

Alexander N Isaev

List of Publications by Year in descending order

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25
papers

261
citations

1477746

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940134

16
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26
all docs

26
docs citations

26
times ranked

210
citing authors

#	ARTICLE	IF	CITATIONS
1	MNDO calculations on hydrogen bonds. Modified function for core-core repulsion. <i>Theoretica Chimica Acta</i> , 1984, 64, 397-401.	0.9	120
2	Proton Conduction by a Chain of Water Molecules in Carbonic Anhydrase. <i>Journal of Physical Chemistry B</i> , 2001, 105, 6420-6426.	1.2	42
3	Intermolecular charge transfer as evidence for unusual O \cdots H \cdots C(sp ³) hydrogen bond. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 180-192.	1.1	16
4	Semiempirical and ab initio calculations on geometry and stability of intermediates. Stability of intermediates for nucleophilic reactions of carbonyl compounds in the gas phase and in solution. <i>Computational and Theoretical Chemistry</i> , 1985, 133, 263-268.	1.5	10
5	O \cdots H \cdots C hydrogen bond in the methane \cdots water complex. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 1978-1985.	0.1	8
6	Two kinds of X H \cdots C(sp ³) hydrogen bond formed by the methide anion: Syn- and anti-orientation of monomers. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 141-149.	1.1	7
7	Ammonia and phosphine complexes with proton donors. Hydrogen bonding from the backside of the N(P) lone pair. <i>Computational and Theoretical Chemistry</i> , 2018, 1142, 28-38.	1.1	7
8	C \cdots O, O \cdots C, and C \cdots C interactions in complexes of carbocations and carboanions. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 817-823.	0.3	6
9	Periodicity in proton conduction along a H \cdots bonded chain. Application to biomolecules. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 607-616.	1.0	5
10	On the question of hydrogen bond proton transfer. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 69-74.	0.1	5
11	Hydrogen bonded D \cdots H \cdots Y (Y = O, S, Hal) molecular complexes: A natural bond orbital analysis. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 601-609.	0.1	5
12	Effect of structural relaxation on the binding energy in a molecular complex. The role of relaxation in the formation of intermediate for nucleophilic reactions of carbonyl compounds. <i>Computational and Theoretical Chemistry</i> , 1999, 490, 249-262.	1.5	4
13	The wave nature of the protonic conductivity mechanism in the active site of carboanhydrase. <i>Russian Journal of Physical Chemistry A</i> , 2007, 81, 924-928.	0.1	4
14	Quantum-Chemical Calculations of a Long Proton Wire. Application of a Harmonic Model to Analysis of the Structure of an Ionic Defect in a Water Chain with an Excess Proton. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2201-2212.	1.1	4
15	The geometry and electronic structure of the ionic defect in a chain of water molecules between a donor and an acceptor. <i>Russian Journal of Physical Chemistry A</i> , 2010, 84, 434-443.	0.1	3
16	Keto-enol tautomerization of a peptide group with proton transfer through a water bridge. <i>Russian Journal of Physical Chemistry A</i> , 2015, 89, 1360-1367.	0.1	3
17	Comparative Analysis of Hydrogen, van der Waals, and Halogen Bonds in Ammonia Complexes with HCl and ClF Molecules. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2394-2406.	0.1	3
18	Nonconventional C(sp ³) \cdots Cl halogen bond in complexes of alkyl carbanions. <i>Chemical Physics Letters</i> , 2021, 763, 138195.	1.2	3

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19	Charge transfer in systems of conjugated bonds in cyanobiphenyl molecules: Quantum-chemical calculations of the structure and vibrational spectra. Russian Journal of Physical Chemistry A, 2009, 83, 430-435.	0.1	2
20	Donor-acceptor interaction and intramolecular proton transfer in aminopolyenes. Russian Journal of Physical Chemistry A, 2009, 83, 2095-2102.	0.1	2
21	The role of intramolecular hydrogen bonds in nucleophilic addition reactions of ketenamines. Russian Journal of Physical Chemistry A, 2012, 86, 1250-1253.	0.1	1
22	syn- and anti-H Bonds in Ammonia and Phosphine Complexes with Proton Donors. Russian Journal of Physical Chemistry A, 2018, 92, 1959-1969.	0.1	1
23	Cooperative interactions of hydrogen bonds in proton-transfer processes involving water molecules. Simulation of biochemical systems. Russian Journal of General Chemistry, 2008, 78, 704-722.	0.3	0
24	Structure of a proton wire in the harmonic model with allowance for the interproton interaction for the first and second neighbors. Russian Journal of Physical Chemistry A, 2014, 88, 2121-2128.	0.1	0
25	Strong dispersion interaction of the carbanionic center in methide anion derivatives with halogen atom of metal halides. Journal of Chemical Sciences, 2022, 134, 1.	0.7	0