

# Sergiy V Rosokha

## List of Publications by Year in descending order

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81  
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4,030  
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172457

29  
h-index

118850

62  
g-index

86  
all docs

86  
docs citations

86  
times ranked

3809  
citing authors

#	ARTICLE	IF	CITATIONS
1	Fresh Look at Electron-Transfer Mechanisms via the Donor/Acceptor Bindings in the Critical Encounter Complex. <i>Accounts of Chemical Research</i> , 2008, 41, 641-653.	15.6	359
2	Halide Recognition through Diagnostic Anion- $\pi$ -Interactions: Molecular Complexes of Cl <sup>-</sup> , Br <sup>-</sup> , and I <sup>-</sup> with Olefinic and Aromatic $\pi$ Receptors. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4650-4652.	13.8	339
3	Intermolecular $\pi$ -to- $\pi$ Bonding between Stacked Aromatic Dyads. Experimental and Theoretical Binding Energies and Near-IR Optical Transitions for Phenalenyl Radical/Radical versus Radical/Cation Dimerizations. <i>Journal of the American Chemical Society</i> , 2004, 126, 13850-13858.	13.7	286
4	Stable (Long-Bonded) Dimers via the Quantitative Self-Association of Different Cationic, Anionic, and Uncharged $\pi$ -Radicals: Structures, Energetics, and Optical Transitions. <i>Journal of the American Chemical Society</i> , 2003, 125, 12161-12171.	13.7	263
5	Molecular and Electronic Structures of the Long-Bonded $\pi$ -Dimers of Tetrathiafulvalene Cation-Radical in Intermolecular Electron Transfer and in (Solid-State) Conductivity. <i>Journal of the American Chemical Society</i> , 2007, 129, 828-838.	13.7	173
6	Donor-Acceptor (Electronic) Coupling in the Precursor Complex to Organic Electron Transfer: Intermolecular and Intramolecular Self-Exchange between Phenothiazine Redox Centers. <i>Journal of the American Chemical Society</i> , 2004, 126, 1388-1401.	13.7	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. <i>Journal of the American Chemical Society</i> , 2007, 129, 3683-3697.	13.7	115
8	Intervalence (Charge-Resonance) Transitions in Organic Mixed-Valence Systems. Through-Space versus Through-Bond Electron Transfer between Bridged Aromatic (Redox) Centers. <i>Journal of the American Chemical Society</i> , 2003, 125, 15950-15963.	13.7	111
9	X-ray Structure Analysis and the Intervalent Electron Transfer in Organic Mixed-Valence Crystals with Bridged Aromatic Cation Radicals. <i>Journal of the American Chemical Society</i> , 2002, 124, 843-855.	13.7	110
10	Isolation of the Latent Precursor Complex in Electron-Transfer Dynamics. Intermolecular Association and Self-Exchange with Acceptor Anion Radicals. <i>Journal of the American Chemical Society</i> , 2003, 125, 2559-2571.	13.7	110
11	Experimental and Computational Probes of the Nature of Halogen Bonding: Complexes of Bromine-Containing Molecules with Bromide Anions. <i>Chemistry - A European Journal</i> , 2013, 19, 8774-8788.	3.3	109
12	Characterizing the Dimerizations of Phenalenyl Radicals by ab Initio Calculations and Spectroscopy: $\pi$ -Bond Formation versus Resonance $\pi$ -Stabilization. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11261-11267.	2.5	90
13	Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcus-Hush Theories with Experiments. <i>Journal of the American Chemical Society</i> , 2003, 125, 3273-3283.	13.7	88
14	Steric Modulations in the Reversible Dimerizations of Phenalenyl Radicals via Unusually Weak Carbon-Centered $\pi$ - and $\pi$ -Bonds. <i>Journal of Organic Chemistry</i> , 2006, 71, 520-526.	3.2	87
15	The Preorganization Step in Organic Reaction Mechanisms. Charge-Transfer Complexes as Precursors to Electrophilic Aromatic Substitutions. <i>Journal of Organic Chemistry</i> , 2002, 67, 1727-1737.	3.2	85
16	Through-Space (Cofacial) $\pi$ -Delocalization among Multiple Aromatic Centers: Toroidal Conjugation in Hexaphenylbenzene-like Radical Cations. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 5133-5136.	13.8	78
17	Quinones as Electron Acceptors. X-Ray Structures, Spectral (EPR, UV-vis) Characteristics and Electron-Transfer Reactivities of Their Reduced Anion Radicals as Separated vs Contact Ion Pairs. <i>Journal of the American Chemical Society</i> , 2006, 128, 16708-16719.	13.7	78
18	Very Fast Electron Migrations within p-Doped Aromatic Cofacial Arrays Leading to Three-Dimensional (Toroidal) $\pi$ -Delocalization. <i>Journal of the American Chemical Society</i> , 2006, 128, 9394-9407.	13.7	78

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19	Conformation, Distance, and Connectivity Effects on Intramolecular Electron Transfer between Phenylene-Bridged Aromatic Redox Centers. Journal of Physical Chemistry A, 2002, 106, 2283-2292.	2.5	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.	13.7	64
21	Anion-π Complexes of Halides with <i>p</i> -Benzoquinones: Structures, Thermodynamics, and Criteria of Charge Transfer to Electron Transfer Transition. Journal of the American Chemical Society, 2019, 141, 9338-9348.	13.7	52
22	Separated versus Contact Ion-Pair Structures in Solution from Their Crystalline States: Dynamic Effects on Dinitrobenzene as a Mixed-Valence Anion. Journal of the American Chemical Society, 2005, 127, 1797-1809.	13.7	50
23	Halogen bonding of electrophilic bromocarbons with pseudohalide anions. Physical Chemistry Chemical Physics, 2014, 16, 12968-12979.	2.8	40
24	X-ray Structures and Electronic Spectra of the π-Halogen Complexes between Halogen Donors and Acceptors with π-Receptors. , 2007, , 137-160.		37
25	The Spectral Elucidation versus the X-ray Structure of the Critical Precursor Complex in Bimolecular Electron Transfers: Application of Experimental/Theoretical Solvent Probes to Ion-Radical (Redox) Dyads. Journal of the American Chemical Society, 2008, 130, 1944-1952.	13.7	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.	3.2	34
27	Reversible Interchange of Charge-Transfer versus Electron-Transfer States in Organic Electron Transfer via Cross-Exchanges between Diamagnetic (Donor/Acceptor) Dyads. Journal of Physical Chemistry B, 2007, 111, 6655-6666.	2.6	33
28	Hybrid Network Formation via Halogen Bonding of the Neutral Bromo-Substituted Organic Molecules with Anionic Metal-Bromide Complexes. Crystal Growth and Design, 2012, 12, 4149-4156.	3.0	32
29	Halogen-bonded assembly of hybrid inorganic/organic 3D-networks from dibromocuprate salts and tetrabromomethane. Chemical Communications, 2007, , 3383.	4.1	31
30	Halogen bond-assisted electron transfer reactions of aliphatic bromosubstituted electrophiles. Physical Chemistry Chemical Physics, 2014, 16, 1809-1813.	2.8	30
31	Intermolecular Electron-Transfer Mechanisms via Quantitative Structures and Ion-Pair Equilibria for Self-Exchange of Anionic (Dinitrobenzene) Donors. Journal of the American Chemical Society, 2005, 127, 7411-7420.	13.7	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.	4.1	29
33	Mulliken-Hush elucidation of the encounter (precursor) complex in intermolecular electron transfer via self-exchange of tetracyanoethylene anion-radical. Chemical Physics, 2006, 324, 117-128.	1.9	28
34	Counter-ion modulation of long-distance π-bonding of the open-shell <i>p</i> -benzoquinone anions. Physical Chemistry Chemical Physics, 2009, 11, 324-332.	2.8	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.	3.2	27
36	Electronic structures of intermolecular charge-transfer states in fast electron transfers with tetrathiafulvalene donor. Thermal and photoactivation of [2 + 4] cycloaddition to <i>o</i> -chloranil acceptor. Photochemical and Photobiological Sciences, 2006, 5, 914.	2.9	27

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37	Unusual structural effects of intermolecular $\pi$ -bonding in the tetracyanopyrazine (ion-radical) dimer. <i>New Journal of Chemistry</i> , 2009, 33, 545-553.	2.8	26
38	Anti-electrostatic Halogen Bonding between Ions of Like Charge. <i>Chemistry - A European Journal</i> , 2021, 27, 16530-16542.	3.3	24
39	Interplay of Halogen and $\pi$ -Charge-Transfer Bondings in Intermolecular Associates of Bromo- or Iododinitrobenzene with Tetramethyl-p-phenylenediamine. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3833-3842.	2.5	23
40	$\pi$ -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. <i>CrystEngComm</i> , 2013, 15, 10638.	2.6	22
41	Electron-transfer reactions of halogenated electrophiles: a different look into the nature of halogen bonding. <i>Faraday Discussions</i> , 2017, 203, 315-332.	3.2	22
42	Effects of Supramolecular Architecture on Halogen Bonding between Diiodine and Heteroaromatic N-Oxides. <i>Crystal Growth and Design</i> , 2018, 18, 1198-1207.	3.0	22
43	Strong electronic coupling in intermolecular (charge-transfer) complexes. Mechanistic relevance to thermal and optical electron transfer from aromatic donors. <i>New Journal of Chemistry</i> , 2002, 26, 851-860.	2.8	21
44	From charge transfer to electron transfer in halogen-bonded complexes of electrophilic bromocarbons with halide anions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4989-4999.	2.8	21
45	Complexes of Diiodine with Heteroaromatic N-Oxides: Effects of Halogen-Bond Acceptors in Halogen Bonding. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7113-7123.	2.5	21
46	Anti-electrostatic halogen bonding in solution. <i>Chemical Science</i> , 2021, 12, 8246-8251.	7.4	20
47	Structural preferences in strong anion- $\pi$ and halogen-bonded complexes: $\pi$ - and $\pi^*$ -holes vs. frontier orbitals interaction. <i>New Journal of Chemistry</i> , 2018, 42, 10572-10583.	2.8	19
48	Diversity and uniformity in anion- $\pi$ complexes of thiocyanate with aromatic, olefinic and quinoidal $\pi$ -acceptors. <i>Dalton Transactions</i> , 2020, 49, 8734-8743.	3.3	19
49	Novel Arene Receptors as Nitric Oxide (NO) Sensors. <i>Journal of the American Chemical Society</i> , 2002, 124, 5620-5621.	13.7	18
50	Computational approaches and sigma-hole interactions: general discussion. <i>Faraday Discussions</i> , 2017, 203, 131-163.	3.2	17
51	Anion- $\pi$ interaction in metal-organic networks formed by metal halides and tetracyanopyrazine. <i>Journal of Molecular Structure</i> , 2017, 1138, 129-135.	3.6	16
52	Resolving the halogen vs. hydrogen bonding dichotomy in solutions: intermolecular complexes of trihalomethanes with halide and pseudohalide anions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21999-22007.	2.8	16
53	Lewis acid effects on donor-acceptor associations and redox reactions: ternary complexes of heteroaromatic N-oxides with boron trifluoride and organic donors. <i>New Journal of Chemistry</i> , 2009, 33, 2317.	2.8	15
54	From weak to strong interactions: structural and electron topology analysis of the continuum from the supramolecular chalcogen bonding to covalent bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8251-8259.	2.8	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. <i>ACS Omega</i> , 2021, 6, 23588-23597.	3.5	14
56	Mechanism and Thermodynamics of Reductive Cleavage of Carbon-Halogen Bonds in the Polybrominated Aliphatic Electrophiles. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1706-1715.	2.5	13
57	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodo- <i>p</i> -benzoquinone with Iodide Anions. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17197-17201.	13.8	13
58	Substituent-Induced Switch of the Role of Charge-Transfer Complexes in the Diels-Alder Reactions of <i>o</i> -Chloroanil and Styrenes. <i>Journal of Organic Chemistry</i> , 2012, 77, 5971-5981.	3.2	10
59	Molecular Bases for Anesthetic Agents: Halothane as a Halogen- and Hydrogen-Bond Donor. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12456-12459.	13.8	10
60	Tris(thianthrene)(2+) bis(dodecamethylcarba-closo-dodecaborate) dichloromethane tetrasolvate: a crossed triple-decker $\pi$ -trimer dication. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o347-o349.	0.4	8
61	Intermolecular $\pi$ -dimer of oxoverdazyl radicals with long-distance multicenter (2e/8c) bonding via nitrogen atoms. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 395-399.	1.9	8
62	From single-point to three-point halogen bonding between zinc( <i>sc</i> ) tetrathiocyanate and tetrabromomethane. <i>CrystEngComm</i> , 2016, 18, 488-495.	2.6	8
63	Effects of structural variations on $\pi$ -dimer formation: long-distance multicenter bonding of cation-radicals of tetrathiafulvalene analogues. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25054-25065.	2.8	8
64	Intermolecular Interactions between Halogen-Substituted <i>p</i> -Benzoquinones and Halide Anions: Anion-Complexes versus Halogen Bonding. <i>ChemPlusChem</i> , 2020, 85, 441-449.	2.8	8
65	One- and two-dimensional coordination networks of the tetracyanoethylene anion-radicals with potassium counter-ions. <i>Polyhedron</i> , 2009, 28, 4136-4140.	2.2	7
66	Trimorphism of a model carcinogen 4-nitroquinoline-N-oxide. <i>CrystEngComm</i> , 2009, 11, 2400.	2.6	7
67	Spectroscopic and Electrochemical Evaluation of Salt Effects on Electron-Transfer Equilibria between Donor/Acceptor and Ion-Radical Pairs in Organic Solvents. <i>ChemPhysChem</i> , 2008, 9, 2406-2413.	2.1	6
68	Structures, Multicenter $\pi$ -Bonding, and Spin Equilibria in the Mixed-Valence Trimers of Tetramethyltetrathiafulvalene Cation-Radicals. <i>Crystal Growth and Design</i> , 2021, 21, 7257-7268.	3.0	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: 'push-pull' deformation of aromatic rings by intramolecular charge transfer. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o464-o466.	0.4	5
71	The halogen bond in solution: general discussion. <i>Faraday Discussions</i> , 2017, 203, 347-370.	3.2	5
72	Halogen Bonding in the Complexes of Brominated Electrophiles with Chloride Anions: From a Weak Supramolecular Interaction to a Covalent Br-Cl Bond. <i>Crystals</i> , 2020, 10, 1075.	2.2	5

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73	Molecular Bases for Anesthetic Agents: Halothane as a Halogen- and Hydrogen-Bond Donor. <i>Angewandte Chemie</i> , 2019, 131, 12586-12589.	2.0	4
74	Efficient energy transfer in phenyl-ethynyl-linked asymmetric BODIPY dimers. <i>Tetrahedron</i> , 2020, 76, 131515.	1.9	4
75	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodo- <i>p</i> -benzoquinone with Iodide Anions. <i>Angewandte Chemie</i> , 2020, 132, 17350-17354.	2.0	4
76	Solvent and Ionic Atmosphere Effects in Anion- $\pi$ Interactions: Complexes of Halide Anions with <i>p</i> -Benzoquinones. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4255-4263.	2.5	3
77	Solid-state chemistry and applications: general discussion. <i>Faraday Discussions</i> , 2017, 203, 459-483.	3.2	2
78	Halide Recognition through Diagnostic $\pi$ -Anion- $\pi$ Interactions: Molecular Complexes of Cl <sup>-</sup> , Br <sup>-</sup> , and I <sup>-</sup> with Olefinic and Aromatic $\pi$ Receptors. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2178-2178.	13.8	1
79	Editorial: Advanced Research in Halogen Bonding. <i>Crystals</i> , 2022, 12, 133.	2.2	1
80	Innentitelbild: Molecular Bases for Anesthetic Agents: Halothane as a Halogen- and Hydrogen-Bond Donor ( <i>Angew. Chem.</i> 36/2019). <i>Angewandte Chemie</i> , 2019, 131, 12436-12436.	2.0	0
81	Frontispiece: $\pi$ - $\pi$ Electrostatic- $\pi$ -Halogen Bonding between Ions of Like Charge. <i>Chemistry - A European Journal</i> , 2021, 27, .	3.3	0