Alexander A Voityuk

List of Publications by Year
in descending order

182 papers	5,419 citations	87888 38 h-index	98798 67 g-index
187 all docs	187 docs citations	187 times ranked	3348 citing authors

#	Article	IF	Citations
1	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C₆₀. Angewandte Chemie, 2022, 134, .	2.0	9
2	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C₆₀. Angewandte Chemie - International Edition, 2022, 61, .	13.8	48
3	Nitrogen-doped molecular bowls as electron donors in photoinduced electron transfer reactions. Nanoscale Advances, 2022, 4, 2180-2188.	4.6	6
4	The Hunter Falls Prey: Photoinduced Oxidation of C₆₀ in Inclusion Complex with Perfluorocycloparaphenylene. ChemPhysChem, 2022, 23, .	2.1	9
5	Photoinduced electron transfer in nano-Saturn complexes of fullerene. Physical Chemistry Chemical Physics, 2021, 23, 2126-2133.	2.8	8
6	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. Journal of Materials Chemistry C, 2021, 9, 9436-9445.	5.5	9
7	Fast nonâ€iterative calculation of solvation energies for water and nonâ€aqueous solvents. Journal of Computational Chemistry, 2021, 42, 1184-1194.	3.3	21
8	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. ChemPhysChem, 2021, 22, 1178-1186.	2.1	7
9	[10]CPPâ€Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. Chemistry - A European Journal, 2021, 27, 8737-8744.	3.3	10
10	Unexpected Disparity in Photoinduced Reactions of C₆₀ and C₇₀ in Water with the Generation of O₂^{â€¢â€“} or ¹O₂. Jacs Au, 2021, 1, 1601-1611.	7.9	9
11	Solvation Free Energies for Aqueous and Nonaqueous Solutions Computed Using PM7 Atomic Charges. Journal of Chemical Information and Modeling, 2021, 61, 4544-4553.	5.4	8
12	Evaluation of charge-transfer rates in fullerene-based donorâ€“acceptor dyads with different density functional approximations. Physical Chemistry Chemical Physics, 2021, 23, 5376-5384.	2.8	18
13	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. Dalton Transactions, 2021, 50, 16214-16222.	3.3	3
14	Cyclo[18]carbon: the smallest all-carbon electron acceptor. Chemical Communications, 2020, 56, 352-355.	4.1	78
15	Photoinduced electron transfer in nanotubeâŠƒC₇₀ inclusion complexes: phenine vs. nanographene nanotubes. Chemical Communications, 2020, 56, 12624-12627.	4.1	16
16	Electron Transfer in a Li⁺-Doped Zn-Porphyrinâ€“[10]CPPâŠƒFullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. Journal of Physical Chemistry B, 2020, 124, 9095-9102.	2.6	16
17	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. Journal of Organic Chemistry, 2020, 85, 11721-11731.	3.2	6
18	Triquinoleneâ€versus Fullereneâ€Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Chargeâ€Shift Reactions. Chemistry - A European Journal, 2020, 26, 10896-10902.	3.3	10

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19	Fast and accurate calculation of hydration energies of molecules and ions. Physical Chemistry Chemical Physics, 2020, 22, 14591-14598.	2.8	36
20	(Invited) Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2020, MA2020-01, 809-809.	0.0	0
21	A simple COSMO-based method for calculation of hydration energies of neutral molecules. Physical Chemistry Chemical Physics, 2019, 21, 18706-18713.	2.8	27
22	Iterative Atomic Charge Partitioning of Valence Electron Density. Journal of Computational Chemistry, 2019, 40, 875-884.	3.3	18
23	Hypsochromic solvent shift of the charge separation band in ionic donorâ€“acceptor Li⁺@C₆₀âŠ‚[10]CPP. Chemical Communications, 2019, 55, 11195-11198.	4.1	23
24	Photoinduced Charge Shift in Li⁺-Doped Giant Nested Fullerenes. Journal of Physical Chemistry C, 2019, 123, 16525-16532.	3.1	13
25	InnenrÃ¼cktitelbild: Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates (Angew. Chem. 21/2019). Angewandte Chemie, 2019, 131, 7217-7217.	2.0	1
26	Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates. Angewandte Chemie - International Edition, 2019, 58, 6932-6937.	13.8	35
27	Allâ€Fullerene Electron Donorâ€“Acceptor Conjugates. Angewandte Chemie, 2019, 131, 7006-7011.	2.0	13
28	Photoinduced electron transfer and unusual environmental effects in fullereneâ€“Zn-porphyrinâ€“BODIPY triads. Physical Chemistry Chemical Physics, 2019, 21, 25098-25107.	2.8	22
29	Peculiar Photoinduced Electron Transfer in Porphyrinâ€“Fullerene Akamptisomers. Chemistry - A European Journal, 2019, 25, 2577-2585.	3.3	9
30	(Invited) Photoinduced Charge Separation in Several Dyads Involving Fullerenes. ECS Meeting Abstracts, 2019, , .	0.0	0
31	Reliable charge assessment on encapsulated fragment for endohedral systems. Scientific Reports, 2018, 8, 2882.	3.3	5
32	Thermally induced hopping model for long-range triplet excitation energy transfer in DNA. Physical Chemistry Chemical Physics, 2018, 20, 4997-5000.	2.8	10
33	Stereocontrolled Photoinduced Electron Transfer in Metalâ€Fullerene Hybrids. Chemistry - A European Journal, 2018, 24, 13020-13025.	3.3	17
34	How abasic sites impact hole transfer dynamics in GC-rich DNA sequences. Physical Chemistry Chemical Physics, 2018, 20, 23123-23131.	2.8	6
35	A simple model for calculating atomic charges in molecules. Physical Chemistry Chemical Physics, 2018, 20, 23328-23337.	2.8	27
36	Direct estimation of the transfer integral for photoinduced electron transfer from TD DFT calculations. Physical Chemistry Chemical Physics, 2017, 19, 31007-31010.	2.8	3

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37	Electronic Couplings for Photoinduced Electron Transfer and Excitation Energy Transfer Computed Using Excited States of Noninteracting Molecules. Journal of Physical Chemistry A, 2017, 121, 5414-5419.	2.5	15
38	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C₆₀ donorâ€“acceptor conjugate. Journal of Computational Chemistry, 2016, 37, 1396-1405.	3.3	10
39	Photoinduced Charge Separation in the Carbon Nano-Onion C₆₀@C₂₄₀. Journal of Physical Chemistry A, 2016, 120, 5798-5804.	2.5	10
40	The Driving Force of Photoinduced Charge Separation in Metalâ€Clusterâ€Encapsulated Triphenylamineâ€[80]fullerenes. Chemistry - A European Journal, 2016, 22, 17305-17310.	3.3	5
41	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	3.3	31
42	Single Amino Acid Mutation Controls Hole Transfer Dynamics in DNA-Methyltransferase HhaI Complexes. Journal of Physical Chemistry Letters, 2015, 6, 3749-3753.	4.6	5
43	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. Journal of Physical Chemistry Letters, 2015, 6, 2434-2438.	4.6	23
44	Interaction of Dark Excited States. Comparison of Computational Approaches. Journal of Physical Chemistry B, 2015, 119, 7417-7421.	2.6	7
45	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donorâ€“acceptor conjugate: a combined molecular dynamics and TD-DFT study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
46	Influence of Base Stacking Geometry on the Nature of Excited States in G-Quadruplexes: A Time-Dependent DFT Study. Journal of Physical Chemistry B, 2015, 119, 3697-3705.	2.6	28
47	On the mechanism of photoinduced dimer dissociation in the plant UVR8 photoreceptor. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5219-5224.	7.1	32
48	Exciton delocalization, charge transfer, and electronic coupling for singlet excitation energy transfer between stacked nucleobases in DNA: An MS-CASPT2 study. Journal of Chemical Physics, 2014, 140, 095102.	3.0	46
49	On the performance of the Kohnâ€“Sham orbital approach in the calculation of electron transfer parameters. The three state model. Physical Chemistry Chemical Physics, 2014, 16, 17154-17162.	2.8	4
50	INDO/X: A New Semiempirical Method for Excited States of Organic and Biological Molecules. Journal of Chemical Theory and Computation, 2014, 10, 4950-4958.	5.3	26
51	Estimation of Electronic Coupling for Singlet Excitation Energy Transfer. Journal of Physical Chemistry C, 2014, 118, 1478-1483.	3.1	14
52	Fragment transition density method to calculate electronic coupling for excitation energy transfer. Journal of Chemical Physics, 2014, 140, 244117.	3.0	44
53	Intermediate neglect of differential overlap for spectroscopy. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 515-527.	14.6	27
54	Effects of dynamic disorder on exciton delocalization and photoinduced charge separation in DNA. Photochemical and Photobiological Sciences, 2013, 12, 1303.	2.9	24

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55	Electron-Hole Transfer in G-Quadruplexes with Different Tetrad Stacking Geometries: A Combined QM and MD Study. Journal of Physical Chemistry B, 2013, 117, 9851-9856.	2.6	45
56	In-silico Assessment of Protein-Protein Electron Transfer. A Case Study: Cytochrome c Peroxidase â€“ Cytochrome c. PLoS Computational Biology, 2013, 9, e1002990.	3.2	23
57	Estimation of Electronic Coupling for Photoinduced Charge Separation and Charge Recombination Using the Fragment Charge Difference Method. Journal of Physical Chemistry C, 2013, 117, 2670-2675.	3.1	30
58	Distance Dependence of Triplet Energy Transfer in Water and Organic Solvents: A QM/MD Study. Journal of Physical Chemistry C, 2012, 116, 22179-22185.	3.1	24
59	DNA Base Pair Stacks with High Electric Conductance: A Systematic Structural Search. ACS Nano, 2012, 6, 8216-8225.	14.6	20
60	MS-CASPT2 Study of Hole Transfer in Guanineâ€“Indole Complexes Using the Generalized Mullikenâ€“Hush Method: Effective Two-State Treatment. Journal of Physical Chemistry B, 2012, 116, 7815-7820.	2.6	4
61	Electronic coupling for charge transfer in donorâ€“bridgeâ€“acceptor systems. Performance of the two-state FCD model. Physical Chemistry Chemical Physics, 2012, 14, 13789.	2.8	42
62	Conformational dependence of the electronic coupling in guanineâ€“tryptophan complexes: A DFT study. International Journal of Quantum Chemistry, 2012, 112, 1838-1843.	2.0	2
63	Electron transfer in DNA. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 780-794.	14.6	35
64	Effects of various halogen anions and cations of alkali metals on energetics of excess charge recombination in stilbene donorâ€“acceptor capped DNA hairpins. Physical Chemistry Chemical Physics, 2011, 13, 16028.	2.8	2
65	Long-Range Electron Transfer in Biomolecules. Tunneling or Hopping?. Journal of Physical Chemistry B, 2011, 115, 12202-12207.	2.6	19
66	Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. Computational and Theoretical Chemistry, 2011, 975, 38-41.	2.5	6
67	Environment effects on tripletâ€“triplet energy transfer in DNA. Chemical Physics Letters, 2011, 512, 118-122.	2.6	7
68	DFT performance for the hole transfer parameters in DNA Ï€ stacks. International Journal of Quantum Chemistry, 2011, 111, 191-201.	2.0	23
69	Tripletâ€“Triplet Energy Transfer in DNA: A Process that Occurs on the Nanosecond Timescale. Angewandte Chemie - International Edition, 2011, 50, 1820-1822.	13.8	28
70	Electron transfer between [4Feâ€“4S] clusters. Chemical Physics Letters, 2010, 495, 131-134.	2.6	15
71	Temperature Effects on Donorâ^'Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2010, 6, 3241-3248.	5.3	7
72	Can Charge Recombination in DNA Hairpins Be Controlled by Counterions?. Journal of Physical Chemistry C, 2010, 114, 20503-20509.	3.1	2

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73	Electron transfer from aromatic amino acids to guanine and adenine radical cations in Ї€ stacked and T-shaped complexes. Organic and Biomolecular Chemistry, 2010, 8, 1870.	2.8	22
74	Triplet Excitation Energy Transfer through Fluorene Ї€ Stack. Journal of Physical Chemistry C, 2010, 114, 20236-20239.	3.1	13
75	An in Silico Design for a DNA Nanomechanical Switch. ACS Nano, 2010, 4, 5737-5742.	14.6	13
76	Conformational dependence of the electronic coupling for singlet excitation energy transfer in DNA. An INDO/S study. Physical Chemistry Chemical Physics, 2010, 12, 7403.	2.8	18
77	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	1.4	9
78	Can Charge Transfer in DNA Significantly Be Modulated by Varying the Ї€ Stack Conformation?. Journal of Physical Chemistry B, 2009, 113, 14365-14368.	2.6	30
79	Solvent Effects on Donorâ^'Acceptor Couplings in Peptides. A Combined QM and MD Study. Journal of Chemical Theory and Computation, 2009, 5, 3312-3320.	5.3	14
80	Stabilization of radical anion states of nucleobases in DNA. Physical Chemistry Chemical Physics, 2009, 11, 10608.	2.8	10
81	Thermochemistry of Ptâ^'Fullerene Complexes: Semiempirical Study. Journal of Physical Chemistry A, 2009, 113, 11801-11808.	2.5	4
82	Charge-on-site scheme to estimate the electronic coupling in electron transfer systems. Chemical Physics Letters, 2008, 451, 153-157.	2.6	8
83	Electronic couplings and on-site energies for hole transfer in DNA: Systematic quantum mechanical/molecular dynamic study. Journal of Chemical Physics, 2008, 128, 115101.	3.0	87
84	Chromophore/DNA Interactions:â€‰ Femto- to Nanosecond Spectroscopy, NMR Structure, and Electron Transfer Theory. Journal of Physical Chemistry B, 2008, 112, 973-989.	2.6	13
85	Thermochemistry of Hydrocarbons. Back to Extended HÃ¼ckel Theory. Journal of Chemical Theory and Computation, 2008, 4, 1877-1885.	5.3	9
86	Ї€ Stack Structure and Hole Transfer Couplings in DNA Hairpins and DNA. A Combined QM/MD Study. Journal of Physical Chemistry B, 2008, 112, 8181-8187.	2.6	21
87	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. Journal of Physical Chemistry C, 2008, 112, 1672-1678.	3.1	16
88	Parameters For Excess Electron Transfer in DNA. Estimation Using Unoccupied Kohnâ^'Sham Orbitals and TD DFT. Journal of Physical Chemistry A, 2008, 112, 9043-9049.	2.5	20
89	Conformations of poly{G}â€“poly{C} Ї€ stacks with high hole mobility. Journal of Chemical Physics, 2008, 128, 045104.	3.0	23
90	How to Switch the Direction of Photoinduced Charge Injection into DNA?. Journal of Physical Chemistry C, 2007, 111, 7207-7210.	3.1	6

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91	Hole Transfer Energetics in Structurally Distorted DNA:Â The Nucleosome Core Particle. Journal of Physical Chemistry B, 2007, 111, 2976-2985.	2.6	13
92	MS-CASPT2 Calculation of Excess Electron Transfer in Stacked DNA Nucleobases. Journal of Physical Chemistry A, 2007, 111, 4714-4719.	2.5	28
93	Fluctuation of the electronic coupling in DNA: Multistate versus two-state model. Chemical Physics Letters, 2007, 439, 162-165.	2.6	33
94	CASSCF/CAS-PT2 Study of Hole Transfer in Stacked DNA Nucleobases. Journal of Physical Chemistry A, 2006, 110, 6426-6432.	2.5	94
95	Accurate Treatment of Energetics and Geometry of Carbon and Hydrocarbon Compounds within Tight-Binding Model. Journal of Chemical Theory and Computation, 2006, 2, 1038-1044.	5.3	12
96	Electronic Coupling Mediated by Stacked [Thymine-Hg-Thymine] Base Pairs. Journal of Physical Chemistry B, 2006, 110, 21010-21013.	2.6	54
97	Femtosecond study of light-induced fluorescence increase of the dark chromoprotein asFP595. Chemical Physics, 2006, 323, 149-160.	1.9	36
98	Donorâ€“acceptor electronic couplings in Ï€-stacks: How many states must be accounted for?. Chemical Physics Letters, 2006, 422, 15-19.	2.6	15
99	Assessment of semiempirical methods for the computation of charge transfer in DNA Ï€-stacks. Chemical Physics Letters, 2006, 427, 177-180.	2.6	51
100	Effects of intra base-pairs flexibility on hole transfer coupling in DNA. Chemical Physics Letters, 2006, 429, 546-550.	2.6	35
101	Modified tight-binding model for fast and accurate estimation of thermochemistry and molecular structure. Parameters and results for hydrocarbons. Chemical Physics Letters, 2006, 433, 216-220.	2.6	6
102	Effect of proton transfer on the electronic coupling in DNA. Chemical Physics, 2006, 325, 567-574.	1.9	26
103	Estimation of electronic coupling in Ï€-stacked donor-bridge-acceptor systems: Correction of the two-state model. Journal of Chemical Physics, 2006, 124, 064505.	3.0	66
104	Computational modeling of Charge Transfer in DNA. , 2006, , 485-511.		5
105	Quantum chemical modeling of charge transfer in DNA. , 2006, , 99-119.		0
106	Charge transfer in DNA: Hole charge is confined to a single base pair due to solvation effects. Journal of Chemical Physics, 2005, 122, 204904.	3.0	68
107	Estimates of electronic coupling for excess electron transfer in DNA. Journal of Chemical Physics, 2005, 123, 034903.	3.0	27
108	Electronic Couplings in DNA Ï€-Stacks:â€‰ Multistate Effects. Journal of Physical Chemistry B, 2005, 109, 17917-17921.	2.6	23

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109	Are Radical Cation States Delocalized over GG and GGG Hole Traps in DNA?. Journal of Physical Chemistry B, 2005, 109, 10793-10796.	2.6	45
110	Environmental Fluctuations Facilitate Electron-Hole Transfer from Guanine to Adenine in DNAÏ€ Stacks. Angewandte Chemie - International Edition, 2004, 43, 624-627.	13.8	120
111	Superexchange Pathways in Charge Transfer through a DNA Ï€-Stack. Israel Journal of Chemistry, 2004, 44, 109-117.	2.3	6
112	Estimate of the Reorganization Energy for Charge Transfer in DNA. Journal of Physical Chemistry B, 2003, 107, 2595-2601.	2.6	104
113	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNAâ€. Journal of Physical Chemistry B, 2002, 106, 7919-7926.	2.6	24
114	Quantum Chemical Modeling of Electron Hole Transfer through Ï€ Stacks of Normal and Modified Pairs of Nucleobases. Journal of Physical Chemistry B, 2002, 106, 3013-3018.	2.6	49
115	Fragment charge difference method for estimating donorâ€“acceptor electronic coupling: Application to DNA Ï€-stacks. Journal of Chemical Physics, 2002, 117, 5607-5616.	3.0	294
116	Superexchange Mediated Charge Hopping in DNA. Journal of Physical Chemistry A, 2002, 106, 7599-7606.	2.5	155
117	Excited-State Photophysics of an Acridine Derivative Selectively Intercalated in Duplex DNA. ChemPhysChem, 2002, 3, 452.	2.1	20
118	Charge transfer in DNA. Sensitivity of electronic couplings to conformational changesDedicated to Professor F. DÃ¶rr on the occasion of his 80th birthday.. Physical Chemistry Chemical Physics, 2001, 3, 5421-5425.	2.8	130
119	Electronic coupling between Watsonâ€“Crick pairs for hole transfer and transport in desoxyribonucleic acid. Journal of Chemical Physics, 2001, 114, 5614-5620.	3.0	228
120	Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results. Chemical Physics, 2001, 269, 83-91.	1.9	77
121	Energetics of excess electron transfer in DNA. Chemical Physics Letters, 2001, 342, 231-238.	2.6	69
122	Energetics of the splitting of pyrimidine photodimers induced by electron transfer to rhodium(III) complexes. A quantum chemical study. International Journal of Quantum Chemistry, 2000, 77, 128-138.	2.0	4
123	Energetics of hole transfer in DNA. Chemical Physics Letters, 2000, 324, 430-434.	2.6	185
124	AM1/d Parameters for Molybdenum. Journal of Physical Chemistry A, 2000, 104, 4089-4094.	2.5	82
125	Electronic Coupling for Charge Transfer and Transport in DNA. Journal of Physical Chemistry B, 2000, 104, 9740-9745.	2.6	249
126	A cyclic intermediate of the splitting reaction of cyclobutane-type pyrimidine dimer cation radicals. A computational finding as challenge for experimental techniques. Computational and Theoretical Chemistry, 1999, 488, 163-168.	1.5	4

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127	Effect of Proton Transfer on the Anionic and Cationic Pathways of Pyrimidine Photodimer Cleavage. A Computational Study. Journal of Physical Chemistry A, 1999, 103, 3569-3574.	2.5	21
128	Extension of the Neglect of Diatomic Differential Overlap Method to Spectroscopy. NDDO-G Parametrization and Results for Organic Molecules. Journal of Physical Chemistry A, 1999, 103, 4553-4559.	2.5	37
129	Structure and rotation barriers for ground and excited states of the isolated chromophore of the green fluorescent protein. Chemical Physics Letters, 1998, 296, 269-276.	2.6	99
130	Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins. Chemical Physics, 1998, 231, 13-25.	1.9	110
131	Splitting of Cyclobutane-Type Uracil Dimer Cation Radicals. Hartreeâ^'Fock, MP2, and Density Functional Studies. Journal of Physical Chemistry A, 1998, 102, 7168-7175.	2.5	21
132	Substrate Oxidation in the Active Site of Xanthine Oxidase and Related Enzymes. A Model Density Functional Study. Inorganic Chemistry, 1998, 37, 176-180.	4.0	50
133	Ab Initio Study on the Structure and Splitting of the Uracil Dimer Anion Radical. Journal of Physical Chemistry A, 1997, 101, 8335-8338.	2.5	42
134	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. Journal of the American Chemical Society, 1997, 119, 3159-3160.	13.7	43
135	Protonation effects on the chromophore of green fluorescent protein. Quantum chemical study of the absorption spectrum. Chemical Physics Letters, 1997, 272, 162-167.	2.6	86
136	Extension of MNDO to d Orbitals:Â Parameters and Results for the Second-Row Elements and for the Zinc Group. The Journal of Physical Chemistry, 1996, 100, 616-626.	2.9	266
137	A Quantum Chemical Study of Photoinduced DNA Repair:Â On the Splitting of Pyrimidine Model Dimers Initiated by Electron Transfer. Journal of the American Chemical Society, 1996, 118, 9750-9758.	13.7	54
138	Extension of MNDO to d orbitals: parameters and results for silicon. Computational and Theoretical Chemistry, 1994, 313, 141-154.	1.5	54
139	Quantum chemical study of molecular ion complexes with hydrogen bonds (Review). Journal of Structural Chemistry, 1993, 33, 899-924.	1.0	1
140	Extension ofMNDO tod orbitals: Parameters and results for the halogens. International Journal of Quantum Chemistry, 1992, 44, 807-829.	2.0	78
141	A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. International Journal of Quantum Chemistry, 1992, 44, 897-930.	2.0	57
142	Extension of the MNDO formalism tod orbitals: Integral approximations and preliminary numerical results. Theoretica Chimica Acta, 1992, 81, 391-404.	0.8	196
143	Structure and energy characteristic of [Mg(H3O)n]2+ and [Mg(H2O)n?1OH]+ complexes according to data from MNDO calculations. Journal of Structural Chemistry, 1992, 32, 590-593.	1.0	1
144	Molecular mechanics calculations of systems with strong hydrogen bonds. Journal of Molecular Structure, 1992, 265, 179-187.	3.6	3

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145	Use of AM1 and PM3 methods for the investigation of energies and structures of compounds O=PXYZ, S=PXYZ. Journal of Structural Chemistry, 1991, 31, 684-685.	1.0	0
146	Stereoelectronic effect in reactions of phosphoester bond rupture. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1990, 39, 2286-2289.	0.0	0
147	Quantum-chemical study of the effect of solvation on the strength of the phosphamide bond in N-phosphorylammonium cations and zwitterions. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 267-270.	0.0	0
148	Quantum-chemical study of the mechanism of the hydrolysis of amides in the gas phase and in aqueous solution. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 1635-1641.	0.0	2
149	Structural features of labile N-phosphorylammonium zwitterions and cations according to data from MNDO calculations and15N NMR spectroscopy. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 1177-1182.	0.0	1
150	Quantum-chemical investigation of the mechanism of nucleophilic addition in the HCNO molecule. Theoretical and Experimental Chemistry, 1989, 25, 662-665.	0.8	0
151	MNDO parameters for the Ca atom. Journal of Structural Chemistry, 1989, 29, 793-795.	1.0	0
152	Diazabicycloalkanes with nitrogen atoms in bridgehead positions.. Chemistry of Heterocyclic Compounds, 1989, 25, 305-310.	1.2	1
153	MNDO calculations of Mg compounds. Journal of Structural Chemistry, 1988, 28, 926-929.	1.0	2
154	Complexes with hydrogen bonds by the MNDO/M method. Journal of Structural Chemistry, 1988, 29, 192-197.	1.0	1
155	Application of the MNDO method to investigation of properties and reactivity of molecules. Journal of Structural Chemistry, 1988, 29, 120-146.	1.0	14
156	Parameters of MNDO method for Zn atom. Journal of Structural Chemistry, 1988, 28, 649-652.	1.0	0
157	MNDO calculations of systems containing hydrogen bonds. Theoretica Chimica Acta, 1987, 72, 223-228.	0.8	47
158	MNDO calculations of systems with hydrogen bonds S-H. Theoretica Chimica Acta, 1987, 71, 327-331.	0.8	3
159	MNDO calculations on systems containing S-H hydrogen bonds. Journal of Structural Chemistry, 1987, 28, 5-8.	1.0	1
160	Revised semiempirical parameters for Br, I, Sn, Hg, and Pb in the MNDO method. Journal of Structural Chemistry, 1987, 28, 9-12.	1.0	3
161	A program for searching for semiempirical parameters by the MNDO method. Journal of Structural Chemistry, 1987, 28, 312-314.	1.0	0
162	The MNDO-85 system of programs for calculating the electronic structure, physicochemical properties, and reactivity of molecular systems by the MDNO, MNDOC, and AM1 semiepirical methods. Journal of Structural Chemistry, 1987, 27, 674-676.	1.0	1

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163	Quantum-chemical study of the influence of the electronegativity of substituents on the reactivity of ?-chloroethylamine derivatives. Journal of Structural Chemistry, 1986, 27, 367-371.	1.0	0
164	The transition state in the half-electron method. Journal of Structural Chemistry, 1984, 24, 593-596.	1.0	0
165	Investigation of electronic structure of chloro complexes of Rhodium(III). Journal of Structural Chemistry, 1984, 25, 351-355.	1.0	0
166	X-ray spectra and model quantum-chemical calculation of SO2 in clathrates based on hydroquinone. Journal of Structural Chemistry, 1984, 25, 371-376.	1.0	2
167	X-ray spectra and electronic structure of the PCl3 molecule. Journal of Structural Chemistry, 1984, 24, 676-682.	1.0	0
168	An x-ray spectral and quantum-chemical study of the electronic structure of ruthenium complexes. Journal of Structural Chemistry, 1984, 24, 837-842.	1.0	0
169	Program for calculating the electronic structure of molecules, complexes, and clusters in the INDO aproximation. Journal of Structural Chemistry, 1983, 23, 821-822.	1.0	0
170	A generalization of the half-electron method for calculations for complex compounds. Journal of Structural Chemistry, 1983, 24, 344-348.	1.0	0
171	One-center parameters dependent on the valence state of the atom. III. Transition elements of periods IV and V. Journal of Structural Chemistry, 1982, 22, 783-786.	1.0	0
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