

Pekka PyykkÄ

List of Publications by Year in descending order

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206
papers

26,086
citations

11639

70
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6294

158
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219
all docs

219
docs citations

219
times ranked

12377
citing authors

#	ARTICLE	IF	CITATIONS
1	Relativistic effects in structural chemistry. <i>Chemical Reviews</i> , 1988, 88, 563-594.	23.0	2,731
2	Strong Closed-Shell Interactions in Inorganic Chemistry. <i>Chemical Reviews</i> , 1997, 97, 597-636.	23.0	2,282
3	Molecular Single-Bond Covalent Radii for Elements 118. <i>Chemistry - A European Journal</i> , 2009, 15, 186-197.	1.7	1,762
4	Theoretical Chemistry of Gold. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 4412-4456.	7.2	1,668
5	Molecular Double-Bond Covalent Radii for Elements 112. <i>Chemistry - A European Journal</i> , 2009, 15, 12770-12779.	1.7	1,106
6	Relativity and the periodic system of elements. <i>Accounts of Chemical Research</i> , 1979, 12, 276-281.	7.6	989
7	Theoretical chemistry of gold. III. <i>Chemical Society Reviews</i> , 2008, 37, 1967.	18.7	631
8	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
9	Spectroscopic nuclear quadrupole moments. <i>Molecular Physics</i> , 2001, 99, 1617-1629.	0.8	505
10	Year-2008 nuclear quadrupole moments. <i>Molecular Physics</i> , 2008, 106, 1965-1974.	0.8	437
11	Theory of the $d^{10}d^{10}$ Closed-Shell Attraction: 1. Dimers Near Equilibrium. <i>Chemistry - A European Journal</i> , 1997, 3, 1451-1457.	1.7	430
12	Relativistic Effects in Chemistry: More Common Than You Thought. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 45-64.	4.8	416
13	Theoretical chemistry of gold. II. <i>Inorganica Chimica Acta</i> , 2005, 358, 4113-4130.	1.2	399
14	Triple-Bond Covalent Radii. <i>Chemistry - A European Journal</i> , 2005, 11, 3511-3520.	1.7	370
15	Molecular Tweezers for Hydrogen: Synthesis, Characterization, and Reactivity. <i>Journal of the American Chemical Society</i> , 2008, 130, 14117-14119.	6.6	356
16	Relativistic Quantum Chemistry. <i>Advances in Quantum Chemistry</i> , 1978, 11, 353-409.	0.4	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. <i>Chemistry - A European Journal</i> , 1998, 4, 118-126.	1.7	344
18	Icosahedral W _{Au} 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 - International Edition</i> , 2002, 41, 2174.	7.2	335

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19	Predicted ligand dependence of the Au(I)-Au(I) attraction in (X _n AuPH ₃) ₂ . <i>Chemical Physics Letters</i> , 1994, 218, 133-138.	1.2	277
20	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur. <i>Inorganic Chemistry</i> , 1998, 37, 624-632.	1.9	255
21	Ab initio Calculations on the (ClAuPH ₃) ₂ Dimer with Relativistic Pseudopotential: Is the Aurophilic Attraction a Correlation Effect?. <i>Angewandte Chemie International Edition in English</i> , 1991, 30, 604-605.	4.4	244
22	Fully numerical hartree-fock methods for molecules. <i>Computer Physics Reports</i> , 1986, 4, 313-344.	2.3	240
23	Theory of d ¹⁰ -d ¹⁰ Closed-Shell Attraction. III. Rings. <i>Inorganic Chemistry</i> , 1998, 37, 3018-3025.	1.9	207
24	Relativity, Gold, Closed-Shell Interactions, and CsAu...NH ₃ . <i>Angewandte Chemie - International Edition</i> , 2002, 41, 3573-3578.	7.2	200
25	The Nuclear Quadrupole Moments of the 20 First Elements: High-Precision Calculations on Atoms and Small Molecules. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1992, 47, 189-196.	0.7	193
26	Theory of the d ¹⁰ -d ¹⁰ Closed-Shell Attraction: 2. Long-Distance Behaviour and Nonadditive Effects in Dimers and Trimers of Type [(X _n Au) ₂] ⁿ⁺ (n = 2, 3; X = Cl, I). <i>Journal of Physical Chemistry</i> , 1998, 102, 1100-1108.	1.0	187
27	The Physics behind Chemistry and the Periodic Table. <i>Chemical Reviews</i> , 2012, 112, 371-384.	23.0	179
28	Ab initio studies of the dimers (HgH ₂) ₂ and (HgMe ₂) ₂ . Metallophilic attraction and the van der Waals radii of mercury. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2489-2493.	1.3	171
29	A transparent interpretation of the relativistic contribution to the N.M.R. heavy atom chemical shift. <i>Molecular Physics</i> , 1987, 61, 195-205.	0.8	167
30	Understanding the eighteen-electron rule. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4336-4340.	0.8	153
31	Luminescent Characterization of Solution Oligomerization Process Mediated Gold-Gold Interactions. DFT Calculations on [Au ₂ Ag ₂ R ₄ L ₂] _n Moieties. <i>Journal of the American Chemical Society</i> , 2000, 122, 7287-7293.	6.6	140
32	A suggested periodic table up to Z ≈ 172, based on Dirac-Fock calculations on atoms and ions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 161-168.	1.3	129
33	Relativistic pseudo-potential analysis of the weak Au(I)-Au(I) attraction. <i>Chemical Physics Letters</i> , 1992, 197, 586-590.	1.2	127
34	Matrix Infrared Spectroscopic and ab Initio Studies of ZnH ₂ , CdH ₂ , and Related Metal Hydride Species. <i>The Journal of Physical Chemistry</i> , 1995, 99, 7925-7934.	2.9	118
35	Two-dimensional, fully numerical molecular calculations. <i>Molecular Physics</i> , 1985, 56, 1411-1418.	0.8	113
36	Calculated energy levels of thallium and eka-thallium (element 113). <i>Physical Review A</i> , 1996, 53, 3926-3933.	1.0	109

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37	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
38	Icosahedral Au ₇₂ : a predicted chiral and spherically aromatic golden fullerene. <i>Chemical Communications</i> , 2008, , 465-467.	2.2	109
39	Aurophilicity: The Effect of the Neutral Ligand <i>L</i> on [ClAu ₂] Systems. <i>Chemistry - A European Journal</i> , 2011, 17, 368-377.	1.7	107
40	A Predicted Organometallic Series Following a 32-Electron Principle: An@C ₂₈ (An = Th, Tj, ET, Qq, O, O, rg, BT, /Overlock, 10, Tf, 5, 131, 238-243.	6.6	106
41	Element 118: The First Rare Gas with an Electron Affinity. <i>Physical Review Letters</i> , 1996, 77, 5350-5352.	2.9	105
42	Year-2017 nuclear quadrupole moments. <i>Molecular Physics</i> , 2018, 116, 1328-1338.	0.8	103
43	Ab Initio Interpretation of the Closed-Shell Intermolecular E.cntdot..cntdot..cntdot.E Attraction in Dipnicogen (H ₂ E-EH ₂) ₂ and Dichalcogen (HE-EH) ₂ Hydride Model Dimers. <i>Inorganic Chemistry</i> , 1995, 34, 4134-4138.	1.9	100
44	Relativity and the Lead-Acid Battery. <i>Physical Review Letters</i> , 2011, 106, 018301.	2.9	100
45	Properties of WAu ₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 11-22.	1.3	97
46	Trends in inversion barriers. I. Group 15 hydrides. <i>Journal of Chemical Physics</i> , 1992, 96, 6807-6819.	1.2	94
47	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
48	Ab-initio-Rechnungen am Dimer (ClAuPH ₃) ₂ mit relativistischem Pseudopotential: Ist die –aurophile Attraktion–ein Korrelationseffekt?. <i>Angewandte Chemie</i> , 1991, 103, 622-623.	1.6	88
49	Towards a 32-Electron Principle: Pu@Pb ₁₂ and Related Systems. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 1427-1430.	7.2	88
50	How Many Hydrogen Atoms Can Be Bound to a Metal? Predicted MH ₁₂ Species. <i>Journal of the American Chemical Society</i> , 2004, 126, 15014-15015.	6.6	87
51	Dirac–Fock one-centre calculations. Part 7.–Divalent systems MH+and MH ₂ (M = Be, Mg, Ca, Sr, Ba, Ra,) Tj ETQq, 1 1 0.784314 rgBT	1.1	86
52	Ab initio study of bonding trends for f ₀ actinide oxyfluoride species. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 393-403.	0.5	86
53	Estimation of Lamb-shift effects for molecules:–Application to the rotation-vibration spectra of water. <i>Physical Review A</i> , 2001, 63, .	1.0	86
54	Introduction to the –Quantum Chemistry 2012– Issue. <i>Chemical Reviews</i> , 2012, 112, 1-3.	23.0	86

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55	Structure of tetrakis(phosphine)nitrido- or -phosphinidyne or arsinidyneultragold(1+): Td or C4v?. <i>Inorganic Chemistry</i> , 1993, 32, 2630-2634.	1.9	85
56	Theory of the d ¹⁰ Closed-Shell Attraction. 4. X(AuL) _n -Centered Systems. <i>Organometallics</i> , 1998, 17, 4842-4852.	1.1	82
57	Aurophilic 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
58	Nuclear quadrupole moment of lithium from combined fully numerical and discrete basis-set calculations on LiH. <i>Chemical Physics Letters</i> , 1984, 112, 1-9.	1.2	79
59	A very short uranium-uranium bond: The predicted metastable U ₂ ²⁺ . <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2415.	1.3	79
60	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
61	5-N5-Metal-7-N7: A New Class of Compounds. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4690-4694.	1.1	77
62	Magic nanoclusters of gold. <i>Nature Nanotechnology</i> , 2007, 2, 273-274.	15.6	76
63	Ab initio study of bonding trends. 4. The 22-electron A=B=C series: possible new anions down to NCB ₄ ⁻ and possible new cations up to FN ₃ ⁺ . <i>The Journal of Physical Chemistry</i> , 1990, 94, 7753-7759.	2.9	75
64	Estimated valence-level Lamb shifts for group 1 and group 11 metal atoms. <i>Physical Review A</i> , 1998, 57, R689-R692.	1.0	75
65	Experimental and Theoretical Studies of the d ⁸ Interaction between Pd(II) and Au(I): Bis(chloro[(phenylthiomethyl)diphenylphosphine]gold(I)) dichloropalladium(II) and Related Systems. <i>Inorganic Chemistry</i> , 2000, 39, 4786-4792.	1.9	75
66	Refitted tetrahedral covalent radii for solids. <i>Physical Review B</i> , 2012, 85, .	1.1	75
67	Ab initio studies of bonding trends. <i>Computational and Theoretical Chemistry</i> , 1991, 234, 279-290.	1.5	74
68	Electric quadrupole moment of the ²⁷ Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. <i>Chemical Physics Letters</i> , 1999, 304, 414-422.	1.2	73
69	Calculated self-energy contributions for annvalence electron using the multiple-commutator method. <i>Physical Review A</i> , 1999, 59, 2707-2711.	1.0	72
70	Relativistic pseudopotential calculations on Xe ₂ , RnXe, and Rn ₂ : The van der Waals properties of radon. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 131-140.	1.0	71
71	Calculated lanthanide contractions for molecular trihalides and fully hydrated ions: The contributions from relativity and 4f-shell hybridization. <i>Chemical Physics Letters</i> , 2006, 429, 8-12.	1.2	71
72	Scandium Cycloheptanitride, ScN ₇ : A Predicted High-Energy Molecule Containing an [7-N7] ₃ -Ligand. <i>Journal of the American Chemical Society</i> , 2001, 123, 9700-9701.	6.6	69

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73	Relativistically parameterized extended h ^{1/4} ckel calculations. IX. An iterative version with applications to some xenon, thorium and uranium compounds. <i>Chemical Physics</i> , 1986, 101, 355-369.	0.9	68
74	Recent developments in the theory of f-element molecules. <i>Inorganica Chimica Acta</i> , 1987, 139, 243-245.	1.2	68
75	Relativistic pseudopotential calculation of bonding trends in XAu _n clusters (X = Bi, N, Al, S; n =) <i>J. Chem. Phys.</i> 110, 7843-14 (1999)	1.2	68
76	Closed-shell interaction in silver and gold chlorides. <i>Journal of Chemical Physics</i> , 1998, 109, 2339-2345.	1.2	68
77	Strong chemical bonds to gold. High level correlated relativistic results for diatomic AuBe ⁺ , AuC ⁺ , AuMg ⁺ , and AuSi ⁺ . <i>Chemical Physics Letters</i> , 1998, 285, 398-403.	1.2	67
78	Icosahedral WAu ₁₂ : 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.. <i>Angewandte Chemie</i> , 2002, 114, 2278.	1.6	66
79	REX calculations. 12. Iteration parameters for the 5f-element organometallics of thorium-neptunium. Geometries of thorium dioxide and uranyl ion revisited. <i>Inorganic Chemistry</i> , 1989, 28, 1801-1805.	1.9	65
80	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
81	Nuclear Quadrupole Moments of Bismuth. <i>Physical Review Letters</i> , 2001, 87, 133003.	2.9	62
82	The nuclear quadrupole moment of ¹⁴ N obtained from finite-element MCHF calculationson N ₂ ⁺ (2p;). <i>J. Chem. Phys.</i> 112, 61 (2000)	1.2	61
83	Two-Dimensional, fully numerical molecular calculations. IV. hartree-fock-slater results on second-row diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 1985, 27, 601-612.	1.0	59
84	The periodic table and the physics that drives it. <i>Nature Reviews Chemistry</i> , 2020, 4, 359-380.	13.8	57
85	Ab initio study of bonding trends among the 14-electron diatomic systems: from B ₂ ⁺ to F ₂ ⁺ . <i>Molecular Physics</i> , 1989, 67, 871-878.	0.8	54
86	Cesium and barium as honorary d elements: CsN and Ba as an example. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 205-210.	0.5	52
87	Bonding and electronic structure in diatomic ThO: Quasirelativistic effective core potential calculations. <i>Computational and Theoretical Chemistry</i> , 1988, 169, 339-354.	1.5	50
88	An ab initio study of the aggregation of LAuX molecules and [LAuL] ⁺ [XAuX] ⁻ ions. <i>Chemical Communications</i> , 1997, , 1111-1112.	2.2	50
89	QED corrections to the binding energy of the eka-radon(Z=118)negative ion. <i>Physical Review A</i> , 2003, 67, .	1.0	50
90	Theoretical Search for Very Short Metal-Actinide Bonds: NUlr and Isoelectronic Systems. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1573-1576.	7.2	49

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91	Relativistic effects in nuclear quadrupole coupling. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 92-104.	0.5	48
92	Aurophilic attraction: the additivity and the combination with hydrogen bonds. <i>Chemical Physics Letters</i> , 2003, 370, 733-740.	1.2	48
93	A London-type formula for the dispersion interactions of endohedral A@B systems. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2954.	1.3	48
94	On bonding in transition-metal helide ions. <i>Molecular Physics</i> , 1984, 52, 23-32.	0.8	46
95	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. <i>Physical Review A</i> , 2001, 64, .	1.0	46
96	Two-dimensional, fully numerical molecular calculations. <i>Molecular Physics</i> , 1987, 60, 597-604.	0.8	45
97	Calculated Structure and Optical Properties of $Tl_2Pt(CN)_4$. <i>Inorganic Chemistry</i> , 1996, 35, 7450-7451.	1.9	45
98	A Study of the Interactions in an Extended Unsupported Gold-Silver Chain. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 750-753.	1.0	45
99	Calculated structures of $[Au=C=Au]^{2+}$ and related systems. <i>Chemical Physics Letters</i> , 2003, 381, 45-52.	1.2	45
100	Predicting new, simple inorganic species by quantum chemical calculations: some successes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14734.	1.3	45
101	Relativistic Theory of Atoms and Molecules II. <i>Lecture Notes in Quantum Chemistry II</i> , 1993, , .	0.3	45
102	Nuclear quadrupole moment of Hg^{201} . <i>Physical Review A</i> , 2005, 71, .	1.0	44
103	Ab initio study of bonding trends 6. The $X \cdot Y$ and $X = Y = Z$ species containing phosphorus. <i>Molecular Physics</i> , 1990, 70, 701-714.	0.8	42
104	Calculated properties of XeH_2 . <i>Chemical Physics Letters</i> , 1995, 246, 239-244.	1.2	42
105	Relativität, Gold, Wechselwirkungen zwischen gefüllten Schalen und $CsAu \cdot \cdot \cdot NH_3$. <i>Angewandte Chemie</i> , 2002, 114, 3723-3728.	1.6	42
106	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
107	An ab initio study of bonding trends in the series BO_3^{2-} , CO_3^{2-} , NO_3^- and $O_4(D_{3h})$. <i>Chemical Physics Letters</i> , 1989, 157, 415-418.	1.2	41
108	Calculations on indium and thallium cyclopentadienyls. Metal-metal interactions and possible new species. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3441-3444.	1.3	41

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109	Coordination of Pyridinethiols in Gold(I) Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 9954-9960.	1.9	40
110	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
111	Linear HThThH: A Candidate for a Th ⁺ Th Triple Bond. <i>Journal of the American Chemical Society</i> , 2005, 127, 13090-13091.	6.6	39
112	Comparative Theoretical Study of N-Heterocyclic Carbenes and Other Ligands Bound to Au. <i>Chemistry - an Asian Journal</i> , 2006, 1, 623-628.	1.7	39
113	Comparative calculations for the A-frame molecules [S(MPH ₃) ₂] (M=Cu, Ag, Au) at levels up to CCSD(T). <i>Chemical Physics Letters</i> , 2005, 405, 148-152.	1.2	38
114	Bonding Trends in Molecular Compounds of Lanthanides: The Double-Bonded Carbene Cations LnCH ₂ ⁺ (Ln=Sc, Y, La–Lu). <i>Chemistry - A European Journal</i> , 2010, 16, 270-275.	1.7	38
115	Auophilic attractions between a closed-shell molecule and a gold cluster. <i>Faraday Discussions</i> , 2011, 152, 169.	1.6	38
116	The large range of uranyl bond lengths: ab initio calculations on simple uranium-oxygen clusters. <i>Inorganic Chemistry</i> , 1991, 30, 3787-3788.	1.9	36
117	Chemical bonds between noble metals and noble gases. <i>Chemical Physics Letters</i> , 1998, 288, 635-641.	1.2	36
118	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
119	Perspective on Norman Ramsey's theories of NMR chemical shifts and nuclear spin-spin coupling. <i>Theoretical Chemistry Accounts</i> , 2000, 103, 214-216.	0.5	31
120	Basis-set limit of the auophilic attraction using the MP2 method: The examples of [ClAuPH ₃] ₂ dimer and [P(AuPH ₃) ₄] ⁺ ion. <i>Journal of Chemical Physics</i> , 2008, 128, 124309.	1.2	31
121	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
122	On the Extreme Oxidation States of Iridium. <i>Chemistry - A European Journal</i> , 2015, 21, 9468-9473.	1.7	31
123	Understanding the Uniqueness of 2p Elements in Periodic Tables. <i>Chemistry - A European Journal</i> , 2020, 26, 15558-15564.	1.7	31
124	Structure and Color of Substituted Pentaphenylbismuth. <i>Angewandte Chemie International Edition in English</i> , 1990, 29, 213-215.	4.4	30
125	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
126	Ab initio study of bonding trends among the 22-electron A _i –B _i –A systems: Evidence for O _i –O _i –O ₂ ⁺ . <i>Chemical Physics Letters</i> , 1989, 156, 337-340.	1.2	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.	1.2	29
128	Complete-active-space multiconfiguration Dirac-Hartree-Fock calculations of hyperfine-structure constants of the gold atom. Physical Review A, 2009, 79, .	1.0	29
129	Formulations of the closed-shell interactions in endohedral systems. Physical Chemistry Chemical Physics, 2010, 12, 6187.	1.3	29
130	Magically magnetic gadolinium. Nature Chemistry, 2015, 7, 680-680.	6.6	29
131	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 55, 627-635.	0.8	28
132	Is the Lamb shift chemically significant?. Chemical Physics Letters, 2001, 348, 497-500.	1.2	28
133	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. Chemical Communications, 2004, , 1982-1983.	2.2	28
134	Calculated Structures of MO ₂₂₊ , MN ₂ , and MP ₂ (M = Mo, W). Journal of Physical Chemistry A, 1997, 101, 8107-8114.	1.1	27
135	The nuclear quadrupole moment of from molecular data for ZrO and ZrS. Chemical Physics Letters, 2000, 318, 222-231.	1.2	27
136	The Formal Oxidation States of Iridium Now Run from $\hat{\alpha}^{\text{III}}$ to +IX. Angewandte Chemie - International Edition, 2015, 54, 1080-1081.	7.2	27
137	Is the chemistry of lawrencium peculiar?. Physical Chemistry Chemical Physics, 2016, 18, 17351-17355.	1.3	27
138	Au ₂₂₊ has bound excited states. Chemical Physics Letters, 2000, 325, 225-231.	1.2	26
139	HgH ₄ and HgH ₆ : further candidates for high-valent mercury compounds. Chemical Communications, 2002, , 1728-1729.	2.2	26
140	Chemical properties of the predicted 32-electron systems Pu@Sn ₁₂ and Pu@Pb ₁₂ . Comptes Rendus Chimie, 2010, 13, 884-888.	0.2	26
141	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series PuO _n F _{8-2n} (n = 0-4). Inorganic Chemistry, 2015, 54, 8825-8831.	1.9	26
142	The nuclear quadrupole moment of ⁴⁵ Sc. Chemical Physics Letters, 2000, 329, 112-118.	1.2	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.	1.0	25
144	Nuclear quadrupole moments of Kr and Xe from molecular data. Chemical Physics Letters, 2001, 346, 155-159.	1.2	25

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145	Study of the MAu6 (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
146	Ab Initio Predictions for New Chemical Species. <i>Physica Scripta</i> , 1990, T33, 52-53.	1.2	24
147	Ab initio studies of bonding trends. <i>Computational and Theoretical Chemistry</i> , 1991, 234, 269-277.	1.5	24
148	Could uranium(XII)hexoxide, UO ₆ (Oh) exist?. <i>Chemical Physics Letters</i> , 2000, 328, 415-419.	1.2	24
149	Structural trends in atomic nuclei from laser spectroscopy of tin. <i>Communications Physics</i> , 2020, 3, .	2.0	24
150	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
151	Vacuum-polarization corrections to the hyperfine-structure splitting of highly charged 83209Bi ions. <i>Physical Review A</i> , 1997, 56, 4508-4516.	1.0	21
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