Pekka Pyykk

List of Publications by Year in Descending Order

214 papers	22,970 citations	65 h-index	149 g-index
219 ext. papers	24,479 ext. citations	6.5 avg, IF	7.7 L-index

#	Paper	IF	Citations
214	Saturnenes Like Th@Au 6 D 6h : Ring-Current Evidence for AuAu Bonding Along the Gold Ring. *Israel Journal of Chemistry*, **2022**, 62,	3.4	1
213	An Essay on Periodic Tables. *Perspectives on the History of Chemistry*, **2021**, 425-438	0	
212	Ab initio electronic factors of the A and B hyperfine structure constants for the 5s25p6sP1o1,3 states in Sn i. *Physical Review A*, **2021**, 103,	2.6	2
211	Structural trends in atomic nuclei from laser spectroscopy of tin. *Communications Physics*, **2020**, 3,	5.4	10
210	The periodic table and the physics that drives it. *Nature Reviews Chemistry*, **2020**, 4, 359-380	34.6	28
209	Understanding the Uniqueness of 2p Elements in Periodic Tables. *Chemistry - A European Journal*, **2020**, 26, 15558-15564	4.8	17
208	An essay on periodic tables. *Pure and Applied Chemistry*, **2019**, 91, 1959-1967	2.1	9
207	In My Element: How did I land in a gold mine?. *Chemistry - A European Journal*, **2019**, 25, 2101-2102	4.8	
206	Simple Estimates for Eutectic Behavior. *ChemPhysChem*, **2019**, 20, 123-127	3.2	4
205	Year-2017 nuclear quadrupole moments. *Molecular Physics*, **2018**, 116, 1328-1338	1.7	65
204	The argon nuclear quadrupole moments. *Molecular Physics*, **2018**, 116, 1682-1686	1.7	2
203	Ab initio calculations of the hyperfine structure of zinc and evaluation of the nuclear quadrupole moment Q(Zn67). *Physical Review A*, **2018**, 97,	2.6	5
202	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. *Angewandte Chemie - International Edition*, **2017**, 56, 10132-10134	16.4	14
201	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. *Angewandte Chemie*, **2017** , 129, 10266-10268	3.6	3
200	Introduction to the Physical and Chemical Properties of Gold **2017**, 29-49		3
199	Is the chemistry of lawrencium peculiar?. *Physical Chemistry Chemical Physics*, **2016**, 18, 17351-5	3.6	21
198	Is the Periodic Table all right (BT OK)?. *EPJ Web of Conferences*, **2016**, 131, 01001	0.3	13

197	Magically magnetic gadolinium. *Nature Chemistry*, **2015**, 7, 680	17.6	19
196	The 32-Electron Principle **2015**, 401-424		1
195	Ab initioMCDHF calculations of electron□ucleus interactions. *Physica Scripta*, **2015**, 90, 054011	2.6	11
194	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series PuO(n)F(8-2n) (n = 0-4). *Inorganic Chemistry*, **2015**, 54, 8825-31	5.1	23
193	Additive covalent radii for single-, double-, and triple-bonded molecules and tetrahedrally bonded crystals: a summary. *Journal of Physical Chemistry A*, **2015**, 119, 2326-37	2.8	340
192	On the Extreme Oxidation States of Iridium. *Chemistry - A European Journal*, **2015**, 21, 9468-73	4.8	24
191	Die formalen Oxidationszahlen des Iridiums reichen nun von □I bis +IX. *Angewandte Chemie*, **2015**, 127, 1094-1095	3.6	8
190	The formal oxidation states of iridium now run from -III to +IX. *Angewandte Chemie - International Edition*, **2015**, 54, 1080-1	16.4	19
189	Preface to The Relativistic Quantum Chemistry Issue of Journal of Computer Chemistry, Japan. *Journal of Computer Chemistry Japan*, **2014**, 13, A2-A3	0.2	1
188	Aspects of bonding in small gold clusters. *International Journal of Mass Spectrometry*, **2013**, 354-355, 15-18	1.9	14
187	Unbridged Au(II)-Au(II) bonds are theoretically allowed. *Chemical Communications*, **2013**, 49, 2103-5	5.8	19
186	The RTAM electronic bibliography, version 17.0, on relativistic theory of atoms and molecules. *Journal of Computational Chemistry*, **2013**, 34, 2667	3.5	16
185	A new, centered 32-electron system: the predicted [U@Si20]6□like isoelectronic series. *Chemical Science*, **2012**, 3, 2843	9.4	36
184	Rare-earth monocarbonyls MCO: comprehensive infrared observations and a transparent theoretical interpretation for M = Sc; Y; La□u. *Chemical Science*, **2012**, 3, 1548	9.4	25
183	The physics behind chemistry and the periodic table. *Chemical Reviews*, **2012**, 112, 371-84	68.1	149
182	Predicting new, simple inorganic species by quantum chemical calculations: some successes. *Physical Chemistry Chemical Physics*, **2012**, 14, 14734-42	3.6	44
181	Refitted tetrahedral covalent radii for solids. *Physical Review B*, **2012**, 85,	3.3	63
180	Relativistic effects in chemistry: more common than you thought. *Annual Review of Physical Chemistry*, **2012**, 63, 45-64	15.7	330

179	Relativity and the lead-acid battery. *Physical Review Letters*, **2011**, 106, 018301	7.4	80
178	Relativity and the mercury battery. *Physical Chemistry Chemical Physics*, **2011**, 13, 16510-2	3.6	13
177	Molecular hydrogen tweezers: structure and mechanisms by neutron diffraction, NMR, and deuterium labeling studies in solid and solution. *Journal of the American Chemical Society*, **2011**, 133, 20245-57	16.4	59
176	A suggested periodic table up to Z□172, based on Dirac-Fock calculations on atoms and ions. *Physical Chemistry Chemical Physics*, **2011**, 13, 161-8	3.6	105
175	Aurophilicity: the effect of the neutral ligand L on [{ClAuL}(2)] systems. *Chemistry - A European Journal*, **2011**, 17, 368-77	4.8	97
174	Aurophilic attractions between a closed-shell molecule and a gold cluster. *Faraday Discussions*, **2011**, 152, 169-78; discussion 203-25	3.6	34
173	Theoretical study of H(2) splitting and storage by boron-nitrogen-based systems: a bimolecular case and some qualitative aspects. *Physical Chemistry Chemical Physics*, **2010**, 12, 149-55	3.6	17
172	Formulations of the closed-shell interactions in endohedral systems. *Physical Chemistry Chemical Physics*, **2010**, 12, 6187-203	3.6	23
171	WAu12(CO)12?. *Chemical Communications*, **2010**, 46, 3762-4	5.8	20
170	Bonding trends in molecular compounds of lanthanides: the double-bonded carbene cations LnCH(2) (+) (Ln=Sc, Y, La-Lu). *Chemistry - A European Journal*, **2010**, 16, 270-5	4.8	34
169	Chemical properties of the predicted 32-electron systems Pu@Sn12 and Pu@Pb12. *Comptes Rendus Chimie*, **2010**, 13, 884-888	2.7	23
168	Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. *Physical Review A*, **2009**, 79,	2.6	27
167	Molecular single-bond covalent radii for elements 1-118. *Chemistry - A European Journal*, **2009**, 15, 186-97	4.8	1416
166	Molecular double-bond covalent radii for elements Li-E112. *Chemistry - A European Journal*, **2009**, 15, 12770-9	4.8	912
165	Theoretical study on the series of [Au(3)Cl (3)M (2)] complexes, with M = Li, Na, K, Rb, Cs. *Journal of Molecular Modeling*, **2009**, 15, 1165-73	2	9
164	Experimental and theoretical treatment of hydrogen splitting and storage in boron□itrogen systems. *Journal of Organometallic Chemistry*, **2009**, 694, 2654-2660	2.3	86
163	Au(n)Hg(m) clusters: mercury aurides, gold amalgams, or van der Waals aggregates?. *Journal of Physical Chemistry A*, **2009**, 113, 12380-5	2.8	18
162	A predicted organometallic series following a 32-electron principle: An@C28 (An = Th, Pa+, U2+, Pu4+). *Journal of the American Chemical Society*, **2009**, 131, 238-43	16.4	96

161	Bonding analysis for sterically uncongested simple aurocarbons CnAum. *Canadian Journal of Chemistry*, **2009**, 87, 798-801	0.9	18
160	Theoretical chemistry of gold. III. *Chemical Society Reviews*, **2008**, 37, 1967-97	58.5	574
159	Molecular tweezers for hydrogen: synthesis, characterization, and reactivity. *Journal of the American Chemical Society*, **2008**, 130, 14117-9	16.4	332
158	Year-2008 nuclear quadrupole moments. *Molecular Physics*, **2008**, 106, 1965-1974	1.7	400
157	From nanostrips to nanorings: the elastic properties of gold-glued polyauronaphthyridines and polyacenes. *Physical Chemistry Chemical Physics*, **2008**, 10, 114-20	3.6	12
156	Deuteron quadrupole coupling in benzene: librational corrections using a temperature-dependent Einstein model, and summary. The symmetries of electric field gradients and conditions for eta = 1. *Physical Chemistry Chemical Physics*, **2008**, 10, 3867-71	3.6	9
155	Basis-set limit of the aurophilic attraction using the MP2 method: the examples of [ClAuPH3]2 dimer and [P(AuPH3)4]+ ion. *Journal of Chemical Physics*, **2008**, 128, 124309	3.9	28
154	Comment on the magnetic dipole hyperfine interaction in the gold atom ground state. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2008**, 41, 115002	1.3	14
153	Bonding trends in MCH2 systems: Simple orbital interpretation and evidence for double bonds. *Chemical Physics Letters*, **2008**, 462, 138-143	2.5	11
152	Theoretical mapping of new L[(N+)]1 family of species with donor–acceptor bonding between N+ and ligand L. *Computational and Theoretical Chemistry*, **2008**, 860, 128-136		11
151	Icosahedral Au(72): a predicted chiral and spherically aromatic golden fullerene. *Chemical Communications*, **2008**, 465-7	5.8	95
150	Structure and bonding of the MCN molecules, M=Cu,Ag,Au,Rg. *Journal of Chemical Physics*, **2008**, 128, 224303	3.9	27
149	Gold as intermolecular glue: a theoretical study of nanostrips based on quinoline-type monomers. *Physical Chemistry Chemical Physics*, **2007**, 9, 3025-30	3.6	9
148	A London-type formula for the dispersion interactions of endohedral A@B systems. *Physical Chemistry Chemical Physics*, **2007**, 9, 2954-8	3.6	38
147	Coordination of pyridinethiols in gold(I) complexes. *Inorganic Chemistry*, **2007**, 46, 9954-60	5.1	36
146	Towards a 32-electron principle: Pu@Pb12 and related systems. *Angewandte Chemie - International Edition*, **2007**, 46, 1427-30	16.4	78
145	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. *Angewandte Chemie*, **2007**, 119, 1449-1452	3.6	16
144	Pocket and antipocket conformations for the CH4@C84 endohedral fullerene. *International Journal of Quantum Chemistry*, **2007**, 107, 1162-1169	2.1	18

143	Hurricanes as Heat Engines: Two Undergraduate Problems. *Journal of Chemical Education*, **2007**, 84, 447	2.4	1
142	Valency and Bonding. A Natural Bond Orbital Donor-Acceptor Perspective. Von Frank Weinhold und Clark Landis.. *Angewandte Chemie*, **2006**, 118, 28-29	3.6	
141	Gold as intermolecular glue: a predicted planar triaurotriazine, C3Au3N3, isomer of gold cyanide. *Chemical Communications*, **2006**, 2890-2	5.8	13
140	Calculated lanthanide contractions for molecular trihalides and fully hydrated ions: The contributions from relativity and 4f-shell hybridization. *Chemical Physics Letters*, **2006**, 429, 8-12	2.5	65
139	Computational study of bonding trends in the metalloactinyl series EThM and MThM? (E=N□O, F+; M, M?=Ir□Pt, Au+). *Chemical Physics Letters*, **2006**, 431, 6-12	2.5	15
138	Understanding the eighteen-electron rule. *Journal of Organometallic Chemistry*, **2006**, 691, 4336-4340	2.3	139
137	Comparative theoretical study of N-heterocyclic carbenes and other ligands bound to Au(I). *Chemistry - an Asian Journal*, **2006**, 1, 623-8	4.5	33
136	A very short uranium-uranium bond: the predicted metastable U(2)2+. *Physical Chemistry Chemical Physics*, **2005**, 7, 2415-7	3.6	71
135	Linear HThThH: a candidate for a Th-Th triple bond. *Journal of the American Chemical Society*, **2005**, 127, 13090-1	16.4	31
134	A small spherical liquid: a DFT molecular dynamics study of WAu12. *Physical Chemistry Chemical Physics*, **2005**, 7, 2208-11	3.6	15
133	Theoretical chemistry of gold. II. *Inorganica Chimica Acta*, **2005**, 358, 4113-4130	2.7	373
132	Comparative calculations for the A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) at levels up to CCSD(T). *Chemical Physics Letters*, **2005**, 405, 148-152	2.5	36
131	Triple-bond covalent radii. *Chemistry - A European Journal*, **2005**, 11, 3511-20	4.8	327
130	Nuclear quadrupole moment of Hg201. *Physical Review A*, **2005**, 71,	2.6	38
129	Degree of accuracy in determining the nuclear electric quadrupole moment of radium. *Physical Review A*, **2005**, 71,	2.6	19
128	Theory of NMR Parameters. From Ramsey to Relativity, 1953 to 1983 **2004**, 7-19		6
127	Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. *Physical Review A*, **2004**, 70,	2.6	5
126	How many hydrogen atoms can be bound to a metal? Predicted MH12 species. *Journal of the American Chemical Society*, **2004**, 126, 15014-5	16.4	82

125	Theoretical chemistry of gold. *Angewandte Chemie - International Edition*, **2004**, 43, 4412-56	16.4	1550
124	Theoretical search for very short metal-actinide bonds: NUIr and isoelectronic systems. *Angewandte Chemie - International Edition*, **2004**, 43, 1573-6	16.4	43
123	Theoretische Chemie des Golds. *Angewandte Chemie*, **2004**, 116, 4512-4557	3.6	277
122	Theoretical Search for Very Short Metal□Actinide Bonds: NUIr and Isoelectronic Systems. *Angewandte Chemie*, **2004**, 116, 1599-1602	3.6	7
121	Al3+□He: stability and spectroscopy. *Chemical Physics Letters*, **2004**, 392, 281-283	2.5	12
120	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. *Chemical Communications*, **2004**, 1982-3	5.8	25
119	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
118	Study of the MAu6 (M = Cr, Mo, W) molecular species: A transition from halogenlike to hydrogenlike chemical behavior for gold. *Physical Chemistry Chemical Physics*, **2004**, 6, 2904-2906	3.6	22
117	The importance of being tetrahedral: the cadmium pyramids CdN; N = 4, 10, 20, 35 and 56. *Physical Chemistry Chemical Physics*, **2004**, 6, 2907-2909	3.6	28
116	Aurophilic attraction in binuclear complexes with Au(I) and Au(III). A theoretical study. *Physical Chemistry Chemical Physics*, **2004**, 6, 900-905	3.6	71
115	Calculated structures of [Au=C=Au]2+ and related systems. *Chemical Physics Letters*, **2003**, 381, 45-52	2.5	41
114	Why are hexavalent uranium cyanides rare while U□ and U□ bonds are common and short?. *Theoretical Chemistry Accounts*, **2003**, 109, 332-340	1.9	75
113	Cesium and barium as honorary d elements: CsN7Ba as an example. *Theoretical Chemistry Accounts*, **2003**, 110, 205-210	1.9	44
112	Strong chemical bonds in heavy diatomics: PtSi, PtTh and AuTh+. *Chemical Physics Letters*, **2003**, 368, 538-541	2.5	15
111	Aurophilic attraction: the additivity and the combination with hydrogen bonds. *Chemical Physics Letters*, **2003**, 370, 733-740	2.5	46
110	QED corrections to the binding energy of the eka-radon (Z=118) negative ion. *Physical Review A*, **2003**, 67,	2.6	41
109	Predicted group 4 tetra-azides M(N3)(4) (M = Ti-Hf, Th): the first examples of linear M-NNN coordination. *Inorganic Chemistry*, **2003**, 42, 3074-8	5.1	31
108	One metal and forty nitrogens. Ab initio predictions for possible new high-energy pentazolides. *Inorganic Chemistry*, **2003**, 42, 8241-9	5.1	35

107	On the nature of the short Pt-Tl bonds in model compounds [H5Pt-TlHn]n-. *Faraday Discussions*, **2003**, 124, 41-51; discussion 53-6, 453-5	3.6	13
106	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He□Rn: A way to absolute nuclear magnetic resonance shielding scales. *Journal of Chemical Physics*, **2003**, 118, 2973-2976	3.9	98
105	Icosahedral WAu12: A Predicted Closed-Shell Species, Stabilized by Aurophilic Attraction and Relativity and in Accord with the 18-Electron Rule. *Angewandte Chemie*, **2002**, 114, 2278	3.6	58
104	Relativität, Gold, Wechselwirkungen zwischen gefüllten Schalen und CsAu?NH3. *Angewandte Chemie*, **2002**, 114, 3723-3728	3.6	31
103	Icosahedral WAu12: a predicted closed-shell species, stabilized by aurophilic attraction and relativity and in accord with the 18-electron rule. *Angewandte Chemie - International Edition*, **2002**, 41, 2174-6	16.4	315
102	Relativity, gold, closed-shell interactions, and CsAu.NH3. *Angewandte Chemie - International Edition*, **2002**, 41, 3573-8, 3512	16.4	169
101	A Study of the Interactions in an Extended Unsupported Gold-Silver Chain. *European Journal of Inorganic Chemistry*, **2002**, 2002, 750-753	2.3	40
100	□-N5- □Metal□-N73-: A New Class of Compounds. *Journal of Physical Chemistry A*, **2002**, 106, 4690-4694	2.8	75
99	HgH4 and HgH6: further candidates for high-valent mercury compounds. *Chemical Communications*, **2002**, 1728-9	5.8	22
98	Possible high-pressure structures of sulfur trioxide. *Chemical Communications*, **2002**, 336-7	5.8	3
97	Ab initio study of bonding trends for f0 actinide oxyfluoride species. *Theoretical Chemistry Accounts* , **2001**, 106, 393-403	1.9	83
96	A note on nodal structures, partial screening, and periodic trends among alkali metals and alkaline earths. *International Journal of Quantum Chemistry*, **2001**, 85, 18-21	2.1	23
95	Nuclear quadrupole moments of Kr and Xe from molecular data. *Chemical Physics Letters*, **2001**, 346, 155-159	2.5	22
94	Is the Lamb shift chemically significant?. *Chemical Physics Letters*, **2001**, 348, 497-500	2.5	24
93	Nuclear quadrupole moments of bismuth. *Physical Review Letters*, **2001**, 87, 133003	7.4	54
92	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. *Physical Review A*, **2001**, 64,	2.6	44
91	Estimation of Lamb-shift effects for molecules: Application to the rotation-vibration spectra of water. *Physical Review A*, **2001**, 63,	2.6	76
90	Magnetic-field-induced quadrupole splitting in gaseous and liquid 131Xe NMR: quadratic and quartic field dependence. *Physical Review Letters*, **2001**, 86, 3268-71	7.4	16

89	Scandium cycloheptanitride, ScN(7): a predicted high-energy molecule containing an [eta(7)-N(7)](3-) ligand. *Journal of the American Chemical Society*, **2001**, 123, 9700-1	16.4	63
88	Spectroscopic nuclear quadrupole moments. *Molecular Physics*, **2001**, 99, 1617-1629	1.7	477
87	The quest for beryllium peroxides. *Inorganic Chemistry*, **2001**, 40, 2270-4	5.1	8
86	Ab initio study of bonding trends among cyanamidophosphates (. *Chemistry - A European Journal*, **2000**, 6, 2145-51	4.8	11
85	Au22+ has bound excited states. *Chemical Physics Letters*, **2000**, 325, 225-231	2.5	24
84	The nuclear quadrupole moment of 45Sc. *Chemical Physics Letters*, **2000**, 329, 112-118	2.5	20
83	Could uranium(XII)hexoxide, UO6 (Oh) exist?. *Chemical Physics Letters*, **2000**, 328, 415-419	2.5	20
82	The nuclear quadrupole moment of from molecular data for ZrO and ZrS. *Chemical Physics Letters*, **2000**, 318, 222-231	2.5	20
81	Perspective on Norman Ramsey's theories of NMR chemical shifts and nuclear spin□spin coupling. *Theoretical Chemistry Accounts*, **2000**, 103, 214-216	1.9	26
80	Structure and stability of gold-substituted diborane, boranes, and borohydride ions. *Theoretical Chemistry Accounts*, **2000**, 103, 399-408	1.9	5
79	Luminescent Characterization of Solution Oligomerization Process Mediated Gold□Gold Interactions. DFT Calculations on [Au2Ag2R4L2]n Moieties. *Journal of the American Chemical Society*, **2000**, 122, 7287-7293	16.4	126
78	Ab initio studies of the dimers (HgH2)2 and (HgMe2)2. Metallophilic attraction and the van der Waals radii of mercury. *Physical Chemistry Chemical Physics*, **2000**, 2, 2489-2493	3.6	163
77	Calculations for XeOn (n = 2□4): Could the Xenon Dioxide Molecule Exist?□*Journal of Physical Chemistry A*, **2000**, 104, 3826-3828	2.8	13
76	Experimental and theoretical studies of the d8-d10 interaction between Pd(II) and Au(I): bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))- dichloropalladium(II) and related systems. *Inorganic Chemistry*, **2000**, 39, 4786-92	5.1	65
75	Relativistic Theory of Atoms and Molecules III. *Lecture Notes in Quantum Chemistry II*, **2000**,	0.6	22
74	Isomerism of Aurated Phosphine Sulfides, Thiophosphinates, Thiophosphonates, and Thiophosphates: Structural and Quantum Chemical Studies. *Inorganic Chemistry*, **1999**, 38, 5870-5875	5.1	16
73	Electric quadrupole moment of the 27Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. *Chemical Physics Letters*, **1999**, 304, 414-422	2.5	67
72	Calculated self-energy contributions for an ns valence electron using the multiple-commutator method. *Physical Review A*, **1999**, 59, 2707-2711	2.6	60

71	Calculations on indium and thallium cyclopentadienyls. Metal–metal interactions and possible new species. *Physical Chemistry Chemical Physics*, **1999**, 1, 3441-3444	3.6	35
70	Predictions for possible new, doubly and triply bridged oxides and peroxides of C, N, P, and S. *Chemical Communications*, **1999**, 495-496	5.8	3
69	Theory of Intermolecular Interactions **1999**, 79-88		
68	Strong chemical bonds to gold. High level correlated relativistic results for diatomic AuBe+, AuC+, AuMg+, and AuSi+. *Chemical Physics Letters*, **1998**, 285, 398-403	2.5	61
67	Chemical bonds between noble metals and noble gases.: Ab initio study of the neutral diatomics NiXe, PdXe and PtXe. *Chemical Physics Letters*, **1998**, 288, 635-641	2.5	33
66	How Do Spin–Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin–Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. *Chemistry - A European Journal*, **1998**, 4, 118-126	4.8	305
65	Relativistic pseudopotential calculations on Xe2, RnXe, and Rn2: The van der Waals properties of radon **1998**, 66, 131-140		61
64	Can triple bonds exist between gold and main-group elements?. *Theoretical Chemistry Accounts*, **1998**, 99, 113-115	1.9	11
63	Theory of the d10–d10Closed-Shell Attraction. 4. X(AuL)nm+Centered Systems. *Organometallics*, **1998**, 17, 4842-4852	3.8	70
62	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur. *Inorganic Chemistry*, **1998**, 37, 624-632	5.1	228
61	Theory of d10–d10 Closed-Shell Attraction. III. Rings. *Inorganic Chemistry*, **1998**, 37, 3018-3025	5.1	190
60	Closed-shell interaction in silver and gold chlorides. *Journal of Chemical Physics*, **1998**, 109, 2339-2345	3.9	60
59	Estimated valence-level Lamb shifts for group 1 and group 11 metal atoms. *Physical Review A*, **1998**, 57, R689-R692	2.6	67
58	How Do Spin–Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin–Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds **1998**, 4, 118		1
57	Hyperfine structure of the state of highly charged ions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1997**, 30, 1427-1435	1.3	10
56	Vacuum-polarization corrections to the hyperfine-structure splitting of highly charged 83209Bi ions. *Physical Review A*, **1997**, 56, 4508-4516	2.6	17
55	An ab initio study of the aggregation of LAuX moleculesand [LAuL]+[XAuX]- ions. *Chemical Communications*, **1997**, 1111-1112	5.8	46
54	Calculated Structures of MO22+, MN2, and MP2 (M = Mo, W). *Journal of Physical Chemistry A*, **1997**, 101, 8107-8114	2.8	23

53	Strong Closed-Shell Interactions in Inorganic Chemistry. *Chemical Reviews*, **1997**, 97, 597-636	68.1	2065
52	Relativistic effects in nuclear quadrupole coupling. *Theoretical Chemistry Accounts*, **1997**, 96, 92-104	1.9	44
51	Theory of the d10□10 Closed-Shell Attraction: 1. Dimers Near Equilibrium. *Chemistry - A European Journal*, **1997**, 3, 1451-1457	4.8	386
50	Theory of the d10□10 Closed-Shell Attraction: 2. Long-Distance Behaviour and Nonadditive Effects in Dimers and Trimers of Type [(x-Au-L)n] (n = 2, 3; X = Cl, I, H; L = PH3, PMe3, -N?CH). *Chemistry - A European Journal*, **1997**, 3, 1458-1465	4.8	162
49	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p; 2P32) and N+ (2p2; 3P2 and 2p2; 1D2). *Chemical Physics Letters*, **1997**, 265, 60-64	2.5	57
48	Calculated energy levels of thallium and eka-thallium (element 113). *Physical Review A*, **1996**, 53, 3926-3933	2.8	100
47	Calculated Structure and Optical Properties of Tl(2)Pt(CN)(4). *Inorganic Chemistry*, **1996**, 35, 7450-7451	5.1	41
46	Element 118: The First Rare Gas with an Electron Affinity. *Physical Review Letters*, **1996**, 77, 5350-5352	7.4	93
45	What did Johan Gadolin Actually do? **1996**, 1-12		3
44	Matrix Infrared Spectroscopic and ab Initio Studies of ZnH2, CdH2, and Related Metal Hydride Species. *The Journal of Physical Chemistry*, **1995**, 99, 7925-7934		109
43	Ab Initio Interpretation of the Closed-Shell Intermolecular E.cntdot..cntdot..cntdot.E Attraction in Dipnicogen (H2E-EH2)2 and Dichalcogen (HE-EH)2 Hydride Model Dimers. *Inorganic Chemistry*, **1995**, 34, 4134-4138	5.1	91
42	Calculated properties of XeH2. *Chemical Physics Letters*, **1995**, 246, 239-244	2.5	35
41	Predicted ligand dependence of the Au(I)□Au(I) attraction in (XAuPH3)2. *Chemical Physics Letters*, **1994**, 218, 133-138	2.5	235
40	ESF works, don't change it. *Nature*, **1994**, 371, 734-734	50.4	
39	Structure of tetrakis(phosphine)nitrido- or -phosphinidyne or arsinidyneultragold(1+): Td or C4v?. *Inorganic Chemistry*, **1993**, 32, 2630-2634	5.1	73
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