Alexander A Voityuk

List of Publications by Year in Descending Order

178 papers	4,648 citations	36 h-index	63 g-index
187 ext. papers	4,991 ext. citations	3.7 avg, IF	6.04 L-index

#	Paper	IF	Citations
178	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. *Dalton Transactions*, **2021**, 50, 16214-16222	4.3	0
177	Fast non-iterative calculation of solvation energies for water and non-aqueous solvents. *Journal of Computational Chemistry*, **2021**, 42, 1184-1194	3.5	3
176	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. *ChemPhysChem*, **2021**, 22, 1178-1186	3.2	3
175	[10]CPP-Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. *Chemistry - A European Journal*, **2021**, 27, 8737-8744	4.8	2
174	Photoinduced electron transfer in nano-Saturn complexes of fullerene. *Physical Chemistry Chemical Physics*, **2021**, 23, 2126-2133	3.6	1
173	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. *Journal of Materials Chemistry C*, **2021**, 9, 9436-9445	7.1	3
172	Unexpected Disparity in Photoinduced Reactions of C and C in Water with the Generation of O or O. *Jacs Au*, **2021**, 1, 1601-1611		1
171	Solvation Free Energies for Aqueous and Nonaqueous Solutions Computed Using PM7 Atomic Charges. *Journal of Chemical Information and Modeling*, **2021**, 61, 4544-4553	6.1	0
170	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. *Physical Chemistry Chemical Physics*, **2021**, 23, 5376-5384	3.6	3
169	Triquinoline- versus Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-Shift Reactions. *Chemistry - A European Journal*, **2020**, 26, 10896-10902	4.8	4
168	Fast and accurate calculation of hydration energies of molecules and ions. *Physical Chemistry Chemical Physics*, **2020**, 22, 14591-14598	3.6	15
167	Cyclo[18]carbon: the smallest all-carbon electron acceptor. *Chemical Communications*, **2020**, 56, 352-355	5.8	43
166	Photoinduced electron transfer in nanotube?C inclusion complexes: phenine . nanographene nanotubes. *Chemical Communications*, **2020**, 56, 12624-12627	5.8	4
165	Electron Transfer in a Li-Doped Zn-Porphyrin-[10]CPP?Fullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. *Journal of Physical Chemistry B*, **2020**, 124, 9095-9102	3.4	4
164	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. *Journal of Organic Chemistry*, **2020**, 85, 11721-11731	4.2	5
163	Iterative Atomic Charge Partitioning of Valence Electron Density. *Journal of Computational Chemistry*, **2019**, 40, 875-884	3.5	11
162	Hypsochromic solvent shift of the charge separation band in ionic donor-acceptor Li@C?[10]CPP. *Chemical Communications*, **2019**, 55, 11195-11198	5.8	11

161	Photoinduced Charge Shift in Li+-Doped Giant Nested Fullerenes. *Journal of Physical Chemistry C*, **2019**, 123, 16525-16532	3.8	6
160	Innenrücktitelbild: All-Fullerene Electron Donor–Acceptor Conjugates (Angew. Chem. 21/2019). *Angewandte Chemie*, **2019**, 131, 7217-7217	3.6	1
159	All-Fullerene Electron Donor-Acceptor Conjugates. *Angewandte Chemie - International Edition*, **2019**, 58, 6932-6937	16.4	19
158	All-Fullerene Electron Donor–Acceptor Conjugates. *Angewandte Chemie*, **2019**, 131, 7006-7011	3.6	8
157	A simple COSMO-based method for calculation of hydration energies of neutral molecules. *Physical Chemistry Chemical Physics*, **2019**, 21, 18706-18713	3.6	10
156	Photoinduced electron transfer and unusual environmental effects in fullerene-Zn-porphyrin-BODIPY triads. *Physical Chemistry Chemical Physics*, **2019**, 21, 25098-25107	3.6	17
155	Peculiar Photoinduced Electron Transfer in Porphyrin-Fullerene Akamptisomers. *Chemistry - A European Journal*, **2019**, 25, 2577-2585	4.8	7
154	Reliable charge assessment on encapsulated fragment for endohedral systems. *Scientific Reports*, **2018**, 8, 2882	4.9	3
153	Thermally induced hopping model for long-range triplet excitation energy transfer in DNA. *Physical Chemistry Chemical Physics*, **2018**, 20, 4997-5000	3.6	5
152	How abasic sites impact hole transfer dynamics in GC-rich DNA sequences. *Physical Chemistry Chemical Physics*, **2018**, 20, 23123-23131	3.6	3
151	A simple model for calculating atomic charges in molecules. *Physical Chemistry Chemical Physics*, **2018**, 20, 23328-23337	3.6	18
150	Stereocontrolled Photoinduced Electron Transfer in Metal-Fullerene Hybrids. *Chemistry - A European Journal*, **2018**, 24, 13020-13025	4.8	14
149	Direct estimation of the transfer integral for photoinduced electron transfer from TD DFT calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 31007-31010	3.6	3
148	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	2.8	12
147	The Driving Force of Photoinduced Charge Separation in Metal-Cluster-Encapsulated Triphenylamine-[80]fullerenes. *Chemistry - A European Journal*, **2016**, 22, 17305-17310	4.8	5
146	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. *Chemistry - A European Journal*, **2016**, 22, 7497-507	4.8	26
145	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C60 donor-acceptor conjugate. *Journal of Computational Chemistry*, **2016**, 37, 1396-405	3.5	8
144	Photoinduced Charge Separation in the Carbon Nano-Onion C60@C240. *Journal of Physical Chemistry A*, **2016**, 120, 5798-804	2.8	10

143	Single Amino Acid Mutation Controls Hole Transfer Dynamics in DNA-Methyltransferase HhaI Complexes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3749-53	6.4	4
142	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. *Journal of Physical Chemistry Letters*, **2015**, 6, 2434-8	6.4	20
141	Interaction of Dark Excited States. Comparison of Computational Approaches. *Journal of Physical Chemistry B*, **2015**, 119, 7417-21	3.4	6
140	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donor–acceptor conjugate: a combined molecular dynamics and TD-DFT study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	12
139	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, 3697-705	3.4	22
138	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	3.9	37
137	On the performance of the Kohn-Sham orbital approach in the calculation of electron transfer parameters. The three state model. *Physical Chemistry Chemical Physics*, **2014**, 16, 17154-62	3.6	4
136	INDO/X: A New Semiempirical Method for Excited States of Organic and Biological Molecules. *Journal of Chemical Theory and Computation*, **2014**, 10, 4950-8	6.4	22
135	Estimation of Electronic Coupling for Singlet Excitation Energy Transfer. *Journal of Physical Chemistry C*, **2014**, 118, 1478-1483	3.8	13
134	Fragment transition density method to calculate electronic coupling for excitation energy transfer. *Journal of Chemical Physics*, **2014**, 140, 244117	3.9	32
133	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, 5219-24	11.5	29
132	Intermediate neglect of differential overlap for spectroscopy. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 515-527	7.9	23
131	Effects of dynamic disorder on exciton delocalization and photoinduced charge separation in DNA. *Photochemical and Photobiological Sciences*, **2013**, 12, 1303-9	4.2	24
130	Electron-hole transfer in G-quadruplexes with different tetrad stacking geometries: a combined QM and MD study. *Journal of Physical Chemistry B*, **2013**, 117, 9851-6	3.4	40
129	In-silico assessment of protein-protein electron transfer. a case study: cytochrome c peroxidase--cytochrome c. *PLoS Computational Biology*, **2013**, 9, e1002990	5	22
128	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	3.8	26
127	Distance Dependence of Triplet Energy Transfer in Water and Organic Solvents: A QM/MD Study. *Journal of Physical Chemistry C*, **2012**, 116, 22179-22185	3.8	19
126	DNA base pair stacks with high electric conductance: a systematic structural search. *ACS Nano*, **2012** , 6, 8216-25	16.7	19

125	MS-CASPT2 study of hole transfer in guanine-indole complexes using the generalized Mulliken-Hush method: effective two-state treatment. *Journal of Physical Chemistry B*, **2012**, 116, 7815-20	3.4	4
124	Electronic coupling for charge transfer in donor-bridge-acceptor systems. Performance of the two-state FCD model. *Physical Chemistry Chemical Physics*, **2012**, 14, 13789-93	3.6	34
123	Conformational dependence of the electronic coupling in guanine–tryptophan complexes: A DFT study. *International Journal of Quantum Chemistry*, **2012**, 112, 1838-1843	2.1	2
122	Electron transfer in DNA. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 780-794	7.9	31
121	Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. *Computational and Theoretical Chemistry*, **2011**, 975, 38-41	2	5
120	Environment effects on triplet–triplet energy transfer in DNA. *Chemical Physics Letters*, **2011**, 512, 118-122	2.5	7
119	DFT performance for the hole transfer parameters in DNA π-stacks. *International Journal of Quantum Chemistry*, **2011**, 111, 191-201	2.1	22
118	Triplet–Triplet Energy Transfer in DNA: A Process that Occurs on the Nanosecond Timescale. *Angewandte Chemie*, **2011**, 123, 1860-1862	3.6	5
117	Triplet-triplet energy transfer in DNA: a process that occurs on the nanosecond timescale. *Angewandte Chemie - International Edition*, **2011**, 50, 1820-2	16.4	24
116	Effects of various halogen anions and cations of alkali metals on energetics of excess charge recombination in stilbene donor-acceptor capped DNA hairpins. *Physical Chemistry Chemical Physics*, **2011**, 13, 16028-32	3.6	2
115	Long-range electron transfer in biomolecules. Tunneling or hopping?. *Journal of Physical Chemistry B*, **2011**, 115, 12202-7	3.4	18
114	Temperature Effects on Donor-Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study. *Journal of Chemical Theory and Computation*, **2010**, 6, 3241-8	6.4	7
113	Can Charge Recombination in DNA Hairpins Be Controlled by Counterions? *Journal of Physical Chemistry C*, **2010**, 114, 20503-20509	3.8	2
112	Electron transfer from aromatic amino acids to guanine and adenine radical cations in pi stacked and T-shaped complexes. *Organic and Biomolecular Chemistry*, **2010**, 8, 1870-5	3.9	19
111	Triplet Excitation Energy Transfer through Fluorene π-Stack. *Journal of Physical Chemistry C*, **2010**, 114, 20236-20239	3.8	12
110	An in silico design for a DNA nanomechanical switch. *ACS Nano*, **2010**, 4, 5737-42	16.7	13
109	Conformational dependence of the electronic coupling for singlet excitation energy transfer in DNA. An INDO/S study. *Physical Chemistry Chemical Physics*, **2010**, 12, 7403-8	3.6	18
108	Electron transfer between [4Fe4S] clusters. *Chemical Physics Letters*, **2010**, 495, 131-134	2.5	12

107	Excess charge delocalization in organic and biological molecules: some theoretical notions. *Theoretical Chemistry Accounts*, **2009**, 123, 29-40	1.9	8
106	Can charge transfer in DNA significantly be modulated by varying the pi stack conformation?. *Journal of Physical Chemistry B*, **2009**, 113, 14365-8	3.4	29
105	Solvent Effects on Donor-Acceptor Couplings in Peptides. A Combined QM and MD Study. *Journal of Chemical Theory and Computation*, **2009**, 5, 3312-20	6.4	14
104	Stabilization of radical anion states of nucleobases in DNA. *Physical Chemistry Chemical Physics*, **2009**, 11, 10608-13	3.6	10
103	Thermochemistry of Pt-fullerene complexes: semiempirical study. *Journal of Physical Chemistry A*, **2009**, 113, 11801-8	2.8	3
102	Electronic couplings and on-site energies for hole transfer in DNA: systematic quantum mechanical/molecular dynamic study. *Journal of Chemical Physics*, **2008**, 128, 115101	3.9	84
101	Chromophore/DNA interactions: femto- to nanosecond spectroscopy, NMR structure, and electron transfer theory. *Journal of Physical Chemistry B*, **2008**, 112, 973-89	3.4	13
100	Thermochemistry of Hydrocarbons. Back to Extended H□kel Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1877-85	6.4	9
99	Pi stack structure and hole transfer couplings in DNA hairpins and DNA. A combined QM/MD study. *Journal of Physical Chemistry B*, **2008**, 112, 8181-7	3.4	21
98	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. *Journal of Physical Chemistry C*, **2008**, 112, 1672-1678	3.8	16
97	Parameters for excess electron transfer in DNA. Estimation using unoccupied Kohn-Sham orbitals and TD DFT. *Journal of Physical Chemistry A*, **2008**, 112, 9043-9	2.8	20
96	Conformations of poly{G}-poly{C} pi stacks with high hole mobility. *Journal of Chemical Physics*, **2008**, 128, 045104	3.9	21
95	Charge-on-site scheme to estimate the electronic coupling in electron transfer systems. *Chemical Physics Letters*, **2008**, 451, 153-157	2.5	8
94	How to Switch the Direction of Photoinduced Charge Injection into DNA?. *Journal of Physical Chemistry C*, **2007**, 111, 7207-7210	3.8	5
93	Hole transfer energetics in structurally distorted DNA: the nucleosome core particle. *Journal of Physical Chemistry B*, **2007**, 111, 2976-85	3.4	11
92	MS-CASPT2 calculation of excess electron transfer in stacked DNA nucleobases. *Journal of Physical Chemistry A*, **2007**, 111, 4714-9	2.8	27
91	Fluctuation of the electronic coupling in DNA: Multistate versus two-state model. *Chemical Physics Letters*, **2007**, 439, 162-165	2.5	31
90	Estimation of electronic coupling in pi-stacked donor-bridge-acceptor systems: correction of the two-state model. *Journal of Chemical Physics*, **2006**, 124, 64505	3.9	57

89	CASSCF/CAS-PT2 study of hole transfer in stacked DNA nucleobases. *Journal of Physical Chemistry A* , **2006**, 110, 6426-32	2.8	90
88	Accurate Treatment of Energetics and Geometry of Carbon and Hydrocarbon Compounds within Tight-Binding Model. *Journal of Chemical Theory and Computation*, **2006**, 2, 1038-44	6.4	12
87	Electronic coupling mediated by stacked [Thymine-Hg-Thymine] base pairs. *Journal of Physical Chemistry B*, **2006**, 110, 21010-3	3.4	54
86	Femtosecond study of light-induced fluorescence increase of the dark chromoprotein asFP595. *Chemical Physics*, **2006**, 323, 149-160	2.3	34
85	Donor□cceptor electronic couplings in □stacks: How many states must be accounted for?. *Chemical Physics Letters*, **2006**, 422, 15-19	2.5	15
84	Assessment of semiempirical methods for the computation of charge transfer in DNA □stacks. *Chemical Physics Letters*, **2006**, 427, 177-180	2.5	49
83	Effects of intra base-pairs flexibility on hole transfer coupling in DNA. *Chemical Physics Letters*, **2006**, 429, 546-550	2.5	34
82	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	2.5	6
81	Effect of proton transfer on the electronic coupling in DNA. *Chemical Physics*, **2006**, 325, 567-574	2.3	24
80	Quantum chemical modeling of charge transfer in DNA **2006**, 99-119		
79	Computational modeling of Charge Transfer in DNA **2006**, 485-511		5
78	Electronic couplings in DNA pi-stacks: multistate effects. *Journal of Physical Chemistry B*, **2005**, 109, 17917-21	3.4	22
77	Are radical cation states delocalized over GG and GGG hole traps in DNA?. *Journal of Physical Chemistry B*, **2005**, 109, 10793-6	3.4	41
76	Charge transfer in DNA: hole charge is confined to a single base pair due to solvation effects. *Journal of Chemical Physics*, **2005**, 122, 204904	3.9	61
75	Estimates of electronic coupling for excess electron transfer in DNA. *Journal of Chemical Physics*, **2005**, 123, 34903	3.9	26
74	Environmental fluctuations facilitate electron-hole transfer from guanine to adenine in DNA pi stacks. *Angewandte Chemie - International Edition*, **2004**, 43, 624-7	16.4	114
73	Environmental Fluctuations Facilitate Electron-Hole Transfer from Guanine to Adenine in DNA □ Stacks. *Angewandte Chemie*, **2004**, 116, 634-637	3.6	11
72	Superexchange Pathways in Charge Transfer through a DNA □Stack. *Israel Journal of Chemistry*, **2004**, 44, 109-117	3.4	6

71	Estimate of the Reorganization Energy for Charge Transfer in DNA. *Journal of Physical Chemistry B*, **2003**, 107, 2595-2601	3.4	96
70	Excited-state photophysics of an acridine derivative selectively intercalated in duplex DNA. *ChemPhysChem*, **2002**, 3, 452-5	3.2	20
69	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNA. *Journal of Physical Chemistry B*, **2002**, 106, 7919-7926	3.4	22
68	Quantum Chemical Modeling of Electron Hole Transfer through Stacks of Normal and Modified Pairs of Nucleobases. *Journal of Physical Chemistry B*, **2002**, 106, 3013-3018	3.4	46
67	Fragment charge difference method for estimating donor–acceptor electronic coupling: Application to DNA stacks. *Journal of Chemical Physics*, **2002**, 117, 5607-5616	3.9	251
66	Superexchange Mediated Charge Hopping in DNA. *Journal of Physical Chemistry A*, **2002**, 106, 7599-7606	2.8	139
65	Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results. *Chemical Physics*, **2001**, 269, 83-91	2.3	73
64	Energetics of excess electron transfer in DNA. *Chemical Physics Letters*, **2001**, 342, 231-238	2.5	62
63	Charge transfer in DNA. Sensitivity of electronic couplings to conformational changes. *Physical Chemistry Chemical Physics*, **2001**, 3, 5421-5425	3.6	119
62	Electronic coupling between Watson–Crick pairs for hole transfer and transport in desoxyribonucleic acid. *Journal of Chemical Physics*, **2001**, 114, 5614-5620	3.9	213
61	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	2.1	3
60	Energetics of hole transfer in DNA. *Chemical Physics Letters*, **2000**, 324, 430-434	2.5	175
59	AM1/d Parameters for Molybdenum. *Journal of Physical Chemistry A*, **2000**, 104, 4089-4094	2.8	72
58	Electronic Coupling for Charge Transfer and Transport in DNA. *Journal of Physical Chemistry B*, **2000**, 104, 9740-9745	3.4	219
57	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		4
56	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	2.8	20
55	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	2.8	30
54	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	2.5	96

53	Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins. *Chemical Physics*, **1998**, 231, 13-25	2.3	102
52	Splitting of Cyclobutane-Type Uracil Dimer Cation Radicals. Hartree□Fock, MP2, and Density Functional Studies. *Journal of Physical Chemistry A*, **1998**, 102, 7168-7175	2.8	21
51	Substrate Oxidation in the Active Site of Xanthine Oxidase and Related Enzymes. A Model Density Functional Study. *Inorganic Chemistry*, **1998**, 37, 176-180	5.1	43
50	Ab Initio Study on the Structure and Splitting of the Uracil Dimer Anion Radical. *Journal of Physical Chemistry A*, **1997**, 101, 8335-8338	2.8	38
49	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	16.4	40
48	Protonation effects on the chromophore of green fluorescent protein. Quantum chemical study of the absorption spectrum. *Chemical Physics Letters*, **1997**, 272, 162-167	2.5	82
47	Extension of MNDO to d Orbitals: Parameters and Results for the Second-Row Elements and for the Zinc Group. *The Journal of Physical Chemistry*, **1996**, 100, 616-626		231
46	A Quantum Chemical Study of Photoinduced DNA Repair: On the Splitting of Pyrimidine Model Dimers Initiated by Electron Transfer. *Journal of the American Chemical Society*, **1996**, 118, 9750-9758	16.4	52
45	Extension of MNDO to d orbitals: parameters and results for silicon. *Computational and Theoretical Chemistry*, **1994**, 313, 141-154		49
44	Quantum chemical study of molecular ion complexes with hydrogen bonds (Review). *Journal of Structural Chemistry*, **1993**, 33, 899-924	0.9	1
43	Extension of MNDO to d orbitals: Parameters and results for the halogens. *International Journal of Quantum Chemistry*, **1992**, 44, 807-829	2.1	68
42	A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, **1992**, 44, 897-930	2.1	52
41	Extension of the MNDO formalism tod orbitals: Integral approximations and preliminary numerical results. *Theoretica Chimica Acta*, **1992**, 81, 391-404		168
40	Structure and energy characteristic of [Mg(H3O)n]2+ and [Mg(H2O)n□OH]+ complexes according to data from MNDO calculations. *Journal of Structural Chemistry*, **1992**, 32, 590-593	0.9	1
39	Molecular mechanics calculations of systems with strong hydrogen bonds. *Journal of Molecular Structure*, **1992**, 265, 179-187	3.4	3
38	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	0.9	
37	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		
36	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		

35	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		2
34	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		1
33	Quantum-chemical investigation of the mechanism of nucleophilic addition in the HCNO molecule. *Theoretical and Experimental Chemistry*, **1989**, 25, 662-665	1.3	
32	MNDO parameters for the Ca atom. *Journal of Structural Chemistry*, **1989**, 29, 793-795	0.9	
31	Diazabicycloalkanes with nitrogen atoms in bridgehead positions.. *Chemistry of Heterocyclic Compounds*, **1989**, 25, 305-310	1.4	
30	MNDO calculations of Mg compounds. *Journal of Structural Chemistry*, **1988**, 28, 926-929	0.9	2
29	Complexes with hydrogen bonds by the MNDO/M method. *Journal of Structural Chemistry*, **1988**, 29, 192-197	0.9	
28	Application of the MNDO method to investigation of properties and reactivity of molecules. *Journal of Structural Chemistry*, **1988**, 29, 120-146	0.9	12
27	Parameters of MNDO method for Zn atom. *Journal of Structural Chemistry*, **1988**, 28, 649-652	0.9	
26	MNDO calculations of systems containing hydrogen bonds. *Theoretica Chimica Acta*, **1987**, 72, 223-228		46
25	MNDO calculations of systems with hydrogen bonds S-H. *Theoretica Chimica Acta*, **1987**, 71, 327-331		3
24	MNDO calculations on systems containing S-H hydrogen bonds. *Journal of Structural Chemistry*, **1987**, 28, 5-8	0.9	1
23	Revised semiempirical parameters for Br, I, Sn, Hg, and Pb in the MNDO method. *Journal of Structural Chemistry*, **1987**, 28, 9-12	0.9	3
22	A program for searching for semiempirical parameters by the MNDO method. *Journal of Structural Chemistry*, **1987**, 28, 312-314	0.9	
21	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	0.9	1
20	Quantum-chemical study of the influence of the electronegativity of substituents on the reactivity of β-chloroethylamine derivatives. *Journal of Structural Chemistry*, **1986**, 27, 367-371	0.9	
19	The transition state in the half-electron method. *Journal of Structural Chemistry*, **1984**, 24, 593-596	0.9	
18	Investigation of electronic structure of chloro complexes of Rhodium(III). *Journal of Structural Chemistry*, **1984**, 25, 351-355	0.9	

17	X-ray spectra and model quantum-chemical calculation of SO2 in clathrates based on hydroquinone. *Journal of Structural Chemistry*, **1984**, 25, 371-376	0.9	2
16	X-ray spectra and electronic structure of the PCl3 molecule. *Journal of Structural Chemistry*, **1984**, 24, 676-682	0.9	
15	An x-ray spectral and quantum-chemical study of the electronic structure of ruthenium complexes. *Journal of Structural Chemistry*, **1984**, 24, 837-842	0.9	
14	Program for calculating the electronic structure of molecules, complexes, and clusters in the INDO aproximation. *Journal of Structural Chemistry*, **1983**, 23, 821-822	0.9	
13	A generalization of the half-electron method for calculations for complex compounds. *Journal of Structural Chemistry*, **1983**, 24, 344-348	0.9	
12	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	0.9	
11	Relaxation of the molecular orbitals in palladium complexes. *Journal of Structural Chemistry*, **1982**, 23, 50-55	0.9	3
10	Use of X-ray spectra to determine the semiempirical parameters of 4d transition metals. *Journal of Structural Chemistry*, **1982**, 23, 355-359	0.9	
9	Change in the electronic structure of the thiocyanate ion on coordination. *Journal of Structural Chemistry*, **1982**, 23, 364-368	0.9	6
8	Study of rotational isomerism in thiophenol, thioanisole, and their polyfluorinated derivatives. *Journal of Structural Chemistry*, **1982**, 23, 194-197	0.9	1
7	Interligand interaction in planar complexes of palladium (II) and platinum (II). *Journal of Structural Chemistry*, **1981**, 22, 282-285	0.9	1
6	Use of the eigenvalues of the matrix of the resonance interaction of the orbitals for an analysis of the M-lig bonds in the complexes cis- and trans-[Pd(NH3)2Cl2]. *Journal of Structural Chemistry*, **1981**, 22, 504-507	0.9	
5	One-center parameters dependent on the valence state of the atom. *Journal of Structural Chemistry*, **1981**, 22, 614-616	0.9	
4	Electronic structure of anions of organic dithioacids and their oxidation-reduction and electron-donor properties. *Bulletin of the Academy of Sciences of the USSR Division of Chemical Science*, **1981**, 30, 765-769		
3	Mutual influence of the ligands in the complexes [Pd(NH3)2X2]. *Journal of Structural Chemistry*, **1980**, 21, 276-280	0.9	2
2	An indo study of the electronic structure of the planar complexes [Pd(NH3)nCl4−n]n−2. *Journal of Structural Chemistry*, **1980**, 21, 281-286	0.9	
1	Quantum Chemical Calculation of Donor–Acceptor Coupling for Charge Transfer in DNA. *Topics in Current Chemistry*,37-72		58