Sergiy V Rosokha

List of Publications by Year
in descending order

81	4,030	172386 29	118793 62
papers	citations	h-index	g-index

86	86	86	3809
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Fresh Look at Electron-Transfer Mechanisms via the Donor/Acceptor Bindings in the Critical Encounter Complex. Accounts of Chemical Research, 2008, 41, 641-653.	7.6	359
2	Halide Recognition through Diagnosticâ€œAnionâ€“Ï€â€•Interactions: Molecular Complexes of Clâ¯, Brâ¯, and Iâ¯ with Olefinic and AromaticÏ€ Receptors. Angewandte Chemie - International Edition, 2004, 43, 4650-4652.	7.2	339
3	Intermolecular Ï€-to-Ï€ Bonding between Stacked Aromatic Dyads. Experimental and Theoretical Binding Energies and Near-IR Optical Transitions for Phenalenyl Radical/Radical versus Radical/Cation Dimerizations. Journal of the American Chemical Society, 2004, 126, 13850-13858.	6.6	286
4	Stable (Long-Bonded) Dimers via the Quantitative Self-Association of Different Cationic, Anionic, and Uncharged Ï€-Radicals:Â Structures, Energetics, and Optical Transitions. Journal of the American Chemical Society, 2003, 125, 12161-12171.	6.6	263
5	Molecular and Electronic Structures of the Long-Bonded Ï€-Dimers of Tetrathiafulvalene Cation-Radical in Intermolecular Electron Transfer and in (Solid-State) Conductivity. Journal of the American Chemical Society, 2007, 129, 828-838.	6.6	173
6	Donorâ¯Acceptor (Electronic) Coupling in the Precursor Complex to Organic Electron Transfer:Â Intermolecular and Intramolecular Self-Exchange between Phenothiazine Redox Centers. Journal of the American Chemical Society, 2004, 126, 1388-1401.	6.6	168
7	Continuum of Outer- and Inner-Sphere Mechanisms for Organic Electron Transfer. Steric Modulation of the Precursor Complex in Paramagnetic (Ion-Radical) Self-Exchanges. Journal of the American Chemical Society, 2007, 129, 3683-3697.	6.6	115
8	Intervalence (Charge-Resonance) Transitions in Organic Mixed-Valence Systems. Through-Space versus Through-Bond Electron Transfer between Bridged Aromatic (Redox) Centers. Journal of the American Chemical Society, 2003, 125, 15950-15963.	6.6	111
9	X-ray Structure Analysis and the Intervalent Electron Transfer in Organic Mixed-Valence Crystals with Bridged Aromatic Cation Radicals. Journal of the American Chemical Society, 2002, 124, 843-855.	6.6	110
10	Isolation of the Latent Precursor Complex in Electron-Transfer Dynamics. Intermolecular Association and Self-Exchange with Acceptor Anion Radicals. Journal of the American Chemical Society, 2003, 125, 2559-2571.	6.6	110
11	Experimental and Computational Probes of the Nature of Halogen Bonding: Complexes of Bromineâ€Containing Molecules with Bromide Anions. Chemistry - A European Journal, 2013, 19, 8774-8788.	1.7	109
12	Characterizing the Dimerizations of Phenalenyl Radicals by ab Initio Calculations and Spectroscopy:â€‰ Ïƒ-Bond Formation versus Resonance Ï€-Stabilization. Journal of Physical Chemistry A, 2005, 109, 11261-11267.	1.1	90
13	Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcusâ¯Hush Theories with Experiments. Journal of the American Chemical Society, 2003, 125, 3273-3283.	6.6	88
14	Steric Modulations in the Reversible Dimerizations of Phenalenyl Radicals via Unusually Weak Carbon-Centered Ï€- and Ïƒ-Bonds. Journal of Organic Chemistry, 2006, 71, 520-526.	1.7	87
15	The Preorganization Step in Organic Reaction Mechanisms. Charge-Transfer Complexes as Precursors to Electrophilic Aromatic Substitutions. Journal of Organic Chemistry, 2002, 67, 1727-1737.	1.7	85
16	Through-Space (Cofacial) Ï€-Delocalization among Multiple Aromatic Centers: Toroidal Conjugation in Hexaphenylbenzene-like Radical Cations. Angewandte Chemie - International Edition, 2005, 44, 5133-5136.	7.2	78
17	Quinones as Electron Acceptors. X-Ray Structures, Spectral (EPR, UVâ¯vis) Characteristics and Electron-Transfer Reactivities of Their Reduced Anion Radicals as Separated vs Contact Ion Pairs. Journal of the American Chemical Society, 2006, 128, 16708-16719.	6.6	78
18	Very Fast Electron Migrations within p-Doped Aromatic Cofacial Arrays Leading to Three-Dimensional (Toroidal) Ï€-Delocalization. Journal of the American Chemical Society, 2006, 128, 9394-9407.	6.6	78

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19	Conformation, Distance, and Connectivity Effects on Intramolecular Electron Transfer between Phenylene-Bridged Aromatic Redox Centersâ€. Journal of Physical Chemistry A, 2002, 106, 2283-2292.	1.1	71
20	Mechanism of Inner-Sphere Electron Transfer via Charge-Transfer (Precursor) Complexes. Redox Energetics of Aromatic Donors with the Nitrosonium Acceptor. Journal of the American Chemical Society, 2001, 123, 8985-8999.	6.6	64
21	Anionâ‹Ï€ Complexes of Halides with p-Benzoquinones: Structures, Thermodynamics, and Criteria of Charge Transfer to Electron Transfer Transition. Journal of the American Chemical Society, 2019, 141, 9338-9348.	6.6	52
22	â€œSeparatedâ€•versus â€œContactâ€•Ion-Pair Structures in Solution from Their Crystalline States:Â Dynamic Effects on Dinitrobenzenide as a Mixed-Valence Anion. Journal of the American Chemical Society, 2005, 127, 1797-1809.	6.6	50
23	Halogen bonding of electrophilic bromocarbons with pseudohalide anions. Physical Chemistry Chemical Physics, 2014, 16, 12968-12979.	1.3	40
24	X-ray Structures and Electronic Spectra of the Ï€-Halogen Complexes between Halogen Donors and Acceptors with Ï€-Receptors. , 2007, , 137-160.		37
25	The Spectral Elucidation versus the X-ray Structure of the Critical Precursor Complex in Bimolecular Electron Transfers:â€‰ Application of Experimental/Theoretical Solvent Probes to Ion-Radical (Redox) Dyads. Journal of the American Chemical Society, 2008, 130, 1944-1952.	6.6	35
26	The Question of Aromaticity in Open-Shell Cations and Anions as Ion-Radical Offsprings of Polycyclic Aromatic and Antiaromatic Hydrocarbons. Journal of Organic Chemistry, 2006, 71, 9357-9365.	1.7	34
27	Reversible Interchange of Charge-Transfer versus Electron-Transfer States in Organic Electron Transfer via Cross-Exchanges between Diamagnetic (Donor/Acceptor) Dyadsâ€. Journal of Physical Chemistry B, 2007, 111, 6655-6666.	1.2	33
28	Hybrid Network Formation via Halogen Bonding of the Neutral Bromo-Substituted Organic Molecules with Anionic Metalâ€“Bromide Complexes. Crystal Growth and Design, 2012, 12, 4149-4156.	1.4	32
29	Halogen-bonded assembly of hybrid inorganic/organic 3D-networks from dibromocuprate salts and tetrabromomethane. Chemical Communications, 2007, , 3383.	2.2	31
30	Halogen bond-assisted electron transfer reactions of aliphatic bromosubstituted electrophiles. Physical Chemistry Chemical Physics, 2014, 16, 1809-1813.	1.3	30
31	Intermolecular Electron-Transfer Mechanisms via Quantitative Structures and Ion-Pair Equilibria for Self-Exchange of Anionic (Dinitrobenzenide) Donors. Journal of the American Chemical Society, 2005, 127, 7411-7420.	6.6	29
32	Continuum of covalent to intermolecular bonding in the halogen-bonded complexes of 1,4-diazabicyclo[2.2.2]octane with bromine-containing electrophiles. Chemical Communications, 2018, 54, 8060-8063.	2.2	29
33	Mullikenâ€“Hush elucidation of the encounter (precursor) complex in intermolecular electron transfer via self-exchange of tetracyanoethylene anion-radical. Chemical Physics, 2006, 324, 117-128.	0.9	28
34	Counter-ion modulation of long-distance Ï€-bonding of the open-shell p-benzoquinone anions. Physical Chemistry Chemical Physics, 2009, 11, 324-332.	1.3	28
35	Molecular Recognition of NO/NO+ via Multicenter (Charge-Transfer) Binding to Bridged Diarene Donors. Effect of Structure on the Optical Transitions and Complexation Thermodynamics. Journal of Organic Chemistry, 2003, 68, 3947-3957.	1.7	27
36	Electronic structures of intermolecular charge-transfer states in fast electron transfers with tetrathiafulvalene donor. Thermal and photoactivation of [2 + 4] cycloaddition to o-chloranil acceptor. Photochemical and Photobiological Sciences, 2006, 5, 914.	1.6	27

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37	Unusual structural effects of intermolecular Ї€-bonding in the tetracyanopyrazine (ion-radical) dimer. New Journal of Chemistry, 2009, 33, 545-553.	1.4	26
38	â€œAntiâ€•electrostaticâ€•Halogen Bonding between Ions of Like Charge. Chemistry - A European Journal, 2021, 27, 16530-16542.	1.7	24
39	Interplay of Halogen and Ї€â€“Ї€ Charge-Transfer Bondings in Intermolecular Associates of Bromo- or Iododinitrobenzene with Tetramethyl-p-phenylenediamine. Journal of Physical Chemistry A, 2015, 119, 3833-3842.	1.1	23
40	Ї€-Bonded molecular wires: self-assembly of mixed-valence cation-radical stacks within the nanochannels formed by inert tetrakis[3,5-bis(trifluoromethyl)phenyl]borate anions. CrystEngComm, 2013, 15, 10638.	1.3	22
41	Electron-transfer reactions of halogenated electrophiles: a different look into the nature of halogen bonding. Faraday Discussions, 2017, 203, 315-332.	1.6	22
42	Effects of Supramolecular Architecture on Halogen Bonding between Diiodine and Heteroaromatic N-Oxides. Crystal Growth and Design, 2018, 18, 1198-1207.	1.4	22
43	Strong electronic coupling in intermolecular (charge-transfer) complexes. Mechanistic relevance to thermal and optical electron transfer from aromatic donors. New Journal of Chemistry, 2002, 26, 851-860.	1.4	21
44	From charge transfer to electron transfer in halogen-bonded complexes of electrophilic bromocarbons with halide anions. Physical Chemistry Chemical Physics, 2015, 17, 4989-4999.	1.3	21
45	Complexes of Diiodine with Heteroaromatic N-Oxides: Effects of Halogen-Bond Acceptors in Halogen Bonding. Journal of Physical Chemistry A, 2019, 123, 7113-7123.	1.1	21
46	â€œAnti-electrostaticâ€•halogen bonding in solution. Chemical Science, 2021, 12, 8246-8251.	3.7	20
47	Structural preferences in strong anionâ€“Ї€ and halogen-bonded complexes: Ї€- and Ї*f*-holes vs. frontier orbitals interaction. New Journal of Chemistry, 2018, 42, 10572-10583.	1.4	19
48	Diversity and uniformity in anionâ€“Ї€ complexes of thiocyanate with aromatic, olefinic and quinoidal Ї€-acceptors. Dalton Transactions, 2020, 49, 8734-8743.	1.6	19
49	Novel Arene Receptors as Nitric Oxide (NO) Sensors. Journal of the American Chemical Society, 2002, 124, 5620-5621.	6.6	18
50	Computational approaches and sigma-hole interactions: general discussion. Faraday Discussions, 2017, 203, 131-163.	1.6	17
51	Anion-Ї€ interaction in metal-organic networks formed by metal halides and tetracyanopyrazine. Journal of Molecular Structure, 2017, 1138, 129-135.	1.8	16
52	Resolving the halogen vs. hydrogen bonding dichotomy in solutions: intermolecular complexes of trihalomethanes with halide and pseudohalide anions. Physical Chemistry Chemical Physics, 2018, 20, 21999-22007.	1.3	16
53	Lewis acid effects on donorâ€“acceptor associations and redox reactions: ternary complexes of heteroaromatic N-oxides with boron trifluoride and organic donors. New Journal of Chemistry, 2009, 33, 2317.	1.4	15
54	From weak to strong interactions: structural and electron topology analysis of the continuum from the supramolecular chalcogen bonding to covalent bonds. Physical Chemistry Chemical Physics, 2022, 24, 8251-8259.	1.3	15

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55	Examining a Transition from Supramolecular Halogen Bonding to Covalent Bonds: Topological Analysis of Electron Densities and Energies in the Complexes of Bromosubstituted Electrophiles. ACS Omega, 2021, 6, 23588-23597.	1.6	14
56	Mechanism and Thermodynamics of Reductive Cleavage of Carbonâ€“Halogen Bonds in the Polybrominated Aliphatic Electrophiles. Journal of Physical Chemistry A, 2016, 120, 1706-1715.	1.1	13
57	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodoâ€•p â€benzoquinone with Iodide Anions. Angewandte Chemie - International Edition, 2020, 59, 17197-17201.	7.2	13
58	Substituent-Induced Switch of the Role of Charge-Transfer Complexes in the Dielsâ€“Alder Reactions of o-Chloranil and Styrenes. Journal of Organic Chemistry, 2012, 77, 5971-5981.	1.7	10
59	Molecular Bases for Anesthetic Agents: Halothane as a Halogenâ€•and HydrogenâEBond Donor. Angewandte Chemie - International Edition, 2019, 58, 12456-12459.	7.2	10
60	Tris(thianthrene)(2+) bis(dodecamethylcarba-closo-dodecaborate) dichloromethane tetrasolvate: a crossed triple-decker Ï€-trimer dication. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o347-o349.	0.4	8
61	Intermolecular Ï€â€dimer of oxoverdazyl radicals with longâ€distance multicenter (2e/8c) bonding via nitrogen atoms. Journal of Physical Organic Chemistry, 2010, 23, 395-399.	0.9	8
62	From single-point to three-point halogen bonding between zinc(<scp>ii</scp>) tetrathiocyanate and tetrabromomethane. CrystEngComm, 2016, 18, 488-495.	1.3	8
63	Effects of structural variations on Ï€-dimer formation: long-distance multicenter bonding of cation-radicals of tetrathiafulvalene analogues. Physical Chemistry Chemical Physics, 2020, 22, 25054-25065.	1.3	8
64	Intermolecular Interactions between Halogenâ€Substituted pâ€Benzoquinones and Halide Anions: Anionâ€Ï€ Complexes versus Halogen Bonding. ChemPlusChem, 2020, 85, 441-449.	1.3	8
65	One- and two-dimensional coordination networks of the tetracyanoethylene anion-radicals with potassium counter-ions. Polyhedron, 2009, 28, 4136-4140.	1.0	7
66	Trimorphism of a model carcinogen 4-nitroquinoline-N-oxide. CrystEngComm, 2009, 11, 2400.	1.3	7
67	Spectroscopic and Electrochemical Evaluation of Salt Effects on Electronâ€Transfer Equilibria between Donor/Acceptor and Ionâ€Radical Pairs in Organic Solvents. ChemPhysChem, 2008, 9, 2406-2413.	1.0	6
68	Structures, Multicenter Ï€-Bonding, and Spin Equilibria in the Mixed-Valence Trimers of Tetramethyltetrathiafulvalene Cation-Radicals. Crystal Growth and Design, 2021, 21, 7257-7268.	1.4	6
69	Charge-Transfer Effects on Arene Structure and Reactivity. , 0, , 435-478.		5
70	2,3,4,5,6-Pentanitroaniline 1,2-dichloroethane disolvate: `pushâ€“pull' deformation of aromatic rings by intramolecular charge transfer. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, o464-o466.	0.4	5
71	The halogen bond in solution: general discussion. Faraday Discussions, 2017, 203, 347-370.	1.6	5
72	Halogen Bonding in the Complexes of Brominated Electrophiles with Chloride Anions: From a Weak Supramolecular Interaction to a Covalent Brâ€“Cl Bond. Crystals, 2020, 10, 1075.	1.0	5

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73	Molecular Bases for Anesthetic Agents: Halothane as a Halogenâ€•and Hydrogenâ€Bond Donor. Angewandte Chemie, 2019, 131, 12586-12589.	1.6	4
74	Efficient energy transfer in phenyl-ethynyl-linked asymmetric BODIPY dimers. Tetrahedron, 2020, 76, 131515.	1.0	4
75	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodoâ€•p â€benzoquinone with Iodide Anions. Angewandte Chemie, 2020, 132, 17350-17354.	1.6	4
76	Solvent and Ionic Atmosphere Effects in Anionâ˜Ï€ Interactions: Complexes of Halide Anions with p-Benzoquinones. Journal of Physical Chemistry A, 2022, 126, 4255-4263.	1.1	3
77	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	1.6	2
78	Halide Recognition through Diagnostic ?Anion-?? Interactions: Molecular Complexes of Cl?, Br?, and I? with Olefinic and Aromatic ? Receptors. Angewandte Chemie - International Edition, 2005, 44, 2178-2178.	7.2	1
79	Editorial: Advanced Research in Halogen Bonding. Crystals, 2022, 12, 133.	1.0	1
80	Innentitelbild: Molecular Bases for Anesthetic Agents: Halothane as a Halogenâ€•and Hydrogenâ€Bond Donor (Angew. Chem. 36/2019). Angewandte Chemie, 2019, 131, 12436-12436.	1.6	0
81	Frontispiece: â€œAntiâ€•electrostaticâ€•Halogen Bonding between Ions of Like Charge. Chemistry - A European Journal, 2021, 27, .	1.7	0