

Pekka Pyykkö

List of Publications by Year in descending order

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26,086
citations

11608

70
h-index

6282

158
g-index

219
all docs

219
docs citations

219
times ranked

12377
citing authors

#	ARTICLE	IF	CITATIONS
1	<i>Saturnenes</i> Like Th@Au ₆ <i>D</i> _{6h} : Ring-Current Evidence for Au ⁺ Au Bonding Along the Gold Ring. Israel Journal of Chemistry, 2022, 62, .	1.0	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, .	1.0	5
4	Understanding the Uniqueness of 2p Elements in Periodic Tables. Chemistry - A European Journal, 2020, 26, 15558-15564.	1.7	31
5	Structural trends in atomic nuclei from laser spectroscopy of tin. Communications Physics, 2020, 3, .	2.0	24
6	The periodic table and the physics that drives it. Nature Reviews Chemistry, 2020, 4, 359-380.	13.8	57
7	An essay on periodic tables. Pure and Applied Chemistry, 2019, 91, 1959-1967.	0.9	18
8	<i>In My Element</i> : How did I land in a gold mine?. Chemistry - A European Journal, 2019, 25, 2101-2102.	1.7	0
9	Simple Estimates for Eutectic Behavior. ChemPhysChem, 2019, 20, 123-127.	1.0	6
10	Year-2017 nuclear quadrupole moments. Molecular Physics, 2018, 116, 1328-1338.	0.8	103
11	The argon nuclear quadrupole moments. Molecular Physics, 2018, 116, 1682-1686.	0.8	2
12	<i>Ab initio</i> calculations of the hyperfine structure of zinc and evaluation of the nuclear quadrupole moment $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle Q \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle (\langle \text{mml:mo} \rangle \langle \text{mml:mmultiscripts} \rangle$	1.0	11
13	Physical Review A, 2018, 97, . Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. Angewandte Chemie - International Edition, 2017, 56, 10132-10134.	7.2	17
14	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. Angewandte Chemie, 2017, 129, 10266-10268.	1.6	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.	0.1	13
17	Is the chemistry of lawrencium peculiar?. Physical Chemistry Chemical Physics, 2016, 18, 17351-17355.	1.3	27
18	On the Extreme Oxidation States of Iridium. Chemistry - A European Journal, 2015, 21, 9468-9473.	1.7	31

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19	The Formal Oxidation States of Iridium Now Run from $+III$ to $+IX$. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1080-1081.	7.2	27
20	Magically magnetic gadolinium. <i>Nature Chemistry</i> , 2015, 7, 680-680.	6.6	29
21	<i>Ab initio</i> MCDHF calculations of electron-nucleus interactions. <i>Physica Scripta</i> , 2015, 90, 054011.	1.2	18
22	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series $PuO_{x}F_{8-2x}$ ($x = 0-4$). <i>Inorganic Chemistry</i> , 2015, 54, 8825-8831.	1.9	26
23	Additive Covalent Radii for Single-, Double-, and Triple-Bonded Molecules and Tetrahedrally Bonded Crystals: A Summary. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2326-2337.	1.1	513
24	Preface to The Relativistic Quantum Chemistry Issue of <i>Journal of Computer Chemistry, Japan</i> . <i>Journal of Computer Chemistry Japan</i> , 2014, 13, A2-A3.	0.0	1
25	Aspects of bonding in small gold clusters. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 15-18.	0.7	15
26	Unbridged Au(II)-Au(II) bonds are theoretically allowed. <i>Chemical Communications</i> , 2013, 49, 2103.	2.2	21
27	The RTAM electronic bibliography, version 17.0, on relativistic theory of atoms and molecules. <i>Journal of Computational Chemistry</i> , 2013, 34, 2667-2667.	1.5	22
28	A new, centered 32-electron system: the predicted $[U@Si_{20}]^{6+}$ -like isoelectronic series. <i>Chemical Science</i> , 2012, 3, 2843.	3.7	42
29	Rare-earth monocarbonyls MCO: comprehensive infrared observations and a transparent theoretical interpretation for $M = Sc; Y; La-Lu$. <i>Chemical Science</i> , 2012, 3, 1548.	3.7	31
30	The Physics behind Chemistry and the Periodic Table. <i>Chemical Reviews</i> , 2012, 112, 371-384.	23.0	179
31	Predicting new, simple inorganic species by quantum chemical calculations: some successes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14734.	1.3	45
32	Refitted tetrahedral covalent radii for solids. <i>Physical Review B</i> , 2012, 85, .	1.1	75
33	Relativistic Effects in Chemistry: More Common Than You Thought. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 45-64.	4.8	416
34	Introduction to the <i>Quantum Chemistry 2012</i> Issue. <i>Chemical Reviews</i> , 2012, 112, 1-3.	23.0	86
35	Auophilic attractions between a closed-shell molecule and a gold cluster. <i>Faraday Discussions</i> , 2011, 152, 169.	1.6	38
36	Relativity and the Lead-Acid Battery. <i>Physical Review Letters</i> , 2011, 106, 018301.	2.9	100

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37	Relativity and the mercury battery. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16510.	1.3	16
38	Molecular Hydrogen Tweezers: Structure and Mechanisms by Neutron Diffraction, NMR, and Deuterium Labeling Studies in Solid and Solution. <i>Journal of the American Chemical Society</i> , 2011, 133, 20245-20257.	6.6	64
39	A suggested periodic table up to $Z \approx 172$, based on Dirac-Fock calculations on atoms and ions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 161-168.	1.3	129
40	Aurophilicity: The Effect of the Neutral Ligand L on $[\{\text{ClAuL}\}]_2$ Systems. <i>Chemistry - A European Journal</i> , 2011, 17, 368-377.	1.7	107
41	Bonding Trends in Molecular Compounds of Lanthanides: The Double-Bonded Carbene Cations LnCH_2^+ ($\text{Ln}=\text{Sc}, \text{Y}, \text{La-Lu}$). <i>Chemistry - A European Journal</i> , 2010, 16, 270-275.	1.7	38
42	Chemical properties of the predicted 32-electron systems Pu@Sn_{12} and Pu@Pb_{12} . <i>Comptes Rendus Chimie</i> , 2010, 13, 884-888.	0.2	26
43	Theoretical study of H_2 splitting and storage by boron-nitrogen-based systems: a bimolecular case and some qualitative aspects. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 149-155.	1.3	18
44	Formulations of the closed-shell interactions in endohedral systems. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6187.	1.3	29
45	$\text{WAu}_{12}(\text{CO})_{12}$. <i>Chemical Communications</i> , 2010, 46, 3762.	2.2	21
46	Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. <i>Physical Review A</i> , 2009, 79, .	1.0	29
47	Molecular Single-Bond Covalent Radii for Elements 1-118. <i>Chemistry - A European Journal</i> , 2009, 15, 186-197.	1.7	1,762
48	Molecular Double-Bond Covalent Radii for Elements 1-118. <i>Chemistry - A European Journal</i> , 2009, 15, 12770-12779.	1.7	1,106
49	Theoretical study on the series of $[\text{Au}_3\text{Cl}_3\text{M}_2]$ complexes, with $\text{M} = \text{Li}, \text{Na}, \text{K}, \text{Rb}, \text{Cs}$. <i>Journal of Molecular Modeling</i> , 2009, 15, 1165-1173.	0.8	9
50	Experimental and theoretical treatment of hydrogen splitting and storage in boron-nitrogen systems. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 2654-2660.	0.8	89
51	Au_nHg_m Clusters: Mercury Aurides, Gold Amalgams, or van der Waals Aggregates?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12380-12385.	1.1	21
52	A Predicted Organometallic Series Following a 32-Electron Principle: $\text{An}@C_{28}$ ($\text{An} = \text{Th}, \text{Tl}, \text{Er}, \text{Yb}, \text{Lu}$). <i>Journal of the American Chemical Society</i> , 2008, 130, 131, 238-243.	6.6	106
53	Bonding trends in MCH_2 systems: Simple orbital interpretation and evidence for double bonds. <i>Chemical Physics Letters</i> , 2008, 462, 138-143.	1.2	13
54	Theoretical mapping of new $(\text{N}^+)\text{L}$ family of species with donor-acceptor bonding between N^+ and ligand L . <i>Computational and Theoretical Chemistry</i> , 2008, 860, 128-136.	1.5	11

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55	Icosahedral Au ₇₂ : a predicted chiral and spherically aromatic golden fullerene. Chemical Communications, 2008, , 465-467.	2.2	109
56	Structure and bonding of the MCN molecules, M=Cu,Ag,Au,Rg. Journal of Chemical Physics, 2008, 128, 224303.	1.2	29
57	Theoretical chemistry of gold. III. Chemical Society Reviews, 2008, 37, 1967.	18.7	631
58	Molecular Tweezers for Hydrogen: Synthesis, Characterization, and Reactivity. Journal of the American Chemical Society, 2008, 130, 14117-14119.	6.6	356
59	Year-2008 nuclear quadrupole moments. Molecular Physics, 2008, 106, 1965-1974.	0.8	437
60	From nanostrips to nanorings: the elastic properties of gold-glued polyaunaphthyridines and polyacenes. Physical Chemistry Chemical Physics, 2008, 10, 114-120.	1.3	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 $\hat{I} = 1$. Physical Chemistry Chemical Physics, 2008, 10, 3867.	1.3	12
62	Basis-set limit of the aurophilic attraction using the MP2 method: The examples of [ClAuPH ₃] ₂ dimer and [P(AuPH ₃) ₄] ⁺ ion. Journal of Chemical Physics, 2008, 128, 124309.	1.2	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.	0.6	17
64	Hurricanes as Heat Engines: Two Undergraduate Problems. Journal of Chemical Education, 2007, 84, 447.	1.1	1
65	Gold as intermolecular glue: a theoretical study of nanostrips based on quinoline-type monomers. Physical Chemistry Chemical Physics, 2007, 9, 3025.	1.3	11
66	A London-type formula for the dispersion interactions of endohedral A@B systems. Physical Chemistry Chemical Physics, 2007, 9, 2954.	1.3	48
67	Coordination of Pyridinethiols in Gold(I) Complexes. Inorganic Chemistry, 2007, 46, 9954-9960.	1.9	40
68	Towards a 32-Electron Principle: Pu@Pb ₁₂ and Related Systems. Angewandte Chemie - International Edition, 2007, 46, 1427-1430.	7.2	88
69	Pocket and antipocket conformations for the CH ₄ @C ₈₄ endohedral fullerene. International Journal of Quantum Chemistry, 2007, 107, 1162-1169.	1.0	21
70	Magic nanoclusters of gold. Nature Nanotechnology, 2007, 2, 273-274.	15.6	76
71	Gold as intermolecular glue: a predicted planar triaurotriazine, C ₃ Au ₃ N ₃ , isomer of gold cyanide. Chemical Communications, 2006, , 2890.	2.2	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.	1.2	71

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73	Computational study of bonding trends in the metalloactinyl series EThM and MThM ²⁺ (E=N ⁺ , O, F ⁺ ; M,) Tj ETQq _{1,1} 0.784314 rgBT /	1.2	16
74	Understanding the eighteen-electron rule. Journal of Organometallic Chemistry, 2006, 691, 4336-4340.	0.8	153
75	Comparative Theoretical Study of N-Heterocyclic Carbenes and Other Ligands Bound to Au. Chemistry - an Asian Journal, 2006, 1, 623-628.	1.7	39
76	Theoretical chemistry of gold. II. Inorganica Chimica Acta, 2005, 358, 4113-4130.	1.2	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.	1.2	38
78	Triple-Bond Covalent Radii. Chemistry - A European Journal, 2005, 11, 3511-3520.	1.7	370
79	Nuclear quadrupole moment of Hg201. Physical Review A, 2005, 71, .	1.0	44
80	Degree of accuracy in determining the nuclear electric quadrupole moment of radium. Physical Review A, 2005, 71, .	1.0	20
81	A very short uranium-uranium bond: The predicted metastable U22+. Physical Chemistry Chemical Physics, 2005, 7, 2415.	1.3	79
82	Linear HThTh: A Candidate for a Th-Th Triple Bond. Journal of the American Chemical Society, 2005, 127, 13090-13091.	6.6	39
83	A small spherical liquid: A DFT molecular dynamics study of WAu12. Physical Chemistry Chemical Physics, 2005, 7, 2208.	1.3	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, .	1.0	5
86	How Many Hydrogen Atoms Can Be Bound to a Metal? Predicted MH12Species. Journal of the American Chemical Society, 2004, 126, 15014-15015.	6.6	87
87	Theoretical Chemistry of Gold. Angewandte Chemie - International Edition, 2004, 43, 4412-4456.	7.2	1,668
88	Theoretical Search for Very Short Metal-Actinide Bonds: NUIr and Isoelectronic Systems. Angewandte Chemie - International Edition, 2004, 43, 1573-1576.	7.2	49
89	Al3+-He: stability and spectroscopy. Chemical Physics Letters, 2004, 392, 281-283.	1.2	12
90	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. Chemical Communications, 2004, , 1982-1983.	2.2	28

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91	Properties of WAu ₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 11-22.	1.3	97
92	Study of the MAu ₆ (M = Cr, Mo, W) molecular species: A transition from halogenlike to hydrogenlike chemical behavior for gold. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2904-2906.	1.3	25
93	The importance of being tetrahedral: the cadmium pyramids CdN _N ; N = 4, 10, 20, 35 and 56. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2907-2909.	1.3	30
94	Auophilic attraction in binuclear complexes with Au(i) and Au(iii). A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 900-905.	1.3	82
95	Calculated structures of [Au=C=Au] ₂ ⁺ and related systems. <i>Chemical Physics Letters</i> , 2003, 381, 45-52.	1.2	45
96	Why are hexavalent uranium cyanides rare while U≡F and U=O bonds are common and short?. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 332-340.	0.5	78
97	Cesium and barium as honorary d elements: CsN ₇ Ba as an example. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 205-210.	0.5	52
98	Strong chemical bonds in heavy diatomics: PtSi, PtTh and AuTh ⁺ . <i>Chemical Physics Letters</i> , 2003, 368, 538-541.	1.2	17
99	Auophilic attraction: the additivity and the combination with hydrogen bonds. <i>Chemical Physics Letters</i> , 2003, 370, 733-740.	1.2	48
100	QED corrections to the binding energy of the eka-radon (Z=118) negative ion. <i>Physical Review A</i> , 2003, 67, .	1.0	50
101	Predicted Group 4 Tetra-azides M(N ₃) ₄ (M = Ti, Hf, Th): The First Examples of Linear M ⁺ NNN Coordination. <i>Inorganic Chemistry</i> , 2003, 42, 3074-3078.	1.9	35
102	One Metal and Forty Nitrogens. Ab Initio Predictions for Possible New High-Energy Pentazolides. <i>Inorganic Chemistry</i> , 2003, 42, 8241-8249.	1.9	39
103	On the nature of the short Pt-Tl bonds in model compounds [H ₅ Pt-TlHn] ⁺ . <i>Faraday Discussions</i> , 2003, 124, 41-51.	1.6	16
104	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He-Rn: A way to absolute nuclear magnetic resonance shielding scales. <i>Journal of Chemical Physics</i> , 2003, 118, 2973-2976.	1.2	109
105	Î ⁵ -N ₅ -Metal-Î ⁷ -N ₇₃ : A New Class of Compounds. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4690-4694.	1.1	77
106	HgH ₄ and HgH ₆ : further candidates for high-valent mercury compounds. <i>Chemical Communications</i> , 2002, , 1728-1729.	2.2	26
107	Possible high-pressure structures of sulfur trioxide Electronic supplementary information (ESI) available: technical details for calculations. See http://www.rsc.org/suppdata/cc/b1/b107778c/ . <i>Chemical Communications</i> , 2002, , 336-337.	2.2	5
108	Icosahedral WAu ₁₂ : A Predicted Closed-Shell Species, Stabilized by Auophilic 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.. <i>Angewandte Chemie</i> , 2002, 114, 2278.	1.6	66

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109	Relativität, Gold, Wechselwirkungen zwischen gefüllten Schalen und CsAu...NH ₃ . Angewandte Chemie, 2002, 114, 3723-3728.	1.6	42
110	Icosahedral WAu ₁₂ : A Predicted Closed-Shell Species, Stabilized by Auophilic 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.	7.2	335
111	Relativity, Gold, Closed-Shell Interactions, and CsAu...NH ₃ . Angewandte Chemie - International Edition, 2002, 41, 3573-3578.	7.2	200
112	A Study of the Interactions in an Extended Unsupported Gold-Silver Chain. European Journal of Inorganic Chemistry, 2002, 2002, 750-753.	1.0	45
113	Scandium Cycloheptanitride, ScN ₇ : A Predicted High-Energy Molecule Containing an [1-7-N ₇] ³⁻ Ligand. Journal of the American Chemical Society, 2001, 123, 9700-9701.	6.6	69
114	Spectroscopic nuclear quadrupole moments. Molecular Physics, 2001, 99, 1617-1629.	0.8	505
115	The Quest for Beryllium Peroxides. Inorganic Chemistry, 2001, 40, 2270-2274.	1.9	13
116	Ab initio study of bonding trends for f ⁰ actinide oxyfluoride species. Theoretical Chemistry Accounts, 2001, 106, 393-403.	0.5	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.	1.0	25
118	Nuclear quadrupole moments of Kr and Xe from molecular data. Chemical Physics Letters, 2001, 346, 155-159.	1.2	25
119	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	1.2	28
120	Nuclear Quadrupole Moments of Bismuth. Physical Review Letters, 2001, 87, 133003.	2.9	62
121	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, .	1.0	46
122	Estimation of Lamb-shift effects for molecules: Application to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	1.0	86
123	Magnetic-Field-Induced Quadrupole Splitting in Gaseous and Liquid ¹³¹ Xe NMR: Quadratic and Quartic Field Dependence. Physical Review Letters, 2001, 86, 3268-3271.	2.9	18
124	Ab Initio Study of Bonding Trends among Cyanamidophosphates ([POn(NCN) ₄] ⁿ⁻) ₃ and Related Systems. Chemistry - A European Journal, 2000, 6, 2145-2151.	1.7	11
125	Au ²²⁺ has bound excited states. Chemical Physics Letters, 2000, 325, 225-231.	1.2	26
126	The nuclear quadrupole moment of ⁴⁵ Sc. Chemical Physics Letters, 2000, 329, 112-118.	1.2	25

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127	Could uranium(III)hexoxide, $\text{UO}_6(\text{OH})$ exist?. Chemical Physics Letters, 2000, 328, 415-419.	1.2	24
128	The nuclear quadrupole moment of from molecular data for ZrO and ZrS . Chemical Physics Letters, 2000, 318, 222-231.	1.2	27
129	Perspective on Norman Ramsey's theories of NMR chemical shifts and nuclear spin-spin coupling. Theoretical Chemistry Accounts, 2000, 103, 214-216.	0.5	31
130	Structure and stability of gold-substituted diborane, boranes, and borohydride ions. Theoretical Chemistry Accounts, 2000, 103, 399-408.	0.5	5
131	Luminescent Characterization of Solution Oligomerization Process Mediated Gold-Gold Interactions. DFT Calculations on $[\text{Au}_2\text{Ag}_2\text{R}_4\text{L}_2]_n$ Moieties. Journal of the American Chemical Society, 2000, 122, 7287-7293.	6.6	140
132	Ab initio studies of the dimers $(\text{HgH}_2)_2$ and $(\text{HgMe}_2)_2$. Metallophilic attraction and the van der Waals radii of mercury. Physical Chemistry Chemical Physics, 2000, 2, 2489-2493.	1.3	171
133	Calculations for $\text{XeO}_n (n=2,4)$: Could the Xenon Dioxide Molecule Exist?. Journal of Physical Chemistry A, 2000, 104, 3826-3828.	1.1	13
134	Experimental and Theoretical Studies of the d π -d π Interaction between Pd(II) and Au(I): Bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I))-dichloropalladium(II) and Related Systems. Inorganic Chemistry, 2000, 39, 4786-4792.	1.9	75
135	Isomerism of Aurated Phosphine Sulfides, Thiophosphinates, Thiophosphonates, and Thiophosphates: Structural and Quantum Chemical Studies. Inorganic Chemistry, 1999, 38, 5870-5875.	1.9	18
136	Electric quadrupole moment of the ^{27}Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. Chemical Physics Letters, 1999, 304, 414-422.	1.2	73
137	Calculated self-energy contributions for annihilation electron using the multiple-commutator method. Physical Review A, 1999, 59, 2707-2711.	1.0	72
138	Calculations on indium and thallium cyclopentadienyls. Metal-metal interactions and possible new species. Physical Chemistry Chemical Physics, 1999, 1, 3441-3444.	1.3	41
139	Predictions for possible new, doubly and triply bridged oxides and peroxides of C, N, P, and S. Chemical Communications, 1999, , 495-496.	2.2	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.	1.2	67
141	Chemical bonds between noble metals and noble gases.. Chemical Physics Letters, 1998, 288, 635-641.	1.2	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.	1.7	344
143	Relativistic pseudopotential calculations on Xe_2 , RnXe , and Rn_2 : The van der Waals properties of radon. , 1998, 66, 131-140.		71
144	Can triple bonds exist between gold and main-group elements?. Theoretical Chemistry Accounts, 1998, 99, 113-115.	0.5	13

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145	Theory of the d ¹⁰ -d ¹⁰ Closed-Shell Attraction. 4. X(AuL) _n m+Centered Systems. Organometallics, 1998, 17, 4842-4852.	1.1	82
146	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur. Inorganic Chemistry, 1998, 37, 624-632.	1.9	255
147	Theory of d ¹⁰ -d ¹⁰ Closed-Shell Attraction. III. Rings. Inorganic Chemistry, 1998, 37, 3018-3025.	1.9	207
148	Closed-shell interaction in silver and gold chlorides. Journal of Chemical Physics, 1998, 109, 2339-2345.	1.2	68
149	Estimated valence-level Lamb shifts for group 1 and group 11 metal atoms. Physical Review A, 1998, 57, R689-R692.	1.0	75
150	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.		2
151	Hyperfine structure of the state of highly charged ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 1427-1435.	0.6	12
152	Vacuum-polarization corrections to the hyperfine-structure splitting of highly charged Bi ions. Physical Review A, 1997, 56, 4508-4516.	1.0	21
153	An ab initio study of the aggregation of LAuX molecules and [LAuL] ⁺ [XAuX] ⁻ ions. Chemical Communications, 1997, , 1111-1112.	2.2	50
154	Calculated Structures of MO ₂ ²⁺ , MN ₂ , and MP ₂ (M = Mo, W). Journal of Physical Chemistry A, 1997, 101, 8107-8114.	1.1	27
155	Strong Closed-Shell Interactions in Inorganic Chemistry. Chemical Reviews, 1997, 97, 597-636.	23.0	2,282
156	Relativistic effects in nuclear quadrupole coupling. Theoretical Chemistry Accounts, 1997, 96, 92-104.	0.5	48
157	Theory of the d ¹⁰ -d ¹⁰ Closed-Shell Attraction: 1. Dimers Near Equilibrium. Chemistry - A European Journal, 1997, 3, 1451-1457.	1.7	430
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159	The nuclear quadrupole moment of ¹⁴ N obtained from finite-element MCHF calculations on N ₂ ⁺ (2p _z). J. Phys. Chem. B, 1998, 102, 7843-7851.	1.2	81
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