Florian Weigend

List of Publications by Year in Descending Order

172 papers	35,167 citations	44 h-index	187 g-index
194 ext. papers	41,005 ext. citations	6.1 avg, IF	7.92 L-index

#	Paper	IF	Citations
172	Introduction of plumbole to f-element chemistry.. *Chemical Science*, **2022**, 13, 945-954	9.4	4
171	Surprises in the Solvent-Induced Self-Ionization in the Uranium Tetrahalide UX (X = Cl, Br, I)/Ethyl Acetate System.. *ACS Omega*, **2022**, 7, 11995-12003	3.9	
170	Electronic structure and bonding in endohedral Zintl clusters.. *Chemical Society Reviews*, **2021**,	58.5	4
169	Paramagnetic NMR Shielding Tensors and Ring Currents: Efficient Implementation and Application to Heavy Element Compounds. *Journal of Physical Chemistry A*, **2021**, 125, 9707-9723	2.8	5
168	-Coordination and Functionalization of the 2-Phosphaethynthiolate Anion at Lanthanum(III)**. *Angewandte Chemie*, **2021**, 133, 9620-9625	3.6	4
167	Using a Porphyrin Diacid Cation to Stabilize a Square-Pyramidal BiX (X = Br, Cl/Br) Unit. *Inorganic Chemistry*, **2021**, 60, 4352-4356	5.1	1
166	Construction of Inorganic Crown Ethers by s-Block-Metal-Templated Si-O Bond Activation. *Angewandte Chemie - International Edition*, **2021**, 60, 10393-10401	16.4	3
165	Tracing the Jahn-Teller Distortion of C60n in Isostructural Fullerides [M(NH3)7]C60 ? NH3, M=Ba, Sr, K. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2021**, 647, 1132-1138	1.3	1
164	Near-Infrared Luminescence in Trinuclear Mixed-Metal Chalcogenolate Complexes of the Types [MTi(EPh)(PPh)] (M = Cu, Ag; E = S, Se) and [Na(thf)][Ti(SPh)]. *Inorganic Chemistry*, **2021**, 60, 8936-8945	5.1	0
163	NMR Indirect Spin-Spin Coupling Constants in a Modern Quasi-Relativistic Density Functional Framework. *Journal of Chemical Theory and Computation*, **2021**, 17, 3974-3994	6.4	10
162	Highly Soluble Supertetrahedra upon Selective Partial Butylation of Chalcogenido Metalate Clusters in Ionic Liquids. *Angewandte Chemie*, **2021**, 133, 17763-17769	3.6	0
161	Reactions of ThX4 (X=F, Cl, Br, I) with Liquid Ammonia-Crystal Structures and a Theoretical Study of Ammine Thorium(IV) Halide Ammoniates. *European Journal of Inorganic Chemistry*, **2021**, 2021, 2787-2796	2.3	0
160	Highly Soluble Supertetrahedra upon Selective Partial Butylation of Chalcogenido Metalate Clusters in Ionic Liquids. *Angewandte Chemie - International Edition*, **2021**, 60, 17622-17628	16.4	3
159	Substantial aromaticity in the anionic heavy-metal cluster [Th@Bi]. *Nature Chemistry*, **2021**, 13, 149-155	17.6	22
158	Photochemistry with Chlorine Trifluoride: Syntheses and Characterization of Difluorooxychloronium(V) Hexafluorido(non)metallates(V), [ClOF][MF] (M=V, Nb, Ta, Ru, Os, Ir, P, Sb). *Chemistry - A European Journal*, **2021**, 27, 2381-2392	4.8	1
157	Planar Iron Hydride Nanoclusters: Combined Spectroscopic and Theoretical Insights into Structures and Building Principles. *ChemistryOpen*, **2021**, 10, 265-271	2.3	
156	Aufbau anorganischer Kronenether durch s-Block-Metall-templatgesteuerte Si-O-Bindungsaktivierung. *Angewandte Chemie*, **2021**, 133, 10481-10490	3.6	1

155	Coordination and Functionalization of the 2-Phosphaethynthiolate Anion at Lanthanum(III)*. *Angewandte Chemie - International Edition*, **2021**, 60, 9534-9539	16.4	6
154	Structure and Reactivity of Alkaline Metal Bis(amido)diazadiarsetidinides. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2021**, 647, 1830-1839	1.3	1
153	The Archetypal Homoleptic Lanthanide Quadruple-Decker Synthesis, Mechanistic Studies, and Quantum Chemical Investigations. *Angewandte Chemie*, **2021**, 133, 24698	3.6	0
152	NON-Ligated N-Heterocyclic Tetrylenes. *European Journal of Inorganic Chemistry*, **2021**, 2021, 3591-3600	2.3	0
151	The Archetypal Homoleptic Lanthanide Quadruple-Decker-Synthesis, Mechanistic Studies, and Quantum Chemical Investigations. *Angewandte Chemie - International Edition*, **2021**, 60, 24493-24499	16.4	3
150	Tetrahedral [Sb(AuMe)4]3 Occurring in Multimetallic Cluster Syntheses: About the Structure-Directing Role of Methyl Groups. *Angewandte Chemie*, **2021**, 133, 25246	3.6	1
149	Tetrahedral [Sb(AuMe)] Occurring in Multimetallic Cluster Syntheses: About the Structure-Directing Role of Methyl Groups. *Angewandte Chemie - International Edition*, **2021**, 60, 25042-25047	16.4	1
148	The Arachno-Zintl Ion (Sn5Sb3)3 and the Effects of Element Composition on the Structures of Isoelectronic Clusters: Another Facet of the Pseudo-Element Concept. *Angewandte Chemie*, **2020**, 132, 14357-14361	3.6	3
147	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107	3.9	255
146	Atom Exchange Versus Reconstruction: (Ge As) (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au (Ge As)(Ge As)]. *Angewandte Chemie - International Edition*, **2020**, 59, 16638-16643	16.4	17
145	Low-Valent Group 14 Phosphinidenide Complexes [({SIDipp}P) M] Exhibit P-M p p Interaction (M=Ge, Sn, Pb). *Chemistry - A European Journal*, **2020**, 26, 192-197	4.8	17
144	Preparation and luminescence properties of a M heterometallic coinage metal chalcogenide cluster. *Dalton Transactions*, **2020**, 49, 593-597	4.3	3
143	An Efficient Coupled-Perturbed Kohn-Sham Implementation of NMR Chemical Shift Computations with Local Hybrid Functionals and Gauge-Including Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 931-943	6.4	19
142	Nuclear Spin-Spin Couplings: Efficient Evaluation of Exact Exchange and Extension to Local Hybrid Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 8529-8539	2.8	10
141	Atom Exchange Versus Reconstruction: (GexAs4)x (x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au6(Ge3As)(Ge2As2)3]3 *Angewandte Chemie*, **2020**, 132, 16781	3.6	
140	A Series of Homoleptic Linear Trimethylsilylchalcogenido Cuprates, Argentates and Aurates Cat[MeSiE-M-ESiMe] (M = Cu, Ag, Au; E = S, Se). *Inorganic Chemistry*, **2020**, 59, 17565-17572	5.1	3
139	Synthesis and Reactivity of Bis(silylene)-Coordinated Calcium and Divalent Lanthanide Complexes. *Chemistry - A European Journal*, **2020**, 26, 14888-14895	4.8	6
138	Segmented Contracted Error-Consistent Basis Sets of Quadruple- Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. *Journal of Chemical Theory and Computation*, **2020**, 16, 5658-5674	6.4	13

137	Stabilizing a metalloid {Zn} unit within a polymetallide environment in [KZnBi]. *Nature Communications*, **2020**, 11, 5122	17.4	15
136	R□ktitelbild: Atom Exchange Versus Reconstruction: (GexAs4□)x□(x=2, 3) as Building Blocks for the Supertetrahedral Zintl Cluster [Au6(Ge3As)(Ge2As2)3]3□(Angew. Chem. 38/2020). *Angewandte Chemie*, **2020**, 132, 16948	3.6	
135	The Arachno-Zintl Ion (Sn Sb) and the Effects of Element Composition on the Structures of Isoelectronic Clusters: Another Facet of the Pseudo-Element Concept. *Angewandte Chemie - International Edition*, **2020**, 59, 14251-14255	16.4	10
134	Synthesis of a Molecule with Five Different Adjacent Pnictogens. *Chemistry - A European Journal*, **2020**, 26, 8536-8540	4.8	8
133	Size Matters: From Two-Dimensional Au -Tl Metallopolymers to Molecular Complexes by Simple Variation of the Steric Demand. *Chemistry - A European Journal*, **2019**, 25, 3799-3808	4.8	8
132	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. *Journal of Physical Chemistry C*, **2019**, 123, 15354-15365	3.8	13
131	The coordination behavior of 2,3-bis(diphenylphosphino)maleic-N-phenylimide towards copper, silver, gold and palladium. *Dalton Transactions*, **2019**, 48, 6863-6871	4.3	4
130	Low-Valent Group 14 NHC-Stabilized Phosphinidenide ate Complexes and NHC-Stabilized K/P-Clusters. *Chemistry - A European Journal*, **2019**, 25, 4914-4919	4.8	7
129	Error-consistent segmented contracted all-electron relativistic basis sets of double- and triple-zeta quality for NMR shielding constants. *Physical Chemistry Chemical Physics*, **2019**, 21, 16658-16664	3.6	27
128	Not Non-Coordinating at All: Coordination Compounds of the Cyclodimethylsiloxanes D (D = MeSiO; = 6, 7) and Group 2 Metal Cations. *Inorganic Chemistry*, **2019**, 58, 15417-15422	5.1	12
127	Tuning the Metal/Chalcogen Composition in Copper(I)-Chalcogenide Clusters with Cyclic (Alkyl)(amino)carbene Ligands. *Inorganic Chemistry*, **2019**, 58, 3338-3348	5.1	14
126	Enhancement of and interference among higher order multipole transitions in molecules near a plasmonic nanoantenna. *Nature Communications*, **2019**, 10, 5775	17.4	13
125	Transition-Metal-Induced Rearrangement of [(PhSn) S] Towards Ternary Cu /Sn/S or Cu /Sn/S Clusters. *Chemistry - A European Journal*, **2019**, 25, 2486-2490	4.8	13
124	NMR Shielding Tensors and Chemical Shifts in Scalar-Relativistic Local Exact Two-Component Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 1028-1043	6.4	27
123	Calculation of Magnetic Shielding Constants with meta-GGA Functionals Employing the Multipole-Accelerated Resolution of the Identity: Implementation and Assessment of Accuracy and Efficiency. *Journal of Chemical Theory and Computation*, **2018**, 14, 191-197	6.4	30
122	(GeP): a binary analogue of P as a precursor to the ternary cluster anion [Cd(GeP)]. *Chemical Communications*, **2018**, 54, 1421-1424	5.8	27
121	Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. *Journal of Chemical Physics*, **2018**, 148, 104110	3.9	36
120	The Identity of "Ternary" A/Tl/Pb or K/Tl/Bi Solid Mixtures and Binary Zintl Anions Isolated From Their Solutions. *Chemistry - A European Journal*, **2018**, 24, 12022-12030	4.8	19

119	[Hg Te (Te)] : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. *Angewandte Chemie - International Edition*, **2018**, 57, 8770-8774	16.4	17
118	[Hg4Te8(Te2)4]8– ein Schwermetall-Porphyrinoid in einer lamellaren Struktur. *Angewandte Chemie*, **2018**, 130, 8906-8910	3.6	7
117	[Co@Sn6Sb6]3– Ein endohedraler 12-Atom-Cluster mit einem nicht-zentrierten inneren Atom. *Angewandte Chemie*, **2018**, 130, 15585-15589	3.6	12
116	[Co@Sn Sb] : An Off-Center Endohedral 12-Vertex Cluster. *Angewandte Chemie - International Edition*, **2018**, 57, 15359-15363	16.4	25
115	Optical properties of trinuclear metal chalcogenolate complexes - room temperature NIR fluorescence in [CuTi(SPh)(PPh)]. *Dalton Transactions*, **2017**, 46, 1502-1509	4.3	10
114	Vibrational circular dichroism spectra for large molecules and molecules with heavy elements. *Journal of Chemical Physics*, **2017**, 146, 054102	3.9	15
113	The chemical space of PbBi and (PbBi): A systematic study for N = 3-13. *Journal of Chemical Physics*, **2017**, 146, 034304	3.9	6
112	Bis(6-methylene-2,2′-bipyridine)phenylphosphine-A Flexible Ligand for the Construction of Trinuclear Coinage-Metal Complexes. *Chemistry - A European Journal*, **2017**, 23, 12198-12209	4.8	14
111	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. *Physical Chemistry Chemical Physics*, **2017**, 19, 12794-12803	3.6	14
110	An NHC-phosphinidenyl as a synthon for new group 13/15 compounds. *Chemical Communications*, **2017**, 53, 7620-7623	5.8	28
109	Synthesis and Reactivity of NHC-Stabilized Iron(II) Mesityl Complexes. *European Journal of Inorganic Chemistry*, **2017**, 2017, 2600-2616	2.3	12
108	A N-Heterocyclic Carbene-Stabilized Coinage Metal-Chalcogenide Framework with Tunable Optical Properties. *Journal of the American Chemical Society*, **2017**, 139, 14045-14048	16.4	50
107	Synthesis and Optical Properties of [CuE(SnPh)(PPhEt)] (E = S, Se, Te) Cluster Molecules. *Inorganic Chemistry*, **2017**, 56, 9330-9336	5.1	10
106	Segmented Contracted Error-Consistent Basis Sets of Double- and Triple-ζ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 3696-3705	6.4	74
105	Coinage Metal Complexes of Bis-Alkynyl-Functionalized N-Heterocyclic Carbenes: Reactivity, Photophysical Properties, and Quantum Chemical Investigations. *Chemistry - A European Journal*, **2017**, 23, 1591-1603	4.8	12
104	A combined experimental and quantum chemical study on thallium(I) tris(pyrazolyl)methanide. *Polyhedron*, **2017**, 125, 74-79	2.7	5
103	{[CuSn5 Sb3](2-) }2 : A Dimer of Inhomogeneous Superatoms. *Angewandte Chemie - International Edition*, **2016**, 55, 11775-80	16.4	37
102	A Controlled Route to a Luminescent 3 d -5 d Sulfido Cluster Containing Unique AuCu (μ-S) Motifs. *Chemistry - A European Journal*, **2016**, 22, 18378-18382	4.8	6

101	Enhancing Electrochemiluminescence of Chalcogenide Clusters by Means of Mn Replacement. *Electrochimica Acta*, **2016**, 210, 79-86	6.7	10
100	Understanding of multimetallic cluster growth. *Nature Communications*, **2016**, 7, 10480	17.4	76
99	Main Group Metal-Actinide Magnetic Coupling and Structural Response Upon U(4+) Inclusion Into Bi, Tl/Bi, or Pb/Bi Cages. *Journal of the American Chemical Society*, **2016**, 138, 9033-6	16.4	57
98	Quasi-Particle Self-Consistent GW for Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 2528-41	6.4	90
97	Quantum Chemical Investigations of Clusters of Heavy Metal Atoms. *Structure and Bonding*, **2016**, 41-62	0.9	1
96	{[CuSn5Sb3]2}2-: Ein Dimer inhomogener Superatome. *Angewandte Chemie*, **2016**, 128, 11950-11955	3.6	14
95	Two-component hybrid time-dependent density functional theory within the Tamm-Dancoff approximation. *Journal of Chemical Physics*, **2015**, 142, 034116	3.9	12
94	Simple but effective: thermally stable Cu-ESiMe3via NHC ligation. *Chemical Communications*, **2015**, 51, 8361-4	5.8	26
93	Error-Balanced Segmented Contracted Gaussian Basis Sets **2015**, 181-194		1
92	[(Pb6I8){Mn(CO)5}6](2-): an octahedral (M6X8)-like cluster with inverted bonding. *Inorganic Chemistry*, **2015**, 54, 3989-94	5.1	13
91	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
90	Ionic-radius-driven selection of the main-group-metal cage for intermetalloid clusters [Ln@Pbx Bi14-x](q-) and [Ln@Pby Bi13-y](q-) (x/q=7/4, 6/3; y/q=4/4, 3/3). *Chemistry - A European Journal*, **2015**, 21, 386-94	4.8	38
89	Off-Diagonal Self-Energy Terms and Partially Self-Consistency in GW Calculations for Single Molecules: Efficient Implementation and Quantitative Effects on Ionization Potentials. *Journal of Chemical Theory and Computation*, **2015**, 11, 5152-60	6.4	36
88	Luminescence in phosphine-stabilized copper chalcogenide cluster molecules--a comparative study. *Inorganic Chemistry*, **2015**, 54, 9413-22	5.1	25
87	{PbSe}: a heavy CO homologue as an unexpected ligand. *Angewandte Chemie - International Edition*, **2015**, 54, 11283-8	16.4	27
86	[V@Ge8As4]3- and [Nb@Ge8As6]3-: encapsulation of electron-poor transition metal atoms. *Chemical Communications*, **2015**, 51, 3866-9	5.8	33
85	PbSe: ein schweres CO-Homolog als ungewöhnlicher Ligand. *Angewandte Chemie*, **2015**, 127, 11437-11442	3.6	11
84	One-Electron Energies from the Two-Component GW Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 969-79	6.4	16

83	Reduction of rhenates(VII) with hydrogen chloride in alcohols: The structural aspects of the trans-tetrachloridomethoxidooxidorhenate(VI) products. *Inorganica Chimica Acta*, **2014**, 411, 26-29	2.7	0
82	Red-luminescent biphosphine stabilized M□Sn□ cluster molecules. *Chemical Communications*, **2014**, 50, 11043-5	5.8	44
81	Superatomic Orbitals under Spin-Orbit Coupling. *Journal of Physical Chemistry Letters*, **2014**, 5, 3286-9	6.4	99
80	Slow magnetic relaxation in trigonal-planar mononuclear Fe(II) and Co(II) bis(trimethylsilyl)amido complexes--a comparative study. *Inorganic Chemistry*, **2014**, 53, 1962-74	5.1	128
79	Phosphorescence lifetimes of organic light-emitting diodes from two-component time-dependent density functional theory. *Journal of Chemical Physics*, **2014**, 141, 224302	3.9	34
78	Extending DFT-based genetic algorithms by atom-to-place re-assignment via perturbation theory: a systematic and unbiased approach to structures of mixed-metallic clusters. *Journal of Chemical Physics*, **2014**, 141, 134103	3.9	30
77	Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100	7.9	710
76	Influence of vibrations on electron transport through nanoscale contacts. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2468-2480	1.3	21
75	The GW-Method for Quantum Chemistry Applications: Theory and Implementation. *Journal of Chemical Theory and Computation*, **2013**, 9, 232-46	6.4	174
74	An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. *Journal of Chemical Physics*, **2013**, 138, 184105	3.9	121
73	Implementation of Two-Component Time-Dependent Density Functional Theory in TURBOMOLE. *Journal of Chemical Theory and Computation*, **2013**, 9, 5341-8	6.4	45
72	Efficient two-component self-consistent field procedures and gradients: implementation in TURBOMOLE and application to. *Molecular Physics*, **2013**, 111, 2617-2624	1.7	28
71	Unusual 14-electron fragments [Pd(□3) -Bi3-x Pbx)]((x+1)-) as pseudo lead atoms in closo-[Pd@Pd2 Pb10 Bi6](4-). *Angewandte Chemie - International Edition*, **2013**, 52, 13544-8	16.4	43
70	Ungewöhnliche 14-Elektronen-Fragmente [Pd(□-Bi3□Pbx)](x+1)□als Pseudo-Bleiatome in closo-[Pd@Pd2Pb10Bi6]4□*Angewandte Chemie*, **2013**, 125, 13786-13790	3.6	26
69	Seminumerical calculation of the Hartree-Fock exchange matrix: application to two-component procedures and efficient evaluation of local hybrid density functionals. *Journal of Computational Chemistry*, **2012**, 33, 810-6	3.5	47
68	Doped semimetal clusters: ternary, intermetalloid anions [Ln@Sn7Bi7]4- and [Ln@Sn4Bi9]4- (Ln = La, Ce) with adjustable magnetic properties. *Journal of the American Chemical Society*, **2012**, 134, 1181-91	16.4	78
67	Zinc chalcogenolate complexes as precursors to ZnE and Mn/ZnE (E = S, Se) clusters. *Inorganic Chemistry*, **2012**, 51, 2747-56	5.1	26
66	Subtle impact of atomic ratio, charge and lewis basicity on structure selection and stability: the Zintl anion [(La@In2Bi11)(□Bi)2(La@In2Bi11)]6-. *Chemistry - A European Journal*, **2012**, 18, 13589-95	4.8	43

65	Making practical use of the pseudo-element concept: an efficient way to ternary intermetalloid clusters by an isoelectronic Pb(-)-Bi combination. *Chemical Communications*, **2012**, 48, 11295-7	5.8	53
64	Error-Balanced Segmented Contracted Basis Sets of Double-ζ to Quadruple-ζ Valence Quality for the Lanthanides. *Journal of Chemical Theory and Computation*, **2012**, 8, 4062-8	6.4	63
63	Probing the Influence of Size and Composition on the Photoelectron Spectra of Cadmium Chalcogenide Cluster Dianions. *Journal of Physical Chemistry C*, **2012**, 116, 13800-13809	3.8	14
62	Structures of small bismuth cluster cations. *Journal of Chemical Physics*, **2012**, 136, 154309	3.9	29
61	Structures and properties of neutral gallium clusters: a theoretical investigation. *Journal of Chemical Physics*, **2011**, 135, 044314	3.9	36
60	Jahn–Teller Distortion Versus Spin–Orbit Splitting: Symmetry of Small Heavy-Metal Atom Clusters. *Journal of Cluster Science*, **2011**, 22, 355-363	3	10
59	Phosphorescence energies of organic light-emitting diodes from spin-flip Tamm-Dancoff approximation time-dependent density functional theory. *ChemPhysChem*, **2011**, 12, 3331-6	3.2	21
58	Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure. *Journal of Computational Chemistry*, **2011**, 32, 3129-34	3.5	6
57	Quantum chemical treatments of metal clusters. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 1245-63	3	34
56	Segmented contracted basis sets for one- and two-component Dirac-Fock effective core potentials. *Journal of Chemical Physics*, **2010**, 133, 174102	3.9	134
55	Bistrimethylsilylamide transition-metal complexes as starting reagents in the synthesis of ternary Cd-Mn-Se cluster complexes. *Inorganic Chemistry*, **2010**, 49, 7331-9	5.1	20
54	Chalcogen chemistry of group(IV) closo-dodecaborates, synthesis, theory and coordination chemistry. *Dalton Transactions*, **2010**, 39, 7504-12	4.3	14
53	Observation and Interpretation of Structural Variety in Alkaline Earth Metal Derivatives of Diphosphanyldisiloxane. *European Journal of Inorganic Chemistry*, **2010**, 2010, 258-265	2.3	14
52	1-D-Tin(II) Phenylchalcogenolato Complexes [Sn(EPh)2] (E = S, Se, Te): Synthesis, Structures, Quantum Chemical Studies and Thermal Behaviour. *European Journal of Inorganic Chemistry*, **2010**, 2010, 410-418	2.3	23
51	Coordination and oligomerisation of the siloxanephosphane cage compound [P(2){(SiMe(2))(2)O}(3)]. *Chemistry - A European Journal*, **2009**, 15, 9642-6	4.8	9
50	Synthesis, Crystal Structure and Bond Situation of [Co7Se7Cp3(CO)4] (Cp = Cyclopentadienyl). *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2009**, 635, 2288-2293	1.3	
49	How photoelectron spectroscopy and quantum chemical studies can help understanding the magnetic properties of molecules: an example from the class of Cu(II)-bis(oxamato) complexes. *Journal of Physical Chemistry B*, **2009**, 113, 10051-4	3.4	3
48	Partial double bond character in chalcogen compounds of stanna-closo-dodecaborate. *Dalton Transactions*, **2009**, 1055-62	4.3	13

47	Neutral and cationic main group element cages of germanium(II) with pyrazolyl ligands: solid state structures, DFT calculations and advanced solution NMR investigations. *Dalton Transactions*, **2009**, 5335-47	4.2	9
46	Approximated electron repulsion integrals: Cholesky decomposition versus resolution of the identity methods. *Journal of Chemical Physics*, **2009**, 130, 164106	3.9	144
45	Self-consistent treatment of spin-orbit interactions with efficient Hartree-Fock and density functional methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 1748-56	3.6	125
44	Binding energy and preferred adsorption sites of CO on gold and silver-gold cluster cations: adsorption kinetics and quantum chemical calculations. *Faraday Discussions*, **2008**, 138, 393-406; discussion 421-34	3.6	52
43	Unique manganese phosphorus complex with a Mn5P7 core: synthesis, molecular structure, and magnetic properties. *Inorganic Chemistry*, **2008**, 47, 1460-4	5.1	14
42	Electron paramagnetic resonance and density-functional theory studies of Cu(II)-bis(oxamato) complexes. *Inorganic Chemistry*, **2008**, 47, 6633-44	5.1	21
41	Hartree-Fock exchange fitting basis sets for H to Rn. *Journal of Computational Chemistry*, **2008**, 29, 167-75	3.5	436
40	Magnetic and optical properties of Cu(II)-bis(oxamato) complexes: combined quantum chemical density functional theory and vibrational spectroscopy studies. *Journal of Physical Chemistry B*, **2008**, 112, 5585-93	3.4	10
39	Stepwise synthesis and coordination compound of an inorganic cryptand. *Angewandte Chemie - International Edition*, **2007**, 46, 4775-9	16.4	25
38	Ein anorganischer Cryptand: schrittweise Synthese und Koordination von Li+-Ionen. *Angewandte Chemie*, **2007**, 119, 4859-4863	3.6	15
37	Spin density distribution in oxamato-type transition metal complexes. *Polyhedron*, **2007**, 26, 1773-1775	2.7	8
36	Quantum chemistry calculations for molecules coupled to reservoirs: formalism, implementation, and application to benzenedithiol. *Journal of Chemical Physics*, **2007**, 126, 174101	3.9	81
35	Silver aggregation caused by Stanna-closo-dodecaborate coordination: syntheses, solid-state structures and theoretical studies. *Inorganic Chemistry*, **2007**, 46, 6775-84	5.1	32
34	Basis-set extensions for two-component spin-orbit treatments of heavy elements. *Physical Chemistry Chemical Physics*, **2006**, 8, 4862-5	3.6	54
33	Accurate Coulomb-fitting basis sets for H to Rn. *Physical Chemistry Chemical Physics*, **2006**, 8, 1057-65	3.6	3695
32	Reactions of mixed silver-gold cluster cations AgmAun + (m+n=4,5,6) with CO: radiative association kinetics and density functional theory computations. *Journal of Chemical Physics*, **2006**, 125, 104308	3.9	55
31	Structural relaxation in charged metal surfaces and cluster ions. *Small*, **2006**, 2, 1497-503	11	56
30	Ab Initio Calculations of Clusters. *Lecture Notes in Physics*, **2005**, 205-219	0.8	

29	Unusual syntheses, structures, and electronic properties of compounds containing ternary, T3-type supertetrahedral M/Sn/S anions [M5Sn(mu3-S)4(SnS4)4](10- (M = Zn, Co). *Inorganic Chemistry*, **2005**, 44, 5686-95	5.1	83
28	Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Physical Chemistry Chemical Physics*, **2005**, 7, 3297-305	3.6	14310
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