Snezana Zaric

List of Publications by Year in Descending Order

142 papers	3,034 citations	32 h-index	48 g-index
144 ext. papers	3,287 ext. citations	4.5 avg, IF	5.44 L-index

#	Paper	IF	Citations
142	Decisive Influence of Environment on Aromatic/Aromatic Interaction Geometries. Comparison of Aromatic/Aromatic Interactions in Crystal Structures of Small Molecules and in Protein Structures. *Crystal Growth and Design*, **2021**, 21, 1898-1904	3.5	3
141	Significant Stacking Interactions of Resonance-Assisted Hydrogen-Bridged (RAHB) Rings at Large Horizontal Displacements. *Crystal Growth and Design*, **2021**, 21, 4947-4958	3.5	
140	Joint Isotherm Calorimetric TitrationDFT Investigation of the Demethoxy-Amination of Fischer Carbenes. *Journal of Organometallic Chemistry*, **2020**, 929, 121582	2.3	1
139	Stacking Interactions between Indenyl Ligands of Transition Metal Complexes: Crystallographic and Density Functional Study. *Crystal Growth and Design*, **2020**, 20, 4491-4502	3.5	2
138	Strong stacking interactions at large horizontal displacements of tropylium and cyclooctatetraenide ligands of transition metal complexes: crystallographic and DFT study. *CrystEngComm*, **2020**, 22, 3831-3839	3.3	2
137	Stacking interactions of aromatic ligands in transition metal complexes. *Coordination Chemistry Reviews*, **2020**, 419, 213338	23.2	13
136	What is the preferred geometry of sulfurisulfide interactions?. *CrystEngComm*, **2020**, 22, 7262-7271	3.3	
135	Role of aromatic amino acids in amyloid self-assembly. *International Journal of Biological Macromolecules*, **2020**, 156, 949-959	7.9	21
134	Stacking interactions of resonance-assisted hydrogen-bridged rings and C-aromatic rings. *Physical Chemistry Chemical Physics*, **2020**, 22, 13721-13728	3.6	5
133	The Affinity of Some Lewis Bases for Hexafluoroisopropanol as a Reference Lewis Acid: An ITC/DFT Study. *ChemPhysChem*, **2020**, 21, 2136-2142	3.2	5
132	What Is Special about Aromatic-Aromatic Interactions? Significant Attraction at Large Horizontal Displacement. *ACS Central Science*, **2020**, 6, 420-425	16.8	23
131	How flexible is the water molecule structure? Analysis of crystal structures and the potential energy surface. *Physical Chemistry Chemical Physics*, **2020**, 22, 4138-4143	3.6	6
130	Phenol and Toluene Stacking Interactions, Including Interactions at Large Horizontal Displacements. Study of Crystal Structures and Calculation of Potential Energy Surfaces. *Crystal Growth and Design*, **2020**, 20, 1025-1034	3.5	9
129	Carbohydrate - Protein aromatic ring interactions beyond CH/interactions: A Protein Data Bank survey and quantum chemical calculations. *International Journal of Biological Macromolecules*, **2020**, 157, 1-9	7.9	9
128	Stacking interactions of the methylated cyclopentadienyl ligands in the crystal structures of transition metal complexes. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2020**, 76, 252-258	1.8	1
127	The Structural Details of Aspirin Molecules and Crystals. *Current Medicinal Chemistry*, **2020**, 27, 99-120	4.3	1
126	Two-dimensional halogen-bonded organic frameworks based on the tetrabromobenzene-1,4-dicarboxylic acid building molecule. *CrystEngComm*, **2020**, 22, 24-34	3.3	8

125	Green Light-Responsive CO-Releasing Polymeric Materials Derived from Ring-Opening Metathesis Polymerization. *ACS Applied Materials & Interfaces*, **2019**, 11, 34376-34384	9.5	15
124	Soft Templating and Disorder in an Applied 1D Cobalt Coordination Polymer Electrocatalyst. *Matter* , **2019**, 1, 1354-1369	12.7	5
123	Influence of chelate ring type on chelate-chelate and chelate-aryl stacking: the case of nickel bis(dithiolene). *Physical Chemistry Chemical Physics*, **2019**, 21, 1198-1206	3.6	5
122	Stacking interaction potential energy surfaces of square-planar metal complexes containing chelate rings. *Advances in Inorganic Chemistry*, **2019**, 159-189	2.1	4
121	Strong stacking interactions of metal-chelate rings are caused by substantial electrostatic component. *Dalton Transactions*, **2019**, 48, 6328-6332	4.3	10
120	Stacking Interactions of Resonance-Assisted Hydrogen-Bridged Rings. A Systematic Study of Crystal Structures and Quantum-Chemical Calculations. *Crystal Growth and Design*, **2019**, 19, 5619-5628	3.5	6
119	Study of stacking interactions between two neutral tetrathiafulvalene molecules in Cambridge Structural Database crystal structures and by quantum chemical calculations. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 1-7	1.8	6
118	Binding of metal ions and water molecules to nucleic acid bases: the influence of water molecule coordination to a metal ion on water-nucleic acid base hydrogen bonds. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 301-309	1.8	0
117	Stacking interactions of borazine: important stacking at large horizontal displacements and dihydrogen bonding governed by electrostatic potentials of borazine. *Physical Chemistry Chemical Physics*, **2019**, 21, 24554-24564	3.6	4
116	Stacking interactions between ruthenium p-cymene complexes: combined crystallographic and density functional study. *CrystEngComm*, **2019**, 21, 7204-7210	3.3	6
115	Significant Differences in the Energy of X-H/Pt Interactions between Cisplatin and Transplatin Molecules. *ChemistrySelect*, **2019**, 4, 12909-12914	1.8	2
114	Influence of hydrogen bonds on edge-to-face interactions between pyridine molecules. *Journal of Molecular Modeling*, **2018**, 24, 60	2	3
113	Recent computational studies on transition-metal carbon–hydrogen bond activation of alkanes. *International Journal of Quantum Chemistry*, **2018**, 118, e25605	2.1	4
112	Influence of metal ion on chelate–aryl stacking interactions. *International Journal of Quantum Chemistry*, **2018**, 118, e25629	2.1	7
111	Unraveling the Role of a Flexible Tetradentate Ligand in the Aerobic Oxidative Carbon-Carbon Bond Formation with Palladium Complexes: A Computational Mechanistic Study. *Journal of the American Chemical Society*, **2018**, 140, 3929-3939	16.4	10
110	Probing the Carbon-Hydrogen Activation of Alkanes Following Photolysis of Tp'Rh(CNR)(carbodiimide): A Computational and Time-Resolved Infrared Spectroscopic Study. *Journal of the American Chemical Society*, **2018**, 140, 1842-1854	16.4	20
109	Chelated metal ions modulate the strength and geometry of stacking interactions: energies and potential energy surfaces for chelate-chelate stacking. *Physical Chemistry Chemical Physics*, **2018**, 20, 14053-14060	3.6	12
108	Insight into the Interactions of Amyloid β-Sheets with Graphene Flakes: Scrutinizing the Role of Aromatic Residues in Amyloids that Interact with Graphene. *ChemPhysChem*, **2018**, 19, 1226-1233	3.2	6

107	Investigation of interactions in Lewis pairs between phosphines and boranes by analyzing crystal structures from the Cambridge Structural Database. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2018**, 74, 255-263	1.8	3
106	Stacking of cyclopentadienyl organometallic sandwich and half-sandwich compounds. Strong interactions of sandwiches at large offsets. *CrystEngComm*, **2018**, 20, 4506-4514	3.3	8
105	Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes. *Coordination Chemistry Reviews*, **2017**, 345, 318-341	23.2	71
104	Is the R Si Moiety in Metal-Silyl Complexes a Z ligand? An Answer from the Interaction Energy. *Chemistry - A European Journal*, **2017**, 23, 17058-17069	4.8	18
103	Unexpected Importance of Aromatic-Aliphatic and Aliphatic Side Chain-Backbone Interactions in the Stability of Amyloids. *Chemistry - A European Journal*, **2017**, 23, 11046-11053	4.8	9
102	Methane Activations by Titanium Neopentylidene Complexes: Electronic Resilience and Steric Control. *Inorganic Chemistry*, **2017**, 56, 9264-9272	5.1	5
101	Stacking interactions between hydrogen-bridged and aromatic rings: study of crystal structures and quantum chemical calculations. *CrystEngComm*, **2017**, 19, 40-46	3.3	11
100	11. Large horizontal displacements of benzene□benzene stacking interactions in co-crystals **2017**, 255-271		2
99	Interactions of Aromatic Residues in Amyloids: A Survey of Protein Data Bank Crystallographic Data. *Crystal Growth and Design*, **2017**, 17, 6353-6362	3.5	10
98	Aliphatic-aromatic stacking interactions in cyclohexane-benzene are stronger than aromatic-aromatic interaction in the benzene dimer. *Physical Chemistry Chemical Physics*, **2016**, 18, 25791-25795	3.6	31
97	Hydrogen Bonding between Metal-Ion Complexes and Noncoordinated Water: Electrostatic Potentials and Interaction Energies. *ChemPhysChem*, **2016**, 17, 2035-42	3.2	9
96	The stacking interactions of bipyridine complexes: the influence of the metal ion type on the strength of interactions. *Journal of Molecular Modeling*, **2016**, 22, 30	2	5
95	Preferred Geometries and Energies of Sulfur□Sulfur Interactions in Crystal Structures. *Crystal Growth and Design*, **2016**, 16, 632-639	3.5	41
94	C□H/O Interactions of Aromatic CH Donors within Proteins: A Crystallographic Study. *Crystal Growth and Design*, **2016**, 16, 1948-1957	3.5	14
93	Parallel interactions of aromatic and heteroaromatic molecules. *Hemijska Industrija*, **2016**, 70, 649-659	0.6	2
92	Very Strong Parallel Interactions Between Two Saturated Acyclic Groups Closed with Intramolecular Hydrogen Bonds Forming Hydrogen-Bridged Rings. *Crystals*, **2016**, 6, 34	2.3	2
91	Coordinating Benzenes Stack Stronger than Noncoordinating Benzenes, even at Large Horizontal Displacements. *Crystal Growth and Design*, **2016**, 16, 4169-4172	3.5	21
90	Parallel Interactions of Aromatic Molecules at Large Horizontal Displacements **2016**, 241-260		

89	Carbon-hydrogen bond activation by a titanium neopentylidene complex. *Journal of Coordination Chemistry*, **2016**, 69, 1759-1768	1.6	7
88	Stacking interactions of hydrogen-bridged rings □stronger than the stacking of benzene molecules. *Chemical Communications*, **2015**, 51, 12989-91	5.8	24
87	Nature of the water/aromatic parallel alignment interactions. *Journal of Computational Chemistry*, **2015**, 36, 171-80	3.5	8
86	Strong Stacking between Organic and Organometallic Molecules as the Key for Material Design **2015**, 409-413		
85	Stacking of metal chelates with benzene: can dispersion-corrected DFT be used to calculate organic-inorganic stacking?. *ChemPhysChem*, **2015**, 16, 761-8	3.2	13
84	Anatase nanoparticles surface modified with fused ring salicylate-type ligands (1-hydroxy-2-naphthoic acids): A combined DFT and experimental study. *Journal of Alloys and Compounds*, **2015**, 630, 226-235	5.7	23
83	Strong Stacking between Organic and Organometallic Molecules as the Key for Material Design **2015**, 409-413		
82	What are the preferred horizontal displacements of aromatic-aromatic interactions in proteins? Comparison with the calculated benzene-benzene potential energy surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 11173-7	3.6	43
81	The effect of substituents on the surface modification of anatase nanoparticles with catecholate-type ligands: a combined DFT and experimental study. *Physical Chemistry Chemical Physics*, **2014**, 16, 20796-805	3.6	41
80	C□H/O interactions of nucleic bases with a water molecule: a crystallographic and quantum chemical study. *CrystEngComm*, **2014**, 16, 10089-10096	3.3	15
79	What are preferred water-aromatic interactions in proteins and crystal structures of small molecules?. *Physical Chemistry Chemical Physics*, **2014**, 16, 23549-53	3.6	12
78	Carbon-hydrogen activation of cycloalkanes by cyclopentadienylcarbonylrhodium--a lifetime enigma. *Journal of the American Chemical Society*, **2014**, 136, 8614-25	16.4	28
77	Stacking Interactions between Square-Planar Metal Complexes with 2,2?-Bipyridine Ligands. Analysis of Crystal Structures and Quantum Chemical Calculations. *Crystal Growth and Design*, **2014**, 14, 3880-3889	3.5	23
76	Experimental and theoretical investigations of the self-association of oxaliplatin. *Physical Chemistry Chemical Physics*, **2014**, 16, 14688-98	3.6	9
75	Stacking of benzene with metal chelates: calculated CCSD(T)/CBS interaction energies and potential-energy curves. *ChemPhysChem*, **2014**, 15, 2458-61	3.2	23
74	Computational study of protein secondary structure elements: Ramachandran plots revisited. *Journal of Molecular Graphics and Modelling*, **2014**, 50, 125-33	2.8	24
73	□Hole Interactions of Covalently-Bonded Nitrogen, Phosphorus and Arsenic: A Survey of Crystal Structures. *Crystals*, **2014**, 4, 12-31	2.3	138
72	Parallel water/aromatic interactions of non-coordinated and coordinated water. *ChemPhysChem*, **2014**, 15, 2386-96	3.2	4

71	Crystallographic and ab initio study of pyridine CHO interactions: linearity of the interactions and influence of pyridine classical hydrogen bonds. *CrystEngComm*, **2013**, 15, 10481	3.3	24
70	Mutual influence of parallel, CH/O, OH/ and lone pair/ interactions in water/benzene/water system. *Computational and Theoretical Chemistry*, **2013**, 1018, 59-65	2	21
69	Surface modification of anatase nanoparticles with fused ring salicylate-type ligands (3-hydroxy-2-naphthoic acids): a combined DFT and experimental study of optical properties. *Nanoscale*, **2013**, 5, 7601-12	7.7	36
68	The influence of water molecule coordination onto the water romatic interaction. Strong interactions of water coordinating to a metal ion. *CrystEngComm*, **2013**, 15, 2099	3.3	10
67	Parallel interactions at large horizontal displacement in pyridine-pyridine and benzene-pyridine dimers. *ChemPhysChem*, **2013**, 14, 237-43	3.2	41
66	Stacking interactions of Ni(acac) chelates with benzene: calculated interaction energies. *ChemPhysChem*, **2013**, 14, 1797-800	3.2	14
65	Influence of supramolecular structures in crystals on parallel stacking interactions between pyridine molecules. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2013**, 69, 389-94	1.8	10
64	Preparation and characterization of zinc-exchanged montmorillonite and its effectiveness as aflatoxin B1 adsorbent. *Materials Chemistry and Physics*, **2012**, 137, 213-220	4.4	14
63	The influence of water molecule coordination to a metal ion on water hydrogen bonds. *Physical Chemistry Chemical Physics*, **2012**, 14, 10896-8	3.6	31
62	Noncovalent Interactions of Systems in Crystal Structures of Transition-Metal Complexes **2012**, 243-274		
61	CH/ interactions in metal-porphyrin complexes with pyrrole and chelate rings as hydrogen acceptors. *Journal of Inorganic Biochemistry*, **2012**, 117, 157-63	4.2	10
60	Surface modification of anatase nanoparticles with fused ring catecholate type ligands: a combined DFT and experimental study of optical properties. *Nanoscale*, **2012**, 4, 1612-9	7.7	48
59	Crystallographic and ab Initio Study of Pyridine Stacking Interactions. Local Nature of Hydrogen Bond Effect in Stacking Interactions. *Crystal Growth and Design*, **2012**, 12, 1060-1063	3.5	62
58	Parallel stacking interactions in square-planar transition-metal complexes containing fused chelate and C6-aromatic rings. *Acta Crystallographica Section B: Structural Science*, **2012**, 68, 261-5		20
57	Are CH?O interactions linear? The case of aromatic CH donors. *CrystEngComm*, **2011**, 13, 5005	3.3	58
56	Geometries of stacking interactions between phenanthroline ligands in crystal structures of square-planar metal complexes. *Journal of Molecular Modeling*, **2011**, 17, 2083-92	2	14
55	What are the preferred horizontal displacements in parallel aromatic-aromatic interactions? Significant interactions at large displacements. *ChemPhysChem*, **2011**, 12, 3511-4	3.2	62
54	Water/Aromatic Parallel Alignment Interactions. Significant Interactions at Large Horizontal Displacements. *Crystal Growth and Design*, **2011**, 11, 2680-2683	3.5	24

53	Understanding the factors affecting the activation of alkane by Cp'Rh(CO)2 (Cp' = Cp or Cp*). *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20178-83	11.5	32
52	Classification of stacking interaction geometries of terpyridyl square-planar complexes in crystal structures. *CrystEngComm*, **2010**,	3.3	3
51	Evidence of Chelate□Chelate Stacking Interactions in Crystal Structures of Transition-Metal Complexes. *Crystal Growth and Design*, **2010**, 10, 3901-3908	3.5	76
50	Protein subunit interfaces: A statistical analysis of hot spots in Sm proteins. *Journal of Molecular Modeling*, **2010**, 16, 1743-51	2	5
49	Oxygen atom transfer catalysis: Ligand effects on the key reaction barrier in molybdenum (VI) dioxo systems. *Journal of Molecular Catalysis A*, **2010**, 324, 15-23		11
48	Influence of natural zeolitic tuff and organozeolites surface charge on sorption of ionizable fumonisin B(1). *Colloids and Surfaces B: Biointerfaces*, **2010**, 76, 272-8	6	22
47	The stereospecific ligand exchange at a pseudo-benzylic T-4 iridium centre in planar-chiral cycloiridium (eta(6)-arene)tricarbonylchromium complexes. *Chemistry - A European Journal*, **2009**, 15, 10830-42	4.8	14
46	A reexamination of correlations of amino acids with particular secondary structures. *Protein Journal* , **2009**, 28, 74-86	3.9	9
45	Intramolecular MLOH/□and MLNH/□Interactions in crystal structures of metal complexes. *Chemical Papers*, **2009**, 63,	1.9	5
44	Parallel alignment of water and aryl rings-crystallographic and theoretical evidence for the interaction. *Chemical Communications*, **2008**, 6546-8	5.8	41
43	Probing the Mechanism of Carbon□Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. *Organometallics*, **2008**, 27, 189-201	3.8	25
42	A reexamination of the propensities of amino acids towards a particular secondary structure: classification of amino acids based on their chemical structure. *Journal of Molecular Modeling*, **2008**, 14, 769-75	2	58
41	Stereoselective □Electrophilic□Cyclometalation of Planar-Prochiral (□6-Arene)tricarbonylchromium Complexes with Asymmetric Metal Centers: pseudo-T-4 [Cp*RhCl2]2 and [Cp*IrCl2]2. *Organometallics*, **2007**, 26, 3336-3345	3.8	88
40	Stacking vs. CH□Interactions between chelate and aryl rings in crystal structures of square-planar transition metal complexes. *CrystEngComm*, **2007**, 9, 793	3.3	61
39	Are chelate rings aromatic? Calculations of magnetic properties of acetylacetonato and o-benzoquinonediimine chelate rings. *Inorganic Chemistry*, **2007**, 46, 7109-14	5.1	66
38	Comparison of structural features of three new cis-dioxomolybdenum(VI) complexes with 2-hydroxy-1-naphthaldehyde-S-methylisothiosemicarbazone: Possible role of intermolecular interactions on the geometry of the cis-MoO2 unit. *Inorganica Chimica Acta*, **2007**, 360, 2197-2206	2.7	23
37	Influence of metal and ligand types on stacking interactions of phenyl rings with square-planar transition metal complexes. *Open Chemistry*, **2007**, 5, 20-31	1.6	7
36	XH/pi interactions with the pi system of porphyrin ring in porphyrin-containing proteins. *Journal of Biological Inorganic Chemistry*, **2007**, 12, 1063-71	3.7	25

35	Orientations of axially coordinated imidazoles and pyridines in crystal structures of model systems of cytochromes. *Journal of Inorganic Biochemistry*, **2006**, 100, 133-42	4.2	7
34	Mechanistic investigation of the oxygen-atom-transfer reactivity of dioxo-molybdenum(VI) complexes. *Chemistry - A European Journal*, **2006**, 12, 7501-9	4.8	49
33	Electron delocalization mediates the metal-dependent capacity for CH/pi interactions of acetylacetonato chelates. *Inorganic Chemistry*, **2006**, 45, 4755-63	5.1	77
32	Stacking Interactions between Chelate and Phenyl Rings in Square-Planar Transition Metal Complexes. *Crystal Growth and Design*, **2006**, 6, 29-31	3.5	80
31	Multi-□□stacked interaction between planar chelate rings in the crystal structure of dichloro(2-hydroxy-1-naphtaldehyde-3-methylisothiosemicarbazonato)iron(III) hemiethanol solvate. *Inorganic Chemistry Communication*, **2006**, 9, 833-835	3.1	11
30	CH/□interactions of □system of acetylacetonato chelate ring: Comparison of CH/□interactions of Ni(II)-acetylacetonato chelate and benzene rings. *Inorganica Chimica Acta*, **2006**, 359, 4427-4430	2.7	23
29	Statistical dependence of protein secondary structure on amino acid bigrams. *Chemical Industry and Chemical Engineering Quarterly*, **2006**, 12, 82-85	0.7	
28	Adsorption of mycotoxins by organozeolites. *Colloids and Surfaces B: Biointerfaces*, **2005**, 46, 20-5	6	87
27	Computational studies on imidazole heme conformations. *Journal of Biological Inorganic Chemistry*, **2005**, 10, 343-54	3.7	33
26	Intramolecular CH□□□interactions in Metal-Porphyrin Complexes. *International Journal of Molecular Sciences*, **2004**, 5, 174-185	6.3	20
25	Intermolecular Interactions between Chelate Rings and Phenyl Rings in Square-Planar Copper(II) Complexes. *European Journal of Inorganic Chemistry*, **2004**, 2004, 2215-2218	2.3	52
24	Very strong metal ligand aromatic cation-□interactions in transition metal complexes: intermolecular interaction in tetraphenylborate salts. *Inorganica Chimica Acta*, **2004**, 357, 4327-4329	2.7	21
23	C-H. . .pi interactions in the metal-porphyrin complexes with chelate ring as the H acceptor. *Journal of Inorganic Biochemistry*, **2004**, 98, 1867-73	4.2	56
22	Theoretical study on orientations of axially coordinated imidazoles in model systems of cytochromes. *Inorganica Chimica Acta*, **2003**, 349, 1-5	2.7	23
21	Crystal structure and modeling calculation of the columnar helix 2,6-Bis(imino)phenoxy iron(III) chloride. *Inorganic Chemistry Communication*, **2003**, 6, 5-9	3.1	9
20	Theoretical study of metal ligand aromatic cation□interactions of [Co(NH3)6]3+ with benzene. *International Journal of Quantum Chemistry*, **2002**, 87, 354-359	2.1	5
19	Theoretical study on intermediate in oxygen transfer reaction in molybdoenzyme model system. *Inorganic Chemistry Communication*, **2002**, 5, 446-448	3.1	6
18	Synthesis and Absolute Configuration of Novel Mono- and Dinuclear Cobalt(III) Complexes Containing S-Phenylalanine. *Journal of Coordination Chemistry*, **2002**, 55, 517-526	1.6	2

17	Energetics of radical transfer in DNA photolyase. *Journal of the American Chemical Society*, **2002**, 124, 3775-82	16.4	49
16	Transition metal complexes with thiosemicarbazide-based ligands. Part XLI. Two crystal structures of cobalt(III) complexes with salicylaldehyde S-methylisothiosemicarbazone and theoretical study on orientations of coordinated pyridines. *Polyhedron*, **2001**, 20, 2231-2240	2.7	18
15	Artificial cytochrome b: computer modeling and evaluation of redox potentials. *Journal of the American Chemical Society*, **2001**, 123, 6040-53	16.4	41
14	Factors determining the orientation of axially coordinated imidazoles in heme proteins. *Biochemistry*, **2001**, 40, 7914-28	3.2	56
13	Theoretical study of cation□interactions of the metal complex cation, [Co(NH3)6]3+, with ethylene and acetylene. *Chemical Physics*, **2000**, 256, 213-223	2.3	17
12	Cation□nteraction with transition-metal complex as cation. *Chemical Physics Letters*, **1999**, 311, 77-80	2.5	39
11	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms 13: Methane, Ethylene, and Acetylene Activation at a Cationic Iridium Center. *ACS Symposium Series*, **1999**, 138-150	0.4	6
10	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 14. □Hydrogen Transfer and Alkene/Alkyne Insertion at a Cationic Iridium Center. *Organometallics*, **1998**, 17, 5139-5147	3.8	27
9	Prediction of the Reactive Intermediates in Alkane Activation by Tris(pyrazolyl borate)rhodium Carbonyl. *Journal of Physical Chemistry A*, **1998**, 102, 1963-1964	2.8	44
8	Ab Initio Calculations of the Geometry and Vibrational Frequencies of the Triplet State of Tungsten Pentacarbonyl Amine: A Model for the Unification of the Preresonance Raman and the Time-Resolved Infrared Experiments. *Journal of the American Chemical Society*, **1997**, 119, 2885-2888	16.4	8
7	Ab Initio Calculations of the Geometries and Bonding Energies of Alkane and Fluoroalkane Complexes with Tungsten Pentacarbonyl. *Journal of Physical Chemistry A*, **1997**, 101, 4646-4652	2.8	52
6	The anisotropic □effect of the nitro group in ammine-nitro cobalt(III) complexes. *Polyhedron*, **1997**, 16, 3565-3569	2.7	
5	Ab Initio and Density Functional Theory Applied to Models for the Oxo-Transfer Reaction of Dioxomolybdenum Enzymes **1997**, 255-277		
4	Methane Metathesis at a Cationic Iridium Center. *Journal of the American Chemical Society*, **1996**, 118, 6068-6069	16.4	105
3	Ligand field analysis of metal-oxygen interactions□ Tris(oxalato)cobaltate(III). *Polyhedron*, **1991**, 10, 2665-2672	2.7	4
2	Investigation of the effect of the aminocarboxylato chelate conformation on the optical activity of the cis(NO2),trans(NH2) -bis(aminocarboxylato)dinitrocobalt/ate(III) isomers. *Polyhedron*, **1988**, 7, 1153-1158	2.7	4
1	The Thermochemistry of Alkyne Insertion into a Palladacycle Outlines the Solvation Conundrum in DFT. *European Journal of Inorganic Chemistry*,	2.3	1