Pekka PyykkÃ¶

List of Publications by Year
in descending order

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206	26,086	11651	6300
papers	citations	70 h-index	158 g-index

219	219	219	12377
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Saturnenes Like Th@Au ₆ D _{6h} : Ringâ€Current Evidence for Auâ”Au Bonding Along the Gold Ring. Israel Journal of Chemistry, 2022, 62, .	2.3	2
2	An Essay on Periodic Tables. Perspectives on the History of Chemistry, 2021, , 425-438.	0.1	0
3	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, .	2.5	5
4	Understanding the Uniqueness of 2p Elements in Periodic Tables. Chemistry - A European Journal, 2020, 26, 15558-15564.	3.3	31
5	Structural trends in atomic nuclei from laser spectroscopy of tin. Communications Physics, 2020, 3, .	5.3	24
6	The periodic table and the physics that drives it. Nature Reviews Chemistry, 2020, 4, 359-380.	30.2	57
7	An essay on periodic tables. Pure and Applied Chemistry, 2019, 91, 1959-1967.	1.9	18
8	In My Element: How did I land in a gold mine?. Chemistry - A European Journal, 2019, 25, 2101-2102.	3.3	0
9	Simple Estimates for Eutectic Behavior. ChemPhysChem, 2019, 20, 123-127.	2.1	6
10	Year-2017 nuclear quadrupole moments. Molecular Physics, 2018, 116, 1328-1338.	1.7	103
11	The argon nuclear quadrupole moments. Molecular Physics, 2018, 116, 1682-1686.	1.7	2
12	Ab initio calculations of the hyperfine structure of zinc and evaluation of the nuclear quadrupole moment <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Q</mml:mi><mml:mo>(</mml:mo><mml:mmultiscripts> Physical Review A, 2018, 97, .	2.5	11
13	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. Angewandte Chemie - International Edition, 2017, 56, 10132-10134.	13.8	17
14	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. Angewandte Chemie, 2017, 129, 10266-10268.	2.0	4
15	Introduction to the Physical and Chemical Properties of Gold. , 2017, , 29-49.		3
16	Is the Periodic Table all right (â€œPT OKâ€)?. EPJ Web of Conferences, 2016, 131, 01001.	0.3	13
17	Is the chemistry of lawrencium peculiar?. Physical Chemistry Chemical Physics, 2016, 18, 17351-17355.	2.8	27
18	On the Extreme Oxidation States of Iridium. Chemistry - A European Journal, 2015, 21, 9468-9473.	3.3	31

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19	The Formal Oxidation States of Iridium Now Run from â˜’III to +IX. Angewandte Chemie - International Edition, 2015, 54, 1080-1081.	13.8	27
20	Magically magnetic gadolinium. Nature Chemistry, 2015, 7, 680-680.	13.6	29
21	Ab initioMCDHF calculations of electronâ€“nucleus interactions. Physica Scripta, 2015, 90, 054011.	2.5	18
22	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series PuO_nF_{8â€“2n} (n = 0â€“4). Inorganic Chemistry, 2015, 54, 8825-8831.	4.0	26
23	Additive Covalent Radii for Single-, Double-, and Triple-Bonded Molecules and Tetrahedrally Bonded Crystals: A Summary. Journal of Physical Chemistry A, 2015, 119, 2326-2337.	2.5	513
24	Preface to The Relativistic Quantum Chemistry Issue of Journal of Computer Chemistry, Japan. Journal of Computer Chemistry Japan, 2014, 13, A2-A3.	0.1	1
25	Aspects of bonding in small gold clusters. International Journal of Mass Spectrometry, 2013, 354-355, 15-18.	1.5	15
26	Unbridged Au(ii)â€“Au(ii) bonds are theoretically allowed. Chemical Communications, 2013, 49, 2103.	4.1	21
27	The RTAM electronic bibliography, version 17.0, on relativistic theory of atoms and molecules. Journal of Computational Chemistry, 2013, 34, 2667-2667.	3.3	22
28	A new, centered 32-electron system: the predicted [U@Si20]6â˜’-like isoelectronic series. Chemical Science, 2012, 3, 2843.	7.4	42
29	Rare-earth monocarbonyls MCO: comprehensive infrared observations and a transparent theoretical interpretation for M = Sc; Y; Laâ€“Lu. Chemical Science, 2012, 3, 1548.	7.4	31
30	The Physics behind Chemistry and the Periodic Table. Chemical Reviews, 2012, 112, 371-384.	47.7	179
31	Predicting new, simple inorganic species by quantum chemical calculations: some successes. Physical Chemistry Chemical Physics, 2012, 14, 14734.	2.8	45
32	Refitted tetrahedral covalent radii for solids. Physical Review B, 2012, 85, .	3.2	75
33	Relativistic Effects in Chemistry: More Common Than You Thought. Annual Review of Physical Chemistry, 2012, 63, 45-64.	10.8	416
34	Introduction to the Quantum Chemistry 2012 Issue. Chemical Reviews, 2012, 112, 1-3.	47.7	86
35	Aurophilic attractions between a closed-shell molecule and a gold cluster. Faraday Discussions, 2011, 152, 169.	3.2	38
36	Relativity and the Lead-Acid Battery. Physical Review Letters, 2011, 106, 018301.	7.8	100

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37	Relativity and the mercury battery. Physical Chemistry Chemical Physics, 2011, 13, 16510.	2.8	16
38	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, 20245-20257.	13.7	64
39	A suggested periodic table up to Z â‰ 172, based on Diracâ€“Fock calculations on atoms and ions. Physical Chemistry Chemical Physics, 2011, 13, 161-168.	2.8	129
40	Aurophilicity: The Effect of the Neutral Ligand L on [{ClAuL}₂] Systems. Chemistry - A European Journal, 2011, 17, 368-377.	3.3	107
41	Bonding Trends in Molecular Compounds of Lanthanides: The Doubleâ€Bonded Carbene Cations LnCH₂⁺ (Ln=Sc, Y, Laâ€“Lu). Chemistry - A European Journal, 2010, 16, 270-275.	3.3	38
42	Chemical properties of the predicted 32-electron systems Pu@Sn12 and Pu@Pb12. Comptes Rendus Chimie, 2010, 13, 884-888.	0.5	26
43	Theoretical study of H₂splitting and storage by boronâ€“nitrogen-based systems: a bimolecular case and some qualitative aspects. Physical Chemistry Chemical Physics, 2010, 12, 149-155.	2.8	18
44	Formulations of the closed-shell interactions in endohedral systems. Physical Chemistry Chemical Physics, 2010, 12, 6187.	2.8	29
45	WAu12(CO)12?. Chemical Communications, 2010, 46, 3762.	4.1	21
46	Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. Physical Review A, 2009, 79, .	2.5	29
47	Molecular Singleâ€Bond Covalent Radii for Elements 1â€“118. Chemistry - A European Journal, 2009, 15, 186-197.	3.3	1,762
48	Molecular Doubleâ€Bond Covalent Radii for Elements Liâ€“E112. Chemistry - A European Journal, 2009, 15, 12770-12779.	3.3	1,106
49	Theoretical study on the series of [Au3Cl3M2] complexes, with M = Li, Na, K, Rb, Cs. Journal of Molecular Modeling, 2009, 15, 1165-1173.	1.8	9
50	Experimental and theoretical treatment of hydrogen splitting and storage in boronâ€“nitrogen systems. Journal of Organometallic Chemistry, 2009, 694, 2654-2660.	1.8	89
51	Au_nHg_m Clusters: Mercury Aurides, Gold Amalgams, or van der Waals Aggregates?. Journal of Physical Chemistry A, 2009, 113, 12380-12385.	2.5	21
52	A Predicted Organometallic Series Following a 32-Electron Principle: An@C₂₈(An = Th,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 131, 238-243.	13.7	106
53	Bonding trends in MCH2 systems: Simple orbital interpretation and evidence for double bonds. Chemical Physics Letters, 2008, 462, 138-143.	2.6	13
54	Theoretical mapping of new Lâ€“(N+)â€“L family of species with donorâ€“acceptor bonding between N+ and ligand L. Computational and Theoretical Chemistry, 2008, 860, 128-136.	1.5	11

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55	Icosahedral Au₇₂: a predicted chiral and spherically aromatic golden fullerene. Chemical Communications, 2008, , 465-467.	4.1	109
56	Structure and bonding of the MCN molecules, M=Cu,Ag,Au,Rg. Journal of Chemical Physics, 2008, 128, 224303.	3.0	29
57	Theoretical chemistry of gold. III. Chemical Society Reviews, 2008, 37, 1967.	38.1	631
58	Molecular Tweezers for Hydrogen: Synthesis, Characterization, and Reactivity. Journal of the American Chemical Society, 2008, 130, 14117-14119.	13.7	356
59	Year-2008 nuclear quadrupole moments. Molecular Physics, 2008, 106, 1965-1974.	1.7	437
60	From nanostrips to nanorings: the elastic properties of gold-glued polyauronaphthyridines and polyacenes. Physical Chemistry Chemical Physics, 2008, 10, 114-120.	2.8	13
61	Deuteron quadrupole coupling in benzene: librational corrections using a temperature-dependent Einstein model, and summary. The symmetries of electric field gradients and conditions for Î· = 1. Physical Chemistry Chemical Physics, 2008, 10, 3867.	2.8	12
62	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.	3.0	31
63	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.	1.5	17
64	Hurricanes as Heat Engines: Two Undergraduate Problems. Journal of Chemical Education, 2007, 84, 447.	2.3	1
65	Gold as intermolecular glue: a theoretical study of nanostrips based on quinoline-type monomers. Physical Chemistry Chemical Physics, 2007, 9, 3025.	2.8	11
66	A London-type formula for the dispersion interactions of endohedral A@B systems. Physical Chemistry Chemical Physics, 2007, 9, 2954.	2.8	48
67	Coordination of Pyridinethiols in Gold(I) Complexes. Inorganic Chemistry, 2007, 46, 9954-9960.	4.0	40
68	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. Angewandte Chemie - International Edition, 2007, 46, 1427-1430.	13.8	88
69	Pocket and antipocket conformations for the CH4@C84 endohedral fullerene. International Journal of Quantum Chemistry, 2007, 107, 1162-1169.	2.0	21
70	Magic nanoclusters of gold. Nature Nanotechnology, 2007, 2, 273-274.	31.5	76
71	Gold as intermolecular glue: a predicted planar triaurotriazine, C3Au3N3, isomer of gold cyanide. Chemical Communications, 2006, , 2890.	4.1	14
72	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.	2.6	71

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73	Computational study of bonding trends in the metalloactinyl series EThM and MThMâ€² (E=Nâˆ’, O, F+; M,) Tj ETQq1 1 0.784314 rgB	2.6	16
74	Understanding the eighteen-electron rule. Journal of Organometallic Chemistry, 2006, 691, 4336-4340.	1.8	153
75	Comparative Theoretical Study of N-Heterocyclic Carbenes and Other Ligands Bound to AuI. Chemistry - an Asian Journal, 2006, 1, 623-628.	3.3	39
76	Theoretical chemistry of gold. II. Inorganica Chimica Acta, 2005, 358, 4113-4130.	2.4	399
77	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.	2.6	38
78	Triple-Bond Covalent Radii. Chemistry - A European Journal, 2005, 11, 3511-3520.	3.3	370
79	Nuclear quadrupole moment ofHg201. Physical Review A, 2005, 71, .	2.5	44
80	Degree of accuracy in determining the nuclear electric quadrupole moment of radium. Physical Review A, 2005, 71, .	2.5	20
81	A very short uraniumâ€“uranium bond: The predicted metastable U22+. Physical Chemistry Chemical Physics, 2005, 7, 2415.	2.8	79
82	Linear HThThH:Â A Candidate for a Thâˆ’Th Triple Bond. Journal of the American Chemical Society, 2005, 127, 13090-13091.	13.7	39
83	A small spherical liquid: A DFT molecular dynamics study of WAu12. Physical Chemistry Chemical Physics, 2005, 7, 2208.	2.8	19
84	Theory of NMR Parameters. From Ramsey to Relativity, 1953 to 1983. , 2004, , 7-19.		8
85	Magnetic-field-induced quadrupole coupling in the nuclear magnetic resonance of noble-gas atoms and molecules. Physical Review A, 2004, 70, .	2.5	5
86	How Many Hydrogen Atoms Can Be Bound to a Metal? Predicted MH12Species. Journal of the American Chemical Society, 2004, 126, 15014-15015.	13.7	87
87	Theoretical Chemistry of Gold. Angewandte Chemie - International Edition, 2004, 43, 4412-4456.	13.8	1,668
88	Theoretical Search for Very Short Metalâ€“Actinide Bonds: NUIr and Isoelectronic Systems. Angewandte Chemie - International Edition, 2004, 43, 1573-1576.	13.8	49
89	Al3+â€“He: stability and spectroscopy. Chemical Physics Letters, 2004, 392, 281-283.	2.6	12
90	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. Chemical Communications, 2004, , 1982-1983.	4.1	28

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91	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	2.8	97
92	Study of the MAu6(Mâ€‰=â€‰Cr, Mo, W) molecular species: A transition from halogenlike to hydrogenlike chemical behavior for gold. Physical Chemistry Chemical Physics, 2004, 6, 2904-2906.	2.8	25
93	The importance of being tetrahedral: the cadmium pyramids CdN; N = 4, 10, 20, 35 and 56. Physical Chemistry Chemical Physics, 2004, 6, 2907-2909.	2.8	30
94	Aurophilic attraction in binuclear complexes with Au(i) and Au(iii). A theoretical study. Physical Chemistry Chemical Physics, 2004, 6, 900-905.	2.8	82
95	Calculated structures of [Au=C=Au]2+ and related systems. Chemical Physics Letters, 2003, 381, 45-52.	2.6	45
96	Why are hexavalent uranium cyanides rare while U?F and U?O bonds are common and short?. Theoretical Chemistry Accounts, 2003, 109, 332-340.	1.4	78
97	Cesium and barium as honorary d elements: CsN 7 Ba as an example. Theoretical Chemistry Accounts, 2003, 110, 205-210.	1.4	52
98	Strong chemical bonds in heavy diatomics: PtSi, PtTh and AuTh+. Chemical Physics Letters, 2003, 368, 538-541.	2.6	17
99	Aurophilic attraction: the additivity and the combination with hydrogen bonds. Chemical Physics Letters, 2003, 370, 733-740.	2.6	48
100	QED corrections to the binding energy of the eka-radon(Z=118)negative ion. Physical Review A, 2003, 67, .	2.5	50
101	Predicted Group 4 Tetra-azides M(N3)4(M = Tiâˆ’Hf, Th):Â The First Examples of Linear Mâˆ’NNN Coordination. Inorganic Chemistry, 2003, 42, 3074-3078.	4.0	35
102	One Metal and Forty Nitrogens. Ab Initio Predictions for Possible New High-Energy Pentazolides. Inorganic Chemistry, 2003, 42, 8241-8249.	4.0	39
103	On the nature of the short Ptâ€“Tl bonds in model compounds [H5Ptâ€“TlHn]nâˆ’. Faraday Discussions, 2003, 124, 41-51.	3.2	16
104	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases Heâ€“Rn: A way to absolute nuclear magnetic resonance shielding scales. Journal of Chemical Physics, 2003, 118, 2973-2976.	3.0	109
105	Î·5-N5-âˆ’Metalâˆ’Î·7-N73-:Â A New Class of Compounds. Journal of Physical Chemistry A, 2002, 106, 4690-4694.	2.5	77
106	HgH4and HgH6: further candidates for high-valent mercury compounds. Chemical Communications, 2002, , 1728-1729.	4.1	26
107	Possible high-pressure structures of sulfur trioxideElectronic supplementary information (ESI) available: technical details for calculations. See http://www.rsc.org/suppdata/cc/b1/b107778c/. Chemical Communications, 2002, , 336-337.	4.1	5
108	Icosahedral WAu12: A Predicted Closed-Shell Species, Stabilized by Aurophilic Attraction and Relativity and in Accord with the 18-Electron Rule This work was supported by The Academy of Finland. The computations were carried out at CSC, Espoo, Finland.. Angewandte Chemie, 2002, 114, 2278.	2.0	66

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109	RelativitÃt, Gold, Wechselwirkungen zwischen gefÃ¼llten Schalen und CsAuâ‹…NH3. Angewandte Chemie, 2002, 114, 3723-3728.	2.0	42
110	Icosahedral WAu12: A Predicted Closed-Shell Species, Stabilized by Aurophilic Attraction and Relativity and in Accord with the 18-Electron Rule This work was supported by The Academy of Finland. The computations were carried out at CSC, Espoo, Finland.. Angewandte Chemie - International Edition, 2002, 41, 2174.	13.8	335
111	Relativity, Gold, Closed-Shell Interactions, and CsAuâ‹…NH3. Angewandte Chemie - International Edition, 2002, 41, 3573-3578.	13.8	200
112	A Study of the Interactions in an Extended Unsupported Gold-Silver Chain. European Journal of Inorganic Chemistry, 2002, 2002, 750-753.	2.0	45
113	Scandium Cycloheptanitride, ScN7:Â A Predicted High-Energy Molecule Containing an [Î·7-N7]3-Ligand. Journal of the American Chemical Society, 2001, 123, 9700-9701.	13.7	69
114	Spectroscopic nuclear quadrupole moments. Molecular Physics, 2001, 99, 1617-1629.	1.7	505
115	The Quest for Beryllium Peroxides. Inorganic Chemistry, 2001, 40, 2270-2274.	4.0	13
116	Ab initio study of bonding trends for f 0 actinide oxyfluoride species. Theoretical Chemistry Accounts, 2001, 106, 393-403.	1.4	86
117	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.	2.0	25
118	Nuclear quadrupole moments of Kr and Xe from molecular data. Chemical Physics Letters, 2001, 346, 155-159.	2.6	25
119	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	2.6	28
120	Nuclear Quadrupole Moments of Bismuth. Physical Review Letters, 2001, 87, 133003.	7.8	62
121	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, .	2.5	46
122	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	2.5	86
123	Magnetic-Field-Induced Quadrupole Splitting in Gaseous and LiquidX131eNMR: Quadratic and Quartic Field Dependence. Physical Review Letters, 2001, 86, 3268-3271.	7.8	18
124	Ab Initio Study of Bonding Trends among Cyanamidophosphates ([POn(NCN)4â^'n]3â^') and Related Systems. Chemistry - A European Journal, 2000, 6, 2145-2151.	3.3	11
125	Au22+ has bound excited states. Chemical Physics Letters, 2000, 325, 225-231.	2.6	26
126	The nuclear quadrupole moment of 45Sc. Chemical Physics Letters, 2000, 329, 112-118.	2.6	25

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127	Could uranium(XII)hexoxide, UO6 (Oh) exist?. Chemical Physics Letters, 2000, 328, 415-419.	2.6	24
128	The nuclear quadrupole moment of from molecular data for ZrO and ZrS. Chemical Physics Letters, 2000, 318, 222-231.	2.6	27
129	Perspective on Norman Ramsey's theories of NMR chemical shifts and nuclear spin-spin coupling. Theoretical Chemistry Accounts, 2000, 103, 214-216.	1.4	31
130	Structure and stability of gold-substituted diborane, boranes, and borohydride ions. Theoretical Chemistry Accounts, 2000, 103, 399-408.	1.4	5
131	Luminescent Characterization of Solution Oligomerization Process Mediated Goldâ^'Gold Interactions. DFT Calculations on [Au2Ag2R4L2]nMoieties. Journal of the American Chemical Society, 2000, 122, 7287-7293.	13.7	140
132	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.	2.8	171
133	Calculations for XeOn(n= 2â^'4):Â Could the Xenon Dioxide Molecule Exist?â€. Journal of Physical Chemistry A, 2000, 104, 3826-3828.	2.5	13
134	Experimental and Theoretical Studies of the d8â^'d10Interaction between Pd(II) and Au(I):Â Bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))â^'dichloropalladium(II) and Related Systems. Inorganic Chemistry, 2000, 39, 4786-4792.	4.0	75
135	Isomerism of Aurated Phosphine Sulfides, Thiophosphinates, Thiophosphonates, and Thiophosphates:â€‰ Structural and Quantum Chemical Studies. Inorganic Chemistry, 1999, 38, 5870-5875.	4.0	18
136	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.	2.6	73
137	Calculated self-energy contributions for annsvalence electron using the multiple-commutator method. Physical Review A, 1999, 59, 2707-2711.	2.5	72
138	Calculations on indium and thallium cyclopentadienyls. Metalâ€“metal interactions and possible new species. Physical Chemistry Chemical Physics, 1999, 1, 3441-3444.	2.8	41
139	Predictions for possible new, doubly and triply bridged oxides and peroxides of C, N, P, and S. Chemical Communications, 1999, , 495-496.	4.1	3
140	Strong chemical bonds to gold. High level correlated relativistic results for diatomic AuBe+, AuC+, AuMg+, and AuSi+. Chemical Physics Letters, 1998, 285, 398-403.	2.6	67
141	Chemical bonds between noble metals and noble gases.. Chemical Physics Letters, 1998, 288, 635-641.	2.6	36
142	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.	3.3	344
143	Relativistic pseudopotential calculations on Xe2, RnXe, and Rn2: The van der Waals properties of radon. International Journal of Quantum Chemistry, 1998, 66, 131-140.	2.0	71
144	Can triple bonds exist between gold and main-group elements?. Theoretical Chemistry Accounts, 1998, 99, 113-115.	1.4	13

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145	Theory of the d10â^'d10Closed-Shell Attraction. 4. X(AuL)nm+Centered Systems. Organometallics, 1998, 17, 4842-4852.	2.3	82
146	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfurâ€. Inorganic Chemistry, 1998, 37, 624-632.	4.0	255
147	Theory of d10â^'d10Closed-Shell Attraction. III. Rings. Inorganic Chemistry, 1998, 37, 3018-3025.	4.0	207
148	Closed-shell interaction in silver and gold chlorides. Journal of Chemical Physics, 1998, 109, 2339-2345.	3.0	68
149	Estimated valence-level Lamb shifts for group 1 and group 11 metal atoms. Physical Review A, 1998, 57, R689-R692.	2.5	75
150	How Do Spinâ€“Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spinâ€“Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. Chemistry - A European Journal, 1998, 4, 118-126.	3.3	2
151	Hyperfine structure of the state of highly charged ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 1427-1435.	1.5	12
152	Vacuum-polarization corrections to the hyperfine-structure splitting of highly charged83209Bi ions. Physical Review A, 1997, 56, 4508-4516.	2.5	21
153	An ab initio study of the aggregation of LAuX molecules and [LAuL]+[XAuX]â^' ions. Chemical Communications, 1997, , 1111-1112.	4.1	50
154	Calculated Structures of MO22+, MN2, and MP2 (M = Mo, W). Journal of Physical Chemistry A, 1997, 101, 8107-8114.	2.5	27
155	Strong Closed-Shell Interactions in Inorganic Chemistry. Chemical Reviews, 1997, 97, 597-636.	47.7	2,282
156	Relativistic effects in nuclear quadrupole coupling. Theoretical Chemistry Accounts, 1997, 96, 92-104.	1.4	48
157	Theory of the d¹⁰â€"d¹⁰ Closedâ€Shell Attraction: 1. Dimers Near Equilibrium. Chemistry - A European Journal, 1997, 3, 1451-1457.	3.3	430
158	Theory of the d¹⁰â€"d¹⁰ Closedâ€Shell Attraction: 2. Longâ€Distance Behaviour and Nonadditive Effects in Dimers and Trimers of Type [(xâ€Auâ€L)_n] (n = 2, 3; X = Cl, I,) Tj ETQq0 0 0 rgBT /Over	3.3	182
159	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p;) Tj ETQq1 1 0.784314 rgBT /Ove	2.6	61
160	Calculated energy levels of thallium and eka-thallium (element 113). Physical Review A, 1996, 53, 3926-3933.	2.5	109
161	Calculated Structure and Optical Properties of Tl2Pt(CN)4. Inorganic Chemistry, 1996, 35, 7450-7451.	4.0	45
162	Element 118: The First Rare Gas with an Electron Affinity. Physical Review Letters, 1996, 77, 5350-5352.	7.8	105

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163	What did Johan Gadolin Actually do?. , 1996, , 1-12.		3
164	Calculated properties of XeH2. Chemical Physics Letters, 1995, 246, 239-244.	2.6	42
165	Matrix Infrared Spectroscopic and ab Initio Studies of ZnH2, CdH2, and Related Metal Hydride Species. The Journal of Physical Chemistry, 1995, 99, 7925-7934.	2.9	118
166	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.	4.0	100
167	Predicted ligand dependence of the Au(I)â€¦Au(I) attraction in (XAuPH3)2. Chemical Physics Letters, 1994, 218, 133-138.	2.6	277
168	ESF works, don't change it. Nature, 1994, 371, 734-734.	27.8	0
169	Structure of tetrakis(phosphine)nitrido- or -phosphinidyne or arsinidyneultragold(1+): Td or C4v?. Inorganic Chemistry, 1993, 32, 2630-2634.	4.0	85
170	Relativistic Theory of Atoms and Molecules II. Lecture Notes in Quantum Chemistry II, 1993, , .	0.3	45
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