167.	2.8	22
130	The relation between high-density and very-high-density amorphous ice. Physical Chemistry Chemical Physics, 2006, 8, 2810.	2.8	35
131	Isobaric annealing of high-density amorphous ice between 0.3 and 1.9 GPa: in situ density values and structural changes. Physical Chemistry Chemical Physics, 2006, 8, 386-397.	2.8	62
132	Modeling the heterogeneous reaction probability for chlorine nitrate hydrolysis on ice. Journal of Geophysical Research, 2006, 111, .	3.3	3
133	Amorphous ices: experiments and numerical simulations. Journal of Physics Condensed Matter, 2006, 18, R919-R977.	1.8	163
134	High Density Amorphous Ice from Cubic Ice. ChemPhysChem, 2006, 7, 1203-1206.	2.1	17
135	Amorphous Ice: Stepwise Formation of Very-High-Density Amorphous Ice from Low-Density Amorphous Ice at 125ÂK. Physical Review Letters, 2006, 96, 025702.	7.8	103
136	The local and intermediate range structures of the five amorphous ices at 80K and ambient pressure: A Faber-Ziman and Bhatia-Thornton analysis. Journal of Chemical Physics, 2006, 125, 194502.	3.0	117
137	Hydrogen chloride-induced surface disordering on ice. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9422-9427.	7.1	88
138	Glass transition in hyperquenched water?. Nature, 2005, 435, E1-E1.	27.8	67
139	Liquid-like relaxation in hyperquenched water at â‰140 K. Physical Chemistry Chemical Physics, 2005, 7, 3210.	2.8	99
140	Correlation in low-dimensional electronic states on metal surfaces. New Journal of Physics, 2005, 7, 102-102.	2.9	15
141	HonPt(110): An atypical chemisorption site at low coverages. Physical Review B, 2004, 70, .	3.2	22
142	Daunomycin Intercalation Stabilizes Distinct Backbone Conformations of DNA. Journal of Biomolecular Structure and Dynamics, 2004, 21, 713-724.	3.5	24
143	Sulfurous acid (H2SO3) on Io?. Icarus, 2004, 169, 242-249.	2.5	20
144	Dynamics of DNA:â€‰ BI and BII Phosphate Backbone Transitions. Journal of Physical Chemistry B, 2004, 108, 2470-2476.	2.6	21

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145	On the Formation of the Sulfonate Ion from Hydrated Sulfur Dioxide. Journal of Physical Chemistry A, 2004, 108, 3859-3864.	2.5	35
146	Extended method for adiabatic mode reordering. Journal of Computational Chemistry, 2003, 24, 386-395.	3.3	1
147	About the Stability of Sulfurous Acid (H2SO3) and Its Dimer.. ChemInform, 2003, 34, no.	0.0	0
148	Reactions of HOBr + HCl + nH2O and HOBr + HBr + nH2O. Chemical Physics Letters, 2003, 372, 569-576.	2.6	7
149	Raman Spectroscopic Study on Hydrogen Bonding in Recovered Ice IV. Journal of Physical Chemistry B, 2003, 107, 2802-2807.	2.6	27
150	Modeling Anhydrous and Aqua Copper(II) Amino Acid Complexes:Â A New Molecular Mechanics Force Field Parametrization Based on Quantum Chemical Studies and Experimental Crystal Data. Inorganic Chemistry, 2003, 42, 2268-2279.	4.0	69
151	Toward elimination of discrepancies between theory and experiment: The gas-phase reaction of N2O5 with H2O. Physical Chemistry Chemical Physics, 2003, 5, 487-495.	2.8	27
152	The low-temperature dynamics of recovered ice XII as studied by differential scanning calorimetry: a comparison with ice V. Physical Chemistry Chemical Physics, 2003, 5, 3507.	2.8	63
153	Pure ices IV and XII from high-density amorphous ice. Canadian Journal of Physics, 2003, 81, 25-32.	1.1	37
154	Structure of a New Dense Amorphous Ice. Physical Review Letters, 2002, 89, 205503.	7.8	200
155	(Meta-)stability domain of ice XII revealed between â‰ˆ158â€“212 K and â‰ˆ0.7â€“1.5 GPa on isobaric heating of high-density amorphous ice. Journal of Chemical Physics, 2002, 116, 3171-3174.	3.0	46
156	The optimal tunneling path for the proton transfer in malonaldehyde. Journal of Chemical Physics, 2002, 117, 1962-1966.	3.0	80
157	An accurate semiclassical method to predict ground-state tunneling splittings. Journal of Chemical Physics, 2002, 117, 1967-1974.	3.0	47
158	Reactions of HOCl + HCl +nH2O and HOCl + HBr +nH2O. Journal of Physical Chemistry A, 2002, 106, 7850-7857.	2.5	19
159	Pure Ice IV from High-Density Amorphous Ice. Journal of Physical Chemistry B, 2002, 106, 5587-5590.	2.6	37
160	The Raman Spectrum of Ice XII and Its Relation to that of a New â€œHigh-Pressure Phase of H2O Iceâ€• Journal of Physical Chemistry B, 2002, 106, 1-6.	2.6	51
161	The structure, modelling and dynamics of 2,7-diisopropoxy-1,8-diarylnaphthalenes. Perkin Transactions II RSC, 2002, , 1510-1519.	1.1	26
162	Towards the Experimental Decomposition Rate of Carbonic Acid (H2CO3) in Aqueous Solution. Chemistry - A European Journal, 2002, 8, 66-73.	3.3	84

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163	About the Stability of Sulfurous Acid (H2SO3) and Its Dimer. Chemistry - A European Journal, 2002, 8, 5644-5651.	3.3	43
164	High-Density Amorphous Ice and its Phase Transition to Ice XII. , 2002, , 325-333.		3
165	A second distinct structural â€œstateâ€•of high-density amorphous ice at 77 K and 1 bar. Physical Chemistry Chemical Physics, 2001, 3, 5355-5357.	2.8	296
166	The structure, modelling and dynamics of hindered 5,6-diarylacenaphthenes. Perkin Transactions II RSC, 2001, , 459-467.	1.1	17
167	Water-Mediated Proton Transfer:Â A Mechanistic Investigation on the Example of the Hydration of Sulfur Oxides. Journal of Physical Chemistry A, 2001, 105, 5137-5145.	2.5	69
168	The Reaction Rate Constant of Chlorine Nitrate Hydrolysis. Chemistry - A European Journal, 2001, 7, 1662-1669.	3.3	11
169	Prediction of the structure of human Janus kinase 2 (JAK2) comprising the two carboxy-terminal domains reveals a mechanism for autoregulation. Protein Engineering, Design and Selection, 2001, 14, 27-37.	2.1	154
170	On the Surprising Kinetic Stability of Carbonic Acid (H2CO3). Angewandte Chemie - International Edition, 2000, 39, 891-894.	13.8	152
171	Toward elimination of discrepancies between theory and experiment: The rate constant of the atmospheric conversion of SO3 to H2SO4. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 8874-8878.	7.1	91
172	On the competing hydrations of sulfur dioxide and sulfur trioxide in our atmosphere. Chemical Communications, 2000, , 999-1000.	4.1	25
173	Temperature-Dependent Ways of Proton TransferA Benchmark Study on Cyclic HF Oligomers. Journal of Physical Chemistry A, 1999, 103, 9022-9028.	2.5	8
174	Predictions of rate constants and estimates for tunneling splittings of concerted proton transfer in small cyclic water clusters. Journal of Chemical Physics, 1998, 109, 2672-2679.	3.0	57
175	Toward Elimination of Discrepancies between Theory and Experiment:â€‰ Double Proton Transfer in Dimers of Carboxylic Acids. Journal of the American Chemical Society, 1998, 120, 12595-12600.	13.7	72
176	Large Curvature Tunneling Effects Reveal Concerted Hydrogen Exchange Rates in Cyclic Hydrogen Fluoride Clusters Comparable to Carboxylic Acid Dimers. Journal of the American Chemical Society, 1998, 120, 404-412.	13.7	29
177	Pressure-annealed high-density amorphous ice made from vitrified water droplets: A systematic calorimetry study on water's second glass transition. Journal of Chemical Physics, 0, , .	3.0	4