Ernst-Walter Knapp

List of Publications by Year
in descending order

169 papers	7,668 citations	47006 47 h-index	62596 80 g-index
176 all docs	176 docs citations	176 times ranked	7095 citing authors

#	Article	IF	Citations
1	Quantification of Local Electric Field Changes at the Active Site of Cytochrome c Oxidase by Fourier Transform Infrared Spectroelectrochemical Titrations. Frontiers in Chemistry, 2021, 9, 669452.	3.6	4
2	Beating Heart of Cytochrome c Oxidase: The Shared Proton of Heme a₃ Propionates. Journal of Physical Chemistry B, 2021, 125, 9668-9677.	2.6	5
3	The redox-coupled proton-channel opening in cytochrome c oxidase. Chemical Science, 2020, 11, 3804-3811.	7.4	6
4	Empirical Conversion of pK_a Values between Different Solvents and Interpretation of the Parameters: Application to Water, Acetonitrile, Dimethyl Sulfoxide, and Methanol. ACS Omega, 2018, 3, 1653-1662.	3.5	92
5	Protonation equilibria of transition metal complexes: From model systems toward the Mn-complex in photosystem II. Coordination Chemistry Reviews, 2017, 345, 16-30.	18.8	15
6	Structural and Vibrational Characterization of the Chromophore Binding Site of Bacterial Phytochrome Agp1. Photochemistry and Photobiology, 2017, 93, 713-723.	2.5	16
7	Influence of Heterogeneity on the Ultrafast Photoisomerization Dynamics of Pfr in Cph1 Phytochrome. Photochemistry and Photobiology, 2017, 93, 703-712.	2.5	13
8	Protonation-State-Dependent Communication in Cytochrome c Oxidase. Biophysical Journal, 2017, 113, 817-828.	0.5	6
9	Redox induced protonation of heme propionates in cytochrome c oxidase: Insights from surface enhanced resonance Raman spectroscopy and QM/MM calculations. Biochimica Et Biophysica Acta - Bioenergetics, 2017, 1858, 103-108.	1.0	15
10	Merging Structural Information from X-ray Crystallography, Quantum Chemistry, and EXAFS Spectra: The Oxygen-Evolving Complex in PSII. Journal of Physical Chemistry B, 2016, 120, 10899-10922.	2.6	16
11	Proton solvation in protic and aprotic solvents. Journal of Computational Chemistry, 2016, 37, 1082-1091.	3.3	53
12	Computing pK_a Values in Different Solvents by Electrostatic Transformation. Journal of Chemical Theory and Computation, 2016, 12, 3360-3369.	5.3	28
13	Chemically Realistic Tetrahedral Lattice Models for Polymer Chains: Application to Polyethylene Oxide. Journal of Chemical Theory and Computation, 2016, 12, 2388-2400.	5.3	1
14	Câ€“H/O Interactions of Aromatic CH Donors within Proteins: A Crystallographic Study. Crystal Growth and Design, 2016, 16, 1948-1957.	3.0	19
15	pK_A in proteins solving the <scp>P</scp>oissonâ€“<scp>B</scp>oltzmann equation with finite elements. Journal of Computational Chemistry, 2015, 36, 2147-2157.	3.3	6
16	ProPairs: A Data Set for Proteinâ€“Protein Docking. Journal of Chemical Information and Modeling, 2015, 55, 1495-1507.	5.4	12
17	Mechanical Rupture of Mono- and Bivalent Transition Metal Complexes in Experiment and Theory. Journal of Physical Chemistry C, 2015, 119, 4333-4343.	3.1	9
18	Optimized distance-dependent atom-pair-based potential DOOP for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2015, 83, 881-890.	2.6	11

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19	pK_a Values in Proteins Determined by Electrostatics Applied to Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2015, 11, 2827-2840.	5.3	38
20	Computing pK_A values of hexaâ€aqua transition metal complexes. Journal of Computational Chemistry, 2015, 36, 69-78.	3.3	26
21	Models for Selfâ€Avoiding Polymer Chains on the Tetrahedral Lattice. Macromolecular Theory and Simulations, 2014, 23, 452-463.	1.4	1
22	Proton Transfer in the K-Channel Analog of B-Type Cytochrome c Oxidase from Thermus thermophilus. Biophysical Journal, 2014, 107, 2177-2184.	0.5	19
23	mFES: A Robust Molecular Finite Element Solver for Electrostatic Energy Computations. Journal of Chemical Theory and Computation, 2014, 10, 5095-5112.	5.3	16
24	Lysine 362 in cytochrome c oxidase regulates opening of the K-channel via changes in p K A and conformation. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1998-2003.	1.0	24
25	Reprint of PSII Manganese Cluster: Protonation of W2, O5, O4 and His337 in the S1 state explored by combined quantum chemical and electrostatic energy computations. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1389-1394.	1.0	7
26	Database of protein complexes with multivalent binding ability: Bivalâ€bind. Proteins: Structure, Function and Bioinformatics, 2014, 82, 744-751.	2.6	10
27	Protein Secondary Structure Classification Revisited: Processing DSSP Information with PSSC. Journal of Chemical Information and Modeling, 2014, 54, 2166-2179.	5.4	30
28	PSII manganese cluster: Protonation of W2, O5, O4 and His337 in the S1 state explored by combined quantum chemical and electrostatic energy computations. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1316-1321.	1.0	18
29	Exploring the Possible Role of Glu286 in CcO by Electrostatic Energy Computations Combined with Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 12432-12441.	2.6	33
30	Geometry motivated alternative view on local protein backbone structures. Protein Science, 2013, 22, 1669-1674.	7.6	8
31	Understanding Selectin Counter-Receptor Binding from Electrostatic Energy Computations and Experimental Binding Studies. Journal of Physical Chemistry B, 2013, 117, 16443-16454.	2.6	15
32	Oxygen-Evolving Mn Cluster in Photosystem II: The Protonation Pattern and Oxidation State in the High-Resolution Crystal Structure. Journal of the American Chemical Society, 2012, 134, 7442-7449.	13.7	158
33	Balanced and Bias-Corrected Computation of Conformational Entropy Differences for Molecular Trajectories. Journal of Chemical Theory and Computation, 2012, 8, 1235-1245.	5.3	30
34	Protein Secondary Structure Prediction with SPARROW. Journal of Chemical Information and Modeling, 2012, 52, 545-556.	5.4	21
35	Multivalency as a Chemical Organization and Action Principle. Angewandte Chemie - International Edition, 2012, 51, 10472-10498.	13.8	854
36	Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. Journal of Physical Chemistry A, 2012, 116, 6885-6893.	2.5	11

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37	Influence of Spacerâ€“Receptor Interactions on the Stability of Bivalent Ligandâ€“Receptor Complexes. Journal of Physical Chemistry B, 2012, 116, 2595-2604.	2.6	31
38	Can oxidation states and the protonation pattern of oxomanganese complexes be recognized from their structures?. CrystEngComm, 2011, 13, 6369.	2.6	24
39	Rubredoxin Function: Redox Behavior from Electrostatics. Journal of Chemical Theory and Computation, 2011, 7, 742-752.	5.3	18
40	Recent advances in anionâ€“Ï€ interactions. CrystEngComm, 2011, 13, 3293.	2.6	144
41	Charge Transport in the ClC-type Chloride-Proton Anti-porter from Escherichia coli. Journal of Biological Chemistry, 2011, 286, 2976-2986.	3.4	17
42	DemQSAR: predicting human volume of distribution and clearance of drugs. Journal of Computer-Aided Molecular Design, 2011, 25, 1121-1133.	2.9	25
43	Prediction using step-wise L1, L2 regularization and feature selection for small data sets with large number of features. BMC Bioinformatics, 2011, 12, 412.	2.6	60
44	Electrostatic pK_a computations in proteins: Role of internal cavities. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3320-3332.	2.6	24
45	Multivalent Binding of Formin-binding Protein 21 (FBP21)-Tandem-WW Domains Fosters Protein Recognition in the Pre-spliceosome. Journal of Biological Chemistry, 2011, 286, 38478-38487.	3.4	25
46	STRATEGIES OF NON-SEQUENTIAL PROTEIN STRUCTURE ALIGNMENTS. , 2010, , .		1
47	Understanding Properties of Cofactors in Proteins: Redox Potentials of Synthetic Cytochromes b. ChemPhysChem, 2010, 11, 1196-1206.	2.1	12
48	Predicting protein complex geometries with a neural network. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1026-1039.	2.6	19
49	Circular permuted proteins in the universe of protein folds. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1618-1630.	2.6	13
50	GIS: a comprehensive source for protein structure similarities. Nucleic Acids Research, 2010, 38, W46-W52.	14.5	6
51	Exploring classification strategies with the CoEPrA 2006 contest. Bioinformatics, 2010, 26, 603-609.	4.1	33
52	Merging Implicit with Explicit Solvent Simulations: Polyethylene Glycol. Journal of Chemical Theory and Computation, 2010, 6, 1871-1883.	5.3	8
53	Statistical Mechanics of the Stability of Multivalent Ligandâ^'Receptor Complexes. Journal of Physical Chemistry C, 2010, 114, 5287-5304.	3.1	28
54	Accurate redox potentials of mononuclear iron, manganese, and nickel model complexes*. Journal of Computational Chemistry, 2009, 30, 203-211.	3.3	47

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55	Energetics of the loopâ€toâ€helix transition leading to the coiledâ€coil structure of influenza virus hemagglutinin HA2 subunits. Proteins: Structure, Function and Bioinformatics, 2009, 74, 291-303.	2.6	17
56	Bound Ligand Conformer Revealed by Flexible Structure Alignment in Absence of Crystal Structures: Indirect Drug Design Probed for HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2009, 5, 659-673.	5.3	0
57	Symmetric Structures in the Universe of Protein Folds. Journal of Chemical Information and Modeling, 2009, 49, 2147-2151.	5.4	16
58	Understanding Rubredoxin Redox Potentials: Role of H-Bonds on Model Complexes. Journal of Chemical Theory and Computation, 2009, 5, 2898-2908.	5.3	17
59	Optimizing pK_A computation in proteins with pH adapted conformations. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1335-1348.	2.6	123
60	Improved pK_a prediction: Combining empirical and semimicroscopic methods. Journal of Computational Chemistry, 2008, 29, 2575-2581.	3.3	33
61	Combined NMR and computational study for azide binding to human manganese superoxide dismutase. Solid State Nuclear Magnetic Resonance, 2008, 34, 6-13.	2.3	9
62	Novel protein folds and their nonsequential structural analogs. Protein Science, 2008, 17, 1374-1382.	7.6	58
63	Statistical Thermodynamics of the Stability of Multivalent Ligand-Receptor Complexes. Physical Review Letters, 2008, 100, 178101.	7.8	48
64	Superimpose: a 3D structural superposition server. Nucleic Acids Research, 2008, 36, W47-W54.	14.5	31
65	3P-271 Exploring the energetics of electron transfer events in photosynthetic reaction centers by electrostatic energy computations(The 46th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2008, 48, S169.	0.1	0
66	The Influence of Aspartate 575PsaBon the Midpoint Potentials of Phylloquinones A1A/A1Band the Fx Iron-Sulfur Cluster in Photosystem I. , 2008, , 101-104.		0
67	Sampling geometries of protein-protein complexes. Genome Informatics, 2008, 20, 260-9.	0.4	1
68	Î±-Helices direct excitation energy flow in the Fennaâ€“Matthewsâ€“Olson protein. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 16862-16867.	7.1	183
69	CONFORMATIONAL ENTROPY OF BIOMOLECULES: BEYOND THE QUASI-HARMONIC APPROXIMATION. , 2007, , .		32
70	Contributions of the Protein Environment to the Midpoint Potentials of the A₁ Phylloquinones and the F_X Ironâ^'Sulfur Cluster in Photosystem I. Biochemistry, 2007, 46, 10804-10816.	2.5	28
71	Protonation States of Ammonia/Ammonium in the Hydrophobic Pore of Ammonia Transporter Protein AmtB. Journal of the American Chemical Society, 2007, 129, 1210-1215.	13.7	41
72	Function of two Î²-carotenes near the D1 and D2 proteins in photosystem II dimers. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 79-87.	1.0	30

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73	Redox potential of the non-heme iron complex in bacterial photosynthetic reaction center. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 1300-1309.	1.0	8
74	EVALUATION OF SEQUENCE ALIGNMENTS OF DISTANTLY RELATED SEQUENCE PAIRS WITH RESPECT TO STRUCTURAL SIMILARITY. , 2007, , .		0
75	Conformational entropy of biomolecules: beyond the quasi-harmonic approximation. Genome Informatics, 2007, 18, 192-205.	0.4	19
76	How photosynthetic reaction centers control oxidation power in chlorophyll pairs P680, P700, and P870. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9855-9860.	7.1	104
77	Electrostatic Influence of PsaC Protein Binding to the PsaA/PsaB Heterodimer in Photosystem I. Biophysical Journal, 2006, 90, 1081-1089.	0.5	26
78	Function of Redox-Active Tyrosine in Photosystem II. Biophysical Journal, 2006, 90, 3886-3896.	0.5	58
79	Energetics of a Possible Proton Exit Pathway for Water Oxidation in Photosystem II. Biochemistry, 2006, 45, 2063-2071.	2.5	167
80	Electrostatic role of the non-heme iron complex in bacterial photosynthetic reaction center. FEBS Letters, 2006, 580, 4567-4570.	2.8	15
81	Stability and fluctuations of amide hydrogen bonds in a bacterial cytochrome c: a molecular dynamics study. Journal of Biological Inorganic Chemistry, 2006, 11, 26-40.	2.6	24
82	Connectivity independent protein-structure alignment: a hierarchical approach. BMC Bioinformatics, 2006, 7, 510.	2.6	48
83	Cationic State of Accessory Chlorophyll and Electron Transfer through Pheophytin to Plastoquinone in Photosystem II. Angewandte Chemie - International Edition, 2006, 45, 1964-1965.	13.8	21
84	Computational studies on imidazole heme conformations. Journal of Biological Inorganic Chemistry, 2005, 10, 343-354.	2.6	36
85	Induced conformational changes upon Cd2+ binding at photosynthetic reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16215-16220.	7.1	22
86	Energetics of Proton Transfer Pathways in Reaction Centers from Rhodobacter sphaeroides. Journal of Biological Chemistry, 2005, 280, 12446-12450.	3.4	24
87	Redox Potentials of Chlorophylls in the Photosystem II Reaction Centerâ€. Biochemistry, 2005, 44, 4118-4124.	2.5	80
88	Control of Quinone Redox Potentials in Photosystem II:Â Electron Transfer and Photoprotection. Journal of the American Chemical Society, 2005, 127, 14714-14720.	13.7	93
89	Oxidation of the Non-Heme Iron Complex in Photosystem II. Biochemistry, 2005, 44, 14772-14783.	2.5	31
90	Role of Ions on Structure and Stability of a Synthetic Gramicidin Ion Channel in Solution. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2005, 109, 10441-10448.	2.6	1

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91	Redox Potentials of Chlorophylls and Î²-Carotene in the Antenna Complexes of Photosystem II. Journal of the American Chemical Society, 2005, 127, 1963-1968.	13.7	23
92	Tuning electron transfer by ester-group of chlorophylls in bacterial photosynthetic reaction center. FEBS Letters, 2005, 579, 712-716.	2.8	20
93	Redox potential of cytochrome c550 in the cyanobacterium Thermosynechococcus elongates. FEBS Letters, 2005, 579, 3190-3194.	2.8	25
94	One-Electron Reduction Potential for Oxygen- and Sulfur-Centered Organic Radicals in Protic and Aprotic Solvents. Journal of the American Chemical Society, 2005, 127, 15730-15737.	13.7	62
95	Problems Evaluating Energetics of Electron Transfer from QA to QB: The Light-Exposed and Dark-Adapted Bacterial Reaction Center. ACS Symposium Series, 2004, , 71-92.	0.5	3
96	Accurate pKa Determination for a Heterogeneous Group of Organic Molecules. ChemPhysChem, 2004, 5, 1513-1522.	2.1	103
97	A molecular docking study of estrogenically active compounds with 1,2-diarylethane and 1,2-diarylethene pharmacophores. Bioorganic and Medicinal Chemistry, 2004, 12, 6527-6537.	3.0	31
98	A Kunitz type protease inhibitor related protein is synthesized in Drosophila prepupal salivary glands and released into the moulting fluid during pupation. Insect Biochemistry and Molecular Biology, 2004, 34, 855-869.	2.7	22
99	Variation of Ser-L223 Hydrogen Bonding with the QB Redox State in Reaction Centers from Rhodobacter sphaeroides. Journal of the American Chemical Society, 2004, 126, 8059-8064.	13.7	55
100	Unfolding of the cold shock protein studied with biased molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2003, 53, 597-606.	2.6	20
101	Redox Potential of Quinones in Photosynthetic Reaction Centers fromRhodobacter sphaeroides:â€‰ Dependence on Protonation of Glu-L212 and Asp-L213. Biochemistry, 2003, 42, 3882-3892.	2.5	54
102	Tuning Heme Redox Potentials in the Cytochrome c Subunit of Photosynthetic Reaction Centers. Journal of Biological Chemistry, 2003, 278, 51993-52001.	3.4	65
103	Redox Potential of Quinones in Both Electron Transfer Branches of Photosystem I. Journal of Biological Chemistry, 2003, 278, 52002-52011.	3.4	103
104	Energetics of Radical Transfer in DNA Photolyase. Journal of the American Chemical Society, 2002, 124, 3775-3782.	13.7	59
105	Driving Forces of Protein Association: The Dimer-Octamer Equilibrium in Arylsulfatase A. Biophysical Journal, 2002, 83, 3066-3078.	0.5	13
106	Protonation and Stability of the Globular Domain of Influenza Virus Hemagglutinin. Biophysical Journal, 2002, 82, 1050-1058.	0.5	60
107	Artificial Cytochromeb:Â Computer Modeling and Evaluation of Redox Potentials. Journal of the American Chemical Society, 2001, 123, 6040-6053.	13.7	49
108	Calculated pH-Dependent Population and Protonation of Carbon-Monoxy-Myoglobin Conformers. Biophysical Journal, 2001, 80, 1141-1150.	0.5	144

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109	Factors Determining the Orientation of Axially Coordinated Imidazoles in Heme Proteinsâ€. Biochemistry, 2001, 40, 7914-7928.	2.5	60
110	The X-ray absorption spectroscopy Debye-Waller factors of an iron compound and of met-myoglobin as a function of temperature. European Biophysics Journal, 2001, 30, 393-403.	2.2	16
111	How to guarantee optimal stability for most representative structures in the protein data bank. Proteins: Structure, Function and Bioinformatics, 2001, 44, 79-96.	2.6	109
112	Negative solubility coefficient of methylated cyclodextrins in water: A theoretical study. Chemical Physics Letters, 2001, 336, 504-510.	2.6	46
113	Structural alignment of ferredoxin and flavodoxin based on electrostatic potentials: Implications for their interactions with photosystem I and ferredoxin-NADP reductase. , 2000, 38, 301-309.		40
114	Metal Ligand Aromatic Cationâ€“Ï€ Interactions in Metalloproteins: Ligands Coordinated to Metal Interact with Aromatic Residues. Chemistry - A European Journal, 2000, 6, 3935-3942.	3.3	120
115	Diffusion of water molecules in crystalline Î²-cyclodextrin hydrates. Journal of Molecular Graphics and Modelling, 2000, 18, 143-152.	2.4	22
116	A statistical mechanical method to optimize energy functions for protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 3977-3981.	7.1	51
117	The Deacylation Step of Acetylcholinesterase:Â Computer Simulation Studies. Journal of the American Chemical Society, 2000, 122, 12254-12262.	13.7	48
118	Electron Transfer between the Quinones in the Photosynthetic Reaction Center and Its Coupling to Conformational Changesâ€. Biochemistry, 2000, 39, 10487-10496.	2.5	110
119	Structural alignment of ferredoxin and flavodoxin based on electrostatic potentials: Implications for their interactions with photosystem I and ferredoxinâ€NADP reductase. Proteins: Structure, Function and Bioinformatics, 2000, 38, 301-309.	2.6	3
120	Simulation of oligopeptide folding or how do residues talk. , 1999, , .		0
121	Electrostatic models for computing protonation and redox equilibria in proteins. European Biophysics Journal, 1999, 28, 533-551.	2.2	250
122	Calculation of protonation patterns in proteins with structural relaxation and molecular ensembles - application to the photosynthetic reaction center. European Biophysics Journal, 1998, 27, 626-637.	2.2	80
123	Energetics of Electron-Transfer and Protonation Reactions of the Quinones in the Photosynthetic Reaction Center ofRhodopseudomonas viridisâ€. Biochemistry, 1998, 37, 2488-2495.	2.5	104
124	An energy function for dynamics simulations of polypeptides in torsion angle space. Journal of Chemical Physics, 1998, 108, 8264-8276.	3.0	13
125	Folding Pathways of a Helixâˆ’Turnâˆ’Helix Model Protein. Journal of Physical Chemistry B, 1997, 101, 6734-6740.	2.6	23
126	Comparison of the Physiologically Equivalent Proteins Cytochrome c6 and Plastocyanin on the Basis of Their Electrostatic Potentials. Tryptophan 63 in Cytochrome c6 May Be Isofunctional with Tyrosine 83 in Plastocyanin. Biochemistry, 1997, 36, 16187-16196.	2.5	53

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127	Computational Simulation and Analysis of Dynamic Association between Plastocyanin and Cytochrome f. Consequences for the Electron-Transfer Reaction. Journal of the American Chemical Society, 1997, 119, 42-52.	13.7	129
128	Structural fluctuations of myoglobin from normal-modes, MÃ¶ssbauer, Raman, and absorption spectroscopy. Biophysical Journal, 1996, 70, 2092-2099.	0.5	93
129	Free Energy Computations on the Shift of the Special Pair Redox Potential:Â Mutants of the Reaction Center ofRhodobacter sphaeroides. Journal of the American Chemical Society, 1996, 118, 3743-3752.	13.7	31
130	Temperature dependent inelastic X-ray scattering of synchrotron radiation on myoglobin analyzed by the MÃ¶ssbauer effect. European Biophysics Journal, 1996, 25, 43-46.	2.2	21
131	Diffusion of two different water models and thermal conductivity in a protein?water system. International Journal of Quantum Chemistry, 1996, 59, 271-279.	2.0	5
132	Polypeptide folding with off-lattice Monte Carlo dynamics: the method. European Biophysics Journal, 1996, 24, 387-403.	2.2	43
133	Protein dynamics with off-lattice Monte Carlo moves. Physical Review E, 1996, 53, 4221-4224.	2.1	24
134	Off-lattice Monte Carlo method with constraints: Long-time dynamics of a protein model without nonbonded interactions. Journal of Computational Chemistry, 1993, 14, 19-29.	3.3	21
135	MÃ¶ssbauer investigations on glass-forming organic liquids. Hyperfine Interactions, 1992, 70, 1125-1128.	0.5	2
136	Long time dynamics of a polymer with rigid body monomer units relating to a protein model: Comparison with the rouse model. Journal of Computational Chemistry, 1992, 13, 793-798.	3.3	18
137	A unified theory of electron transfer and internal conversion based on solitary electronic states. Journal of Chemical Physics, 1989, 90, 354-365.	3.0	11
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139	Dynamics of hierarchical Brownian oscillators. Physical Review B, 1988, 38, 9474-9482.	3.2	0
140	Continuous-time random walks on a long-range hierarchical model. Physical Review B, 1988, 38, 6774-6778.	3.2	4
141	Relaxation in Self-Similar Hierarchical Spaces. Physical Review Letters, 1988, 60, 2386-2389.	7.8	11
142	Equivalence of dynamics in ultrametric and hierarchical spaces. Physical Review B, 1988, 38, 2664-2668.	3.2	5
143	Reply to â€˜â€˜Comment on: â€˜Cytochrome oxidation in bacterial photosynthesisâ€™â€‰â€™. Journal of Chemical Physics, 1988, 89, 3394-3395.	3.0	6
144	Electron transfer and protein dynamics. Journal of Chemical Physics, 1987, 87, 3880-3887.	3.0	34

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145	Analysis of optical spectra from single crystals of Rhodopseudomonas viridis reaction centers. Proceedings of the National Academy of Sciences of the United States of America, 1985, 82, 8463-8467.	7.1	145
146	Correlation of structural and spectroscopic properties of a photosynthetic reaction center. Chemical Physics Letters, 1985, 119, 1-4.	2.6	72
147	Recombination of radicals in solution. A theoretical study on the influence of twoâ€•and manyâ€•site hopping on the microwave field effect. Journal of Chemical Physics, 1985, 83, 2913-2922.	3.0	1
148	Vibrational line shapes in liquids. The role of resonant intermolecular coupling. Journal of Chemical Physics, 1984, 81, 643-652.	3.0	40
149	The interdependence of small linewidth and frequency changes of a vibration in liquid mixtures of CDCl3and CCl4. Journal of Chemical Physics, 1984, 81, 3774-3778.	3.0	24
150	Exciton-phonon self-trapping: A continuous transition. Chemical Physics Letters, 1984, 106, 191-196.	2.6	28
151	Two-site-hopping time correlation functions. Application to radical pair recombination. Chemical Physics Letters, 1984, 110, 259-264.	2.6	3
152	Exchange narrowing of correlated inhomogeneities. The dimer lineshape. Chemical Physics Letters, 1984, 103, 479-483.	2.6	18
153	On the lineshapes of vibronically resolved molecular aggregate spectra. application to pseudoisocyanin (PIC). Chemical Physics Letters, 1984, 111, 481-486.	2.6	93
154	Analysis of the optical absorption spectra of diradical oligomers in diacetylene crystals. Chemical Physics, 1984, 84, 321-331.	1.9	10
155	A consistent picture of protein dynamics.. Proceedings of the National Academy of Sciences of the United States of America, 1984, 81, 7088-7092.	7.1	162
156	The influence of protein dynamics on MÃ¶ssbauer spectra. Journal of Chemical Physics, 1983, 78, 4701-4711.	3.0	93
157	The concentration dependence of the vibrational linewidth and shift in liquid binary mixtures: An analytical model. Journal of Chemical Physics, 1982, 76, 4730-4735.	3.0	97
158	Protein dynamics. Journal of Molecular Biology, 1982, 161, 177-194.	4.2	357
159	On the theory of homogeneous and inhomogeneous line broadening. An exactly solvable model. Journal of Chemical Physics, 1981, 74, 89-95.	3.0	68
160	Concentration dependence of the vibrational energy relaxation of O2 in liquid mixtures. Chemical Physics, 1981, 63, 203-208.	1.9	5
161	Proton conduction in linear hydrogen-bonded systems. Chemical Physics, 1980, 46, 215-229.	1.9	53
162	Magnetic field effect on the hyperfineâ€•induced electron spin motion in radicals undergoing diamagneticâ€“paramagnetic exchange. Journal of Chemical Physics, 1979, 71, 1878-1883.	3.0	80

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163	Vibrational dephasing of diatomic molecules in liquids: role of anharmonicity of the diatom. Chemical Physics Letters, 1978, 58, 221-224.	2.6	14
164	Vibrational energy relaxation of diatomic molecules isolated in rareâ€gas matrices: Role of orientational motions. Journal of Chemical Physics, 1978, 68, 4056-4065.	3.0	54
165	Quantumâ€mechanical treatment of collisionâ€induced dissociation. Journal of Chemical Physics, 1977, 67, 4969-4975.	3.0	58
166	Close-coupling calculation of quantum-mechanical probabilities for collision-induced dissociation. Chemical Physics Letters, 1977, 49, 379-383.	2.6	26
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