Roger A Klein

List of Publications by Year
in descending order

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48	3,980	279798 23	214800 47
papers	citations	h-index	g-index

50	50	50	4350
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie, 2015, 127, 2636-2638.	2.0	17
2	Improved General Understanding of the Hydrogenâ€Bonding Phenomena: A Reply. Angewandte Chemie - International Edition, 2015, 54, 2600-2602.	13.8	42
3	Antiâ€Electrostatic Hydrogen Bonds. Angewandte Chemie - International Edition, 2014, 53, 11214-11217.	13.8	171
4	What is a hydrogen bond? Resonance covalency in the supramolecular domain. Chemistry Education Research and Practice, 2014, 15, 276-285.	2.5	97
5	What is a hydrogen bond? Mutually consistent theoretical and experimental criteria for characterizing H-bonding interactions. Molecular Physics, 2012, 110, 565-579.	1.7	195
6	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
7	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
8	Crystalline ethane-1,2-diol does not have intra-molecular hydrogen bonding: Experimental and theoretical charge density studies. Journal of Molecular Structure, 2010, 964, 126-133.	3.6	66
9	Pople versus Dunning basis-sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standard. Chemical Physics Letters, 2006, 419, 254-258.	2.6	24
10	Single point calculations using geometries derived at a lower level of theory: Caveats to be observed in using compound levels of theory or â€˜double-barrellingâ€™. Chemical Physics Letters, 2006, 423, 413-416.	2.6	3
11	Modified van der Waals atomic radii for hydrogen bonding based on electron density topology. Chemical Physics Letters, 2006, 425, 128-133.	2.6	71
12	Hydrogen bonding in strained cyclic vicinal diols: The birth of the hydrogen bond. Chemical Physics Letters, 2006, 429, 633-637.	2.6	48
13	Reply to the comment on â€˜Pople versus Dunning basis-sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standardâ€™ by R.A. Klein and M.A. Zottola [Chem. Phys. Lett. 419 (2006) 254â€“258]. Chemical Physics Letters, 2006, 430, 464-465.	2.6	1
14	Lack of intramolecular hydrogen bonding in glucopyranose: Vicinal hydroxyl groups exhibit negative cooperativity. Chemical Physics Letters, 2006, 433, 165-169.	2.6	24
15	Re-examination of the Solvolysis of Acyl Chlorides. Rethinking the Role of Both Carbonyl and Chloride. Journal of Physical Chemistry A, 2004, 108, 9328-9330.	2.5	2
16	Ab Initio Calculations of17O NMR-Chemical Shifts for Water. The Limits of PCM Theory and the Role of Hydrogen-Bond Geometry and Cooperativity. Journal of Physical Chemistry A, 2004, 108, 5851-5863.	2.5	70
17	Barriers to internal rotation around the Câ€“N bond in 3-(o-aryl)-5-methyl-rhodanines using NMR spectroscopy and computational studies. Electron density topological analysis of the transition states. Organic and Biomolecular Chemistry, 2004, 2, 2426-2436.	2.8	14
18	Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. Journal of Computational Chemistry, 2003, 24, 1120-1131.	3.3	79

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19	Electron Density Topological Analysis of Hydrogen Bonding in Glucopyranose and Hydrated Glucopyranose. Journal of the American Chemical Society, 2002, 124, 13931-13937.	13.7	110
20	Ab initio conformational studies on diols and binary diol-water systems using DFT methods. Intramolecular hydrogen bonding and 1:1 complex formation with water. Journal of Computational Chemistry, 2002, 23, 585-599.	3.3	104
21	Binary Diolâ^'Water Systems Studied by 17O Nuclear Magnetic Resonance Spectroscopy. Interpretation of the Effect of Diol Structure on 17O-Water Chemical Shift. Formation of Networks of Water Molecules Stabilized by Weak Câ^'HÂ·Â·Â·O Interactions. Journal of Physical Chemistry A, 2001, 105, 9298-9304.	2.5	10
22	The critical role of force-fields in property prediction. New Journal of Chemistry, 1999, 23, 153-164.	2.8	22
23	Aspects of conformational mobility in charged oligosaccharides. Computational and Theoretical Chemistry, 1997, 395-396, 313-332.	1.5	1
24	UNIQUAC interaction parameters for molecules with î—¸OH group on adjacent carbon atoms in aqueous solution determined by molecular mechanicsâ€"glycols, glycerol and glucose. Fluid Phase Equilibria, 1997, 132, 117-137.	2.5	35
25	UNIQUAC interaction parameters for alkane/amine systems determined by Molecular Mechanics. Fluid Phase Equilibria, 1996, 115, 59-72.	2.5	21
26	The aqueous solution structure of a lipoteichoic acid from Streptococcus pneumoniae strain R6 containing 2,4-diamino-2,4,6-trideoxy-galactose: evidence for conformational mobility of the galactopyranose ring. Carbohydrate Research, 1996, 281, 79-98.	2.3	26
27	The aqueous solution structure of the tetrasaccharide-ribitol repeat-unit from the lipoteichoic acid of Streptococcus pneumoniae strain R6 determined using a combination of NMR spectroscopy and computer calculations. Carbohydrate Research, 1994, 256, 189-222.	2.3	18
28	Reporter resonances in the NMR spectra of oligosaccharides containing sialic acid linked to galactopyranose rings. Carbohydrate Research, 1994, 254, 289-294.	2.3	19
29	Isolation and Structural Characterization of Sialic Acid-Containing Glycopeptides of the O-GlycosidicType from the Urine of Two Patients with an Hereditary Deliciency in Î±-N-Acetylgalactosaminidase Activity. Biological Chemistry Hoppe-Seyler, 1989, 370, 661-672.	1.4	46
30	MS and NMR analysis of the cross-reacting determinant glycan from Trypanosoma brucei brucei MITat 1.6 variant specific glycoprotein. Biochemical and Biophysical Research Communications, 1987, 146, 1055-1063.	2.1	38
31	Lectin interactions with the variant surface glycoprotein from Trypanosoma brucei brucei incorporated into liposomes. Biochemical and Biophysical Research Communications, 1986, 141, 1274-1278.	2.1	4
32	The trypanocidal activity of bromoacetyl-<scp>l</scp>-carnitine and Î±-difluoromethylornithine in Trypanosoma brucei brucei infected rats. Biochemical Society Transactions, 1986, 14, 1093-1094.	3.4	0
33	Mass spectrometric localization of carbon-carbon double bonds: A critical review of recent methods. Chemistry and Physics of Lipids, 1986, 39, 285-311.	3.2	60
34	Double bond location in fatty acids. A critical analysis of the feasibility of using specifically deuterated pyrrolidides for mass spectral analysis. Biological Mass Spectrometry, 1986, 13, 429-437.	0.5	6
35	A study of the membrane attachment site of the membrane-form variant surface glycoprotein from Trypanosoma brucei brucei using lipid vesicles as a model of the plasma membrane. Molecular and Biochemical Parasitology, 1986, 20, 191-197.	1.1	13
36	Threonine uptake in Trypanosoma brucei. Molecular and Biochemical Parasitology, 1984, 11, 215-223.	1.1	3

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37	Pyruvate kinase: A carnitine regulated site of ATP production in Trypanosoma brucei brucei. Comparative Biochemistry and Physiology Part B: Comparative Biochemistry, 1984, 78, 595-599.	0.2	8
38	The measurement of motility in micro-organisms and its biochemical significance. Biochemical Society Transactions, 1984, 12, 627-630.	3.4	0
39	The role of threonine in the metabolism of acetyl coenzyme A by Trypanosoma brucei brucei. Comparative Biochemistry and Physiology Part B: Comparative Biochemistry, 1983, 74, 277-281.	0.2	12
40	Bromoacetyl-l-carnitine: Biochemical and antitrypanosomal actions against Trypanosoma brucei brucei. Biochemical Pharmacology, 1983, 32, 3447-3451.	4.4	11
41	Characterization of DNA and protein synthesis in Trypanosoma brucei by using inhibitors. Biochemical Society Transactions, 1983, 11, 366-367.	3.4	6
42	The Movement of Molecules Across Membranes: The Thermodynamic Analysis of the Dependence on Structure, Pressure, and Temperature. , 1983, , 301-317.		1
43	Thermodynamics and membrane processes. Quarterly Reviews of Biophysics, 1982, 15, 667-759.	5.7	28
44	Carnitine stimulates ATP synthesis in Trypanosoma brucei brucei. FEBS Letters, 1982, 141, 271-274.	2.8	8
45	The use of 13-methyltetradecanoic acid as an indicator of adipose tissue turnover. Lipids, 1980, 15, 572-579.	1.7	24
46	Stereospecificity of the threonine dehydrogenase from bloodstream Trypanosoma brucei. Comparative Biochemistry and Physiology Part B: Comparative Biochemistry, 1980, 66, 143-146.	0.2	1
47	Threonine as a Preferred Source of 2-Carbon Units for Lipid Synthesis in Trypanosoma brucei. Biochemical Society Transactions, 1976, 4, 48-50.	3.4	27
48	The Enzymic Hydrolysis of Acetyl-Coenzyme A by Trypanosomatid Flagellates. Biochemical Society Transactions, 1976, 4, 285-287.	3.4	13