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	Relativistic effects in structural chemistry. Chemical Reviews, 1988, 88, 563-594.	47.7	2,731
2	Strong Closed-Shell Interactions in Inorganic Chemistry. Chemical Reviews, 1997, 97, 597-636.	47.7	2,282
3	Molecular Singleâ€Bond Covalent Radii for Elements 1â€“118. Chemistry - A European Journal, 2009, 15, 186-197.	3.3	1,762
4	Theoretical Chemistry of Gold. Angewandte Chemie - International Edition, 2004, 43, 4412-4456.	13.8	1,668
5	Molecular Doubleâ€Bond Covalent Radii for Elements Liâ€“E112. Chemistry - A European Journal, 2009, 15, 12770-12779.	3.3	1,106
6	Relativity and the periodic system of elements. Accounts of Chemical Research, 1979, 12, 276-281.	15.6	989
7	Theoretical chemistry of gold. III. Chemical Society Reviews, 2008, 37, 1967.	38.1	631
8	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
9	Spectroscopic nuclear quadrupole moments. Molecular Physics, 2001, 99, 1617-1629.	1.7	505
10	Year-2008 nuclear quadrupole moments. Molecular Physics, 2008, 106, 1965-1974.	1.7	437
11	Theory of the d¹⁰â€“d¹⁰ Closedâ€Shell Attraction: 1. Dimers Near Equilibrium. Chemistry - A European Journal, 1997, 3, 1451-1457.	3.3	430
12	Relativistic Effects in Chemistry: More Common Than You Thought. Annual Review of Physical Chemistry, 2012, 63, 45-64.	10.8	416
13	Theoretical chemistry of gold. II. Inorganica Chimica Acta, 2005, 358, 4113-4130.	2.4	399
14	Triple-Bond Covalent Radii. Chemistry - A European Journal, 2005, 11, 3511-3520.	3.3	370
15	Molecular Tweezers for Hydrogen: Synthesis, Characterization, and Reactivity. Journal of the American Chemical Society, 2008, 130, 14117-14119.	13.7	356
16	Relativistic Quantum Chemistry. Advances in Quantum Chemistry, 1978, 11, 353-409.	0.8	344
17	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
18	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

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19	Predicted ligand dependence of the Au(I)â€¦Au(I) attraction in (XAuPH3)2. Chemical Physics Letters, 1994, 218, 133-138.	2.6	277
20	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
21	Ab initio Calculations on the(ClAuPH3)2 Dimer with Relativistic Pseudopotential: Is theâ€œAurophilic Attractionâ€•a Correlation Effect?. Angewandte Chemie International Edition in English, 1991, 30, 604-605.	4.4	244
22	Fully numerical hartree-fock methods for molecules. Computer Physics Reports, 1986, 4, 313-344.	2.2	240
23	Theory of d10â^'d10Closed-Shell Attraction. III. Rings. Inorganic Chemistry, 1998, 37, 3018-3025.	4.0	207
24	Relativity, Gold, Closed-Shell Interactions, and CsAuâ‹…NH3. Angewandte Chemie - International Edition, 2002, 41, 3573-3578.	13.8	200
25	The Nuclear Quadrupole Moments of the 20 First Elements: High-Precision Calculations on Atoms and Small Molecules. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1992, 47, 189-196.	1.5	193
26	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 ET Q q 0 0 1 gBT /Over	3.8	182
27	The Physics behind Chemistry and the Periodic Table. Chemical Reviews, 2012, 112, 371-384.	47.7	179
28	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
29	A transparent interpretation of the relativistic contribution to the N.M.R. â€˜heavy atom chemical shiftâ€™. Molecular Physics, 1987, 61, 195-205.	1.7	167
30	Understanding the eighteen-electron rule. Journal of Organometallic Chemistry, 2006, 691, 4336-4340.	1.8	153
31	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
32	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
33	Relativistic pseudo-potential analysis of the weak Au(I)â€¦Au(I) attraction. Chemical Physics Letters, 1992, 197, 586-590.	2.6	127
34	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
35	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 56, 1411-1418.	1.7	113
36	Calculated energy levels of thallium and eka-thallium (element 113). Physical Review A, 1996, 53, 3926-3933.	2.5	109

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37	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
38	Icosahedral Au₇₂: a predicted chiral and spherically aromatic golden fullerene. Chemical Communications, 2008, , 465-467.	4.1	109
39	Aurophilicity: The Effect of the Neutral Ligand L on [{ClAuL}₂] Systems. Chemistry - A European Journal, 2011, 17, 368-377.	3.3	107
40	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
41	Element 118: The First Rare Gas with an Electron Affinity. Physical Review Letters, 1996, 77, 5350-5352.	7.8	105
42	Year-2017 nuclear quadrupole moments. Molecular Physics, 2018, 116, 1328-1338.	1.7	103
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.	4.0	100
44	Relativity and the Lead-Acid Battery. Physical Review Letters, 2011, 106, 018301.	7.8	100
45	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	2.8	97
46	Trends in inversion barriers. I. Groupâ€15 hydrides. Journal of Chemical Physics, 1992, 96, 6807-6819.	3.0	94
47	Experimental and theoretical treatment of hydrogen splitting and storage in boronâ€“nitrogen systems. Journal of Organometallic Chemistry, 2009, 694, 2654-2660.	1.8	89
48	Abâ€initioâ€Rechnungen am Dimer (ClAuPH₃)₂ mit relativistischem Pseudopotential: Ist die â€žaurophile Attraktionâ€œ ein Korrelationseffekt?. Angewandte Chemie, 1991, 103, 622-623.	2.0	88
49	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. Angewandte Chemie - International Edition, 2007, 46, 1427-1430.	13.8	88
50	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
51	Diracâ€“Fock one-centre calculations. Part 7.â€”Divalent systems MH+and MH2(M = Be, Mg, Ca, Sr, Ba, Ra,) Tj ETQq1 1 0.784314 rgBT	11	86
52	Ab initio study of bonding trends for f 0 actinide oxyfluoride species. Theoretical Chemistry Accounts, 2001, 106, 393-403.	1.4	86
53	Estimation of Lamb-shift effects for molecules:â€ƒApplication to the rotation-vibration spectra of water. Physical Review A, 2001, 63, .	2.5	86
54	Introduction to the Quantum Chemistry 2012 Issue. Chemical Reviews, 2012, 112, 1-3.	47.7	86

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55	Structure of tetrakis(phosphine)nitrido- or -phosphinidyne or arsinidyneultragold(1+): Td or C4v?. Inorganic Chemistry, 1993, 32, 2630-2634.	4.0	85
56	Theory of the d10â^'d10Closed-Shell Attraction. 4. X(AuL)nm+Centered Systems. Organometallics, 1998, 17, 4842-4852.	2.3	82
57	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
58	Nuclear quadrupole moment of lithium from combined fully numerical and discrete basis-set calculations on LiH. Chemical Physics Letters, 1984, 112, 1-9.	2.6	79
59	A very short uraniumâ€“uranium bond: The predicted metastable U22+. Physical Chemistry Chemical Physics, 2005, 7, 2415.	2.8	79
60	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
61	Î·5-N5-â^'Metalâ^'Î·7-N73-:Â A New Class of Compounds. Journal of Physical Chemistry A, 2002, 106, 4690-4694.	2.5	77
62	Magic nanoclusters of gold. Nature Nanotechnology, 2007, 2, 273-274.	31.5	76
63	Ab initio study of bonding trends. 4. The 22-electron A=B=C series: possible new anions down to NCB4- and possible new cations up to FNF3+. The Journal of Physical Chemistry, 1990, 94, 7753-7759.	2.9	75
64	Estimated valence-level Lamb shifts for group 1 and group 11 metal atoms. Physical Review A, 1998, 57, R689-R692.	2.5	75
65	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
66	Refitted tetrahedral covalent radii for solids. Physical Review B, 2012, 85, .	3.2	75
67	Ab initio studies of bonding trends. Computational and Theoretical Chemistry, 1991, 234, 279-290.	1.5	74
68	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
69	Calculated self-energy contributions for annsvalence electron using the multiple-commutator method. Physical Review A, 1999, 59, 2707-2711.	2.5	72
70	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
71	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
72	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

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73	Relativistically parameterized extended hÃ¼ckel calculations. IX. An iterative version with applications to some xenon, thorium and uranium compounds. Chemical Physics, 1986, 101, 355-369.	1.9	68
74	Recent developments in the theory of f-element molecules. Inorganica Chimica Acta, 1987, 139, 243-245.	2.4	68
75	Relativistic pseudopotential calculation of bonding trends in XAum+n clusters (X = Bâ^'N, Alâ^'S; n =) Tj ETQq1 1 0.784314 rgBT /Over	2.6	68
76	Closed-shell interaction in silver and gold chlorides. Journal of Chemical Physics, 1998, 109, 2339-2345.	3.0	68
77	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
78	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
79	REX calculations. 12. Iteration parameters for the 5f-element organometallics of thorium-neptunium. Geometries of thorium dioxide and uranyl ion revisited. Inorganic Chemistry, 1989, 28, 1801-1805.	4.0	65
80	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
81	Nuclear Quadrupole Moments of Bismuth. Physical Review Letters, 2001, 87, 133003.	7.8	62
82	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	61
83	Two-Dimensional, fully numerical molecular calculations. IV. hartree-fock-slater results on second-row diatomic molecules. International Journal of Quantum Chemistry, 1985, 27, 601-612.	2.0	59
84	The periodic table and the physics that drives it. Nature Reviews Chemistry, 2020, 4, 359-380.	30.2	57
85	Ab initiostudy of bonding trends among the 14-electron diatomic systems: from B24-to F24+. Molecular Physics, 1989, 67, 871-878.	1.7	54
86	Cesium and barium as honorary d elements: CsN 7 Ba as an example. Theoretical Chemistry Accounts, 2003, 110, 205-210.	1.4	52
87	Bonding and electronic structure in diatomic ThO: Quasirelativistic effective core potential calculations. Computational and Theoretical Chemistry, 1988, 169, 339-354.	1.5	50
88	An ab initio study of the aggregation of LAuX molecules and [LAuL]+[XAuX]â^' ions. Chemical Communications, 1997, , 1111-1112.	4.1	50
89	QED corrections to the binding energy of the eka-radon(Z=118)negative ion. Physical Review A, 2003, 67, .	2.5	50
90	Theoretical Search for Very Short Metalâ€"Actinide Bonds: NUIr and Isoelectronic Systems. Angewandte Chemie - International Edition, 2004, 43, 1573-1576.	13.8	49

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91	Relativistic effects in nuclear quadrupole coupling. Theoretical Chemistry Accounts, 1997, 96, 92-104.	1.4	48
92	Aurophilic attraction: the additivity and the combination with hydrogen bonds. Chemical Physics Letters, 2003, 370, 733-740.	2.6	48
93	A London-type formula for the dispersion interactions of endohedral A@B systems. Physical Chemistry Chemical Physics, 2007, 9, 2954.	2.8	48
94	On bonding in transition-metal helide ions. Molecular Physics, 1984, 52, 23-32.	1.7	46
95	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, .	2.5	46
96	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1987, 60, 597-604.	1.7	45
97	Calculated Structure and Optical Properties of Tl2Pt(CN)4. Inorganic Chemistry, 1996, 35, 7450-7451.	4.0	45
98	A Study of the Interactions in an Extended Unsupported Gold-Silver Chain. European Journal of Inorganic Chemistry, 2002, 2002, 750-753.	2.0	45
99	Calculated structures of [Au=C=Au]2+ and related systems. Chemical Physics Letters, 2003, 381, 45-52.	2.6	45
100	Predicting new, simple inorganic species by quantum chemical calculations: some successes. Physical Chemistry Chemical Physics, 2012, 14, 14734.	2.8	45
101	Relativistic Theory of Atoms and Molecules II. Lecture Notes in Quantum Chemistry II, 1993, , .	0.3	45
102	Nuclear quadrupole moment ofHg201. Physical Review A, 2005, 71, .	2.5	44
103	Ab initiostudy of bonding trends 6. The X â‰¡ Y and X = Y = Z species containing phosphorus. Molecular Physics, 1990, 70, 701-714.	1.7	42
104	Calculated properties of XeH2. Chemical Physics Letters, 1995, 246, 239-244.	2.6	42
105	RelativitÃt, Gold, Wechselwirkungen zwischen gefÃ¼llten Schalen und CsAuâ‹…NH3. Angewandte Chemie, 2002, 114, 3723-3728.	2.0	42
106	A new, centered 32-electron system: the predicted [U@Si20]6â^'-like isoelectronic series. Chemical Science, 2012, 3, 2843.	7.4	42
107	An ab initio study of bonding trends in the series BO33â^', CO32â^', NO3â^' and O4(D3h). Chemical Physics Letters, 1989, 157, 415-418.	2.6	41
108	Calculations on indium and thallium cyclopentadienyls. Metalâ€“metal interactions and possible new species. Physical Chemistry Chemical Physics, 1999, 1, 3441-3444.	2.8	41

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109	Coordination of Pyridinethiols in Gold(I) Complexes. Inorganic Chemistry, 2007, 46, 9954-9960.	4.0	40
110	One Metal and Forty Nitrogens. Ab Initio Predictions for Possible New High-Energy Pentazolides. Inorganic Chemistry, 2003, 42, 8241-8249.	4.0	39
111	Linear HThThH:Â A Candidate for a Thâ‹¯Th Triple Bond. Journal of the American Chemical Society, 2005, 127, 13090-13091.	13.7	39
112	Comparative Theoretical Study of N-Heterocyclic Carbenes and Other Ligands Bound to AuI. Chemistry - an Asian Journal, 2006, 1, 623-628.	3.3	39
113	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
114	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
115	Aurophilic attractions between a closed-shell molecule and a gold cluster. Faraday Discussions, 2011, 152, 169.	3.2	38
116	The large range of uranyl bond lengths: ab initio calculations on simple uranium-oxygen clusters. Inorganic Chemistry, 1991, 30, 3787-3788.	4.0	36
117	Chemical bonds between noble metals and noble gases.. Chemical Physics Letters, 1998, 288, 635-641.	2.6	36
118	Predicted Group 4 Tetra-azides M(N3)4(M = Tiâ‹¯Hf, Th):Â The First Examples of Linear Mâ‹¯NNN Coordination. Inorganic Chemistry, 2003, 42, 3074-3078.	4.0	35
119	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
120	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
121	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
122	On the Extreme Oxidation States of Iridium. Chemistry - A European Journal, 2015, 21, 9468-9473.	3.3	31
123	Understanding the Uniqueness of 2p Elements in Periodic Tables. Chemistry - A European Journal, 2020, 26, 15558-15564.	3.3	31
124	Structure and Color of Substituted Pentaphenylbismuth. Angewandte Chemie International Edition in English, 1990, 29, 213-215.	4.4	30
125	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
126	Ab initio study of bonding trends among the 22-electron Aî—»Bî—»A systems: Evidence for Oî—»Oî—»O2+. Chemical Physics Letters, 1989, 156, 337-340.	2.6	29

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127	Structure and bonding of the MCN molecules, M=Cu,Ag,Au,Rg. Journal of Chemical Physics, 2008, 128, 224303.	3.0	29
128	Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. Physical Review A, 2009, 79, .	2.5	29
129	Formulations of the closed-shell interactions in endohedral systems. Physical Chemistry Chemical Physics, 2010, 12, 6187.	2.8	29
130	Magically magnetic gadolinium. Nature Chemistry, 2015, 7, 680-680.	13.6	29
131	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 55, 627-635.	1.7	28
132	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	2.6	28
133	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. Chemical Communications, 2004, , 1982-1983.	4.1	28
134	Calculated Structures of MO22+, MN2, and MP2 (M = Mo, W). Journal of Physical Chemistry A, 1997, 101, 8107-8114.	2.5	27
135	The nuclear quadrupole moment of from molecular data for ZrO and ZrS. Chemical Physics Letters, 2000, 318, 222-231.	2.6	27
136	The Formal Oxidation States of Iridium Now Run from â˜’III to +IX. Angewandte Chemie - International Edition, 2015, 54, 1080-1081.	13.8	27
137	Is the chemistry of lawrencium peculiar?. Physical Chemistry Chemical Physics, 2016, 18, 17351-17355.	2.8	27
138	Au22+ has bound excited states. Chemical Physics Letters, 2000, 325, 225-231.	2.6	26
139	HgH4and HgH6: further candidates for high-valent mercury compounds. Chemical Communications, 2002, , 1728-1729.	4.1	26
140	Chemical properties of the predicted 32-electron systems Pu@Sn12 and Pu@Pb12. Comptes Rendus Chimie, 2010, 13, 884-888.	0.5	26
141	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
142	The nuclear quadrupole moment of 45Sc. Chemical Physics Letters, 2000, 329, 112-118.	2.6	25
143	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
144	Nuclear quadrupole moments of Kr and Xe from molecular data. Chemical Physics Letters, 2001, 346, 155-159.	2.6	25

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145	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
146	Ab InitioPredictions for New Chemical Species. Physica Scripta, 1990, T33, 52-53.	2.5	24
147	Ab initio studies of bonding trends. Computational and Theoretical Chemistry, 1991, 234, 269-277.	1.5	24
148	Could uranium(XII)hexoxide, UO6 (Oh) exist?. Chemical Physics Letters, 2000, 328, 415-419.	2.6	24
149	Structural trends in atomic nuclei from laser spectroscopy of tin. Communications Physics, 2020, 3, .	5.3	24
150	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
151	Vacuum-polarization corrections to the hyperfine-structure splitting of highly charged83209Bi ions. Physical Review A, 1997, 56, 4508-4516.	2.5	21
152	Pocket and antipocket conformations for the CH4@C84 endohedral fullerene. International Journal of Quantum Chemistry, 2007, 107, 1162-1169.	2.0	21
153	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
154	WAu12(CO)12?. Chemical Communications, 2010, 46, 3762.	4.1	21
155	Unbridged Au(ii)â€“Au(ii) bonds are theoretically allowed. Chemical Communications, 2013, 49, 2103.	4.1	21
156	Degree of accuracy in determining the nuclear electric quadrupole moment of radium. Physical Review A, 2005, 71, .	2.5	20
157	Struktur und Farbe von substituiertem Pentaphenylbismut. Angewandte Chemie, 1990, 102, 211-213.	2.0	19
158	A small spherical liquid: A DFT molecular dynamics study of WAu12. Physical Chemistry Chemical Physics, 2005, 7, 2208.	2.8	19
159	Isomerism of Aurated Phosphine Sulfides, Thiophosphinates, Thiophosphonates, and Thiophosphates:â€‰Structural and Quantum Chemical Studies. Inorganic Chemistry, 1999, 38, 5870-5875.	4.0	18
160	Magnetic-Field-Induced Quadrupole Splitting in Gaseous and LiquidX131eNMR: Quadratic and Quartic Field Dependence. Physical Review Letters, 2001, 86, 3268-3271.	7.8	18
161	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
162	Ab initioMCDHF calculations of electronâ€“nucleus interactions. Physica Scripta, 2015, 90, 054011.	2.5	18

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163	An essay on periodic tables. Pure and Applied Chemistry, 2019, 91, 1959-1967.	1.9	18
164	Strong chemical bonds in heavy diatomics: PtSi, PtTh and AuTh+. Chemical Physics Letters, 2003, 368, 538-541.	2.6	17
165	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
166	Chemistry of the 5g Elements: Relativistic Calculations on Hexafluorides. Angewandte Chemie - International Edition, 2017, 56, 10132-10134.	13.8	17
167	Calculated properties of PS2+and PS3â€“. Journal of the Chemical Society Chemical Communications, 1990, , 933-934.	2.0	16
168	On the nature of the short Ptâ€“Tl bonds in model compounds [H5Ptâ€“TlHn]nâ˜. Faraday Discussions, 2003, 124, 41-51.	3.2	16
169	Computational study of bonding trends in the metalloactinyl series EThM and MThMâ€² (E=Nâ˜, O, F+; M,) Tj ETQq1 1 0.784314 rgB	2.6	16
170	Relativity and the mercury battery. Physical Chemistry Chemical Physics, 2011, 13, 16510.	2.8	16
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