Attila KovÃ¡cs

List of Publications by Year
in descending order

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85 papers	1,722 citations	331670 21 h-index	315739 38 g-index
89 all docs	89 docs citations	89 times ranked	1791 citing authors

#	Article	IF	Citations
1	The Thermodynamic Properties of the f-Elements and their Compounds. Part 2. The Lanthanide and Actinide Oxides. Journal of Physical and Chemical Reference Data, 2014, 43, .	4.2	241
2	Quantum Chemical Calculations and Experimental Investigations of Molecular Actinide Oxides. Chemical Reviews, 2015, 115, 1725-1759.	47.7	103
3	Considerations on the influence of extreme events on the phosphorus transport from river catchments to the sea. Water Science and Technology, 2005, 51, 193-204.	2.5	78
4	Ionization Energies for the Actinide Mono- and Dioxides Series, from Th to Cm: Theory versus Experiment. Journal of Physical Chemistry A, 2010, 114, 6007-6015.	2.5	73
5	Structural Characteristics of Intramolecular Hydrogen Bonding in Benzene Derivatives. Accounts of Chemical Research, 2002, 35, 887-894.	15.6	72
6	How accurate are electronic structure methods for actinoid chemistry?. Theoretical Chemistry Accounts, 2011, 129, 657-666.	1.4	65
7	Structure and Vibrations of Lanthanide Trihalides: An Assessment of Experimental and Theoretical Data. Journal of Physical and Chemical Reference Data, 2004, 33, 377-404.	4.2	60
8	Intramolecular Hydrogen Bonding in Fluorophenol Derivatives:Â 2-Fluorophenol, 2,6-Difluorophenol, and 2,3,5,6-Tetrafluorohydroquinone. Journal of Physical Chemistry A, 1999, 103, 3110-3114.	2.5	59
9	Computed Vibrational Frequencies of Actinide Oxides AnO^{0/+/2+} and AnO₂^{0/+/2+} (An = Th, Pa, U, Np, Pu, Am, Cm). Journal of Physical Chemistry A, 2011, 115, 6646-6656.	2.5	50
10	Theoretical Study of Bond Distances and Dissociation Energies of Actinide Oxides AnO and AnO₂. Inorganic Chemistry, 2012, 51, 4841-4849.	4.0	39
11	Planar and Perpendicular X2Eâ‹EX2 (E = B, Al, Ga, In, Tl; X = H, F, Cl, Br, I). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1803-1809.	1.2	36
12	Vibrational Analysis of N-Acetyl-Î±-<scp>d</scp>-glucosamine and Î²-<scp>d</scp>-Glucuronic Acid. Journal of Physical Chemistry B, 2008, 112, 5728-5735.	2.6	34
13	Benchmarking density functionals in conjunction with <scp>G</scp>rimme's dispersion correction for noble gas dimers (Ne₂, Ar₂, Kr₂, Xe₂,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	4.0	32
14	Title is missing!. Structural Chemistry, 2000, 11, 193-201.	2.0	29
15	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 2001, 63, 723-732.	1.4	29
16	A Theoretical Study of the Structure and Bonding of UOX4(X=F, Cl, Br, I) Molecules: The Importance of InverseTransInfluence. ChemPhysChem, 2006, 7, 455-462.	2.1	29
17	Vibrational Analysis of Î±-<scp>d</scp>-Glucose Trapped in Ar Matrix. Journal of Physical Chemistry B, 2009, 113, 2151-2159.	2.6	29
18	Theoretical Study of the Structure and Bonding in ThC₂ and UC₂. Journal of Physical Chemistry A, 2012, 116, 747-755.	2.5	28

#	Article	IF	Citations
19	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 2001, 66, 573-581.	1.4	26
20	Structural, spectroscopic and computational studies of the HgL2Cl2 complex (L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td (3,5-dim 2005, 29, 833.	2.8	26
21	Long-Range Effects in Oligopeptides. A Theoretical Study of the Î²-Sheet Structure of Glyn (n = 2â˜10). Journal of Physical Chemistry A, 2004, 108, 6869-6873.	2.5	23
22	Theoretical Study of Actinide Complexes with Macropa. ACS Omega, 2020, 5, 26431-26440.	3.5	22
23	Chemical Vapor Deposition of Gallium Nitride from the GaCl3+NH3 System. Theoretical Study of the Structure and Thermodynamics of Potential Intermediates Formed in the Gaseous Phase. Inorganic Chemistry, 2002, 41, 3067-3075.	4.0	20
24	Investigation of the density-functional theory-derived scaled quantum mechanical method for cage-like systems: the vibrational analysis of adamantane. Molecular Physics, 1999, 96, 161-167.	1.7	19
25	A terminal neptunium(V)â€“mono(oxo) complex. Nature Chemistry, 2022, 14, 342-349.	13.6	19
26	Solidâ€State Structure of Trisâ€Cyclopentadienide Uranium(III) and Plutonium(III). Chemistry - A European Journal, 2018, 24, 2841-2844.	3.3	18
27	Reactions of divalent transition metal halides with 3,5-dimethyl-1-(hydroxymethyl)-pyrazole. Journal of Thermal Analysis and Calorimetry, 2007, 89, 267-275.	3.6	17
28	A theoretical study of AmO_nand CmO_n(n = 1, 2). Physical Chemistry Chemical Physics, 2008, 10, 1114-1117.	2.8	17
29	Structure and Other Molecular Properties of Actinide Trichlorides AnCl₃ (An = Thâ€“Cm). Journal of Physical Chemistry A, 2013, 117, 11357-11363.	2.5	17
30	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 1999, 56, 493-501.	1.4	16
31	Comparative Study of Complexes of Rare Earths and Actinides with 2,6-Bis(1,2,4-triazin-3-yl)pyridine. Inorganics, 2019, 7, 26.	2.7	16
32	Molecular structure and thermodynamic properties of the gaseous ThC2 and ThC4 species. Journal of Nuclear Materials, 2008, 372, 391-393.	2.7	15
33	Theoretical study of actinide monocarbides (ThC, UC, PuC, and AmC). Journal of Chemical Physics, 2016, 145, 244310.	3.0	15
34	Pentavalent Curium, Berkelium, and Californium in Nitrate Complexes: Extending Actinide Chemistry and Oxidation States. Inorganic Chemistry, 2018, 57, 9453-9467.	4.0	15
35	FACILE SYNTHESIS OF 1,2,3,4,5,6-HEXAHYDROPHOSPHININE 1-OXIDES BY THE HYDROGENATION OF 1,2-DIHYDROPHOSPHININE 1-OXIDES. Phosphorus, Sulfur and Silicon and the Related Elements, 1992, 70, 219-227.	1.6	13
36	â€˜Lanthanide contractionâ€™ in [Ln(BTP)3](CF3SO3)3 complexes. Structural Chemistry, 2015, 26, 1287-1295.	2.0	13

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37	Relativistic Multireference Quantum Chemical Study of the Electronic Structure of Actinide Trioxide Molecules. Journal of Physical Chemistry A, 2017, 121, 2523-2530.	2.5	13
38	Theoretical Study of Actinide(III)-DOTA Complexes. ACS Omega, 2021, 6, 13321-13330.	3.5	13
39	Theoretical study of the Pu and Am dicarbide molecules. Structural Chemistry, 2012, 23, 1281-1289.	2.0	12
40	Insight into the Crystalline Structure of ThF4 with the Combined Use of Neutron Diffraction, 19F Magic-Angle Spinning-NMR, and Density Functional Theory Calculations. Inorganic Chemistry, 2018, 57, 15350-15360.	4.0	12
41	Hydrogen bonding in peptide secondary structures. International Journal of Quantum Chemistry, 2005, 105, 302-312.	2.0	11
42	Theoretical Study of Thorium and Uranium Tetracarbide Molecules. European Journal of Inorganic Chemistry, 2014, 2014, 1062-1071.	2.0	11
43	Joint Raman spectroscopic and quantum chemical analysis of the vibrational features of Cs 2 RuO 4. Journal of Raman Spectroscopy, 2015, 46, 661-668.	2.5	11
44	Trisâ€{hydridotris(1â€pyrazolyl)borato}actinide Complexes: Synthesis, Spectroscopy, Crystal Structure, Bonding Properties and Magnetic Behaviour. Chemistry - A European Journal, 2020, 26, 11293-11306.	3.3	11
45	Comparative study of two watershed scale models to calculate diffuse phosphorus pollution. Water Science and Technology, 2006, 53, 281-288.	2.5	10
46	Impacts of the climate change on runoff and diffuse phosphorus load to Lake Balaton (Hungary). Water Science and Technology, 2009, 59, 417-423.	2.5	10
47	Comparison ofab initio and density functional methods for vibrational analysis of TeCl4. Journal of Computational Chemistry, 1998, 19, 308-318.	3.3	9
48	Spectroscopic and thermal studies of [Fe(dioximato)2(amine)2] mixed chelates. Journal of Coordination Chemistry, 2007, 60, 379-392.	2.2	9
49	Mass spectrometric study of the vaporization behaviour of Î±-Na2NpO4: Thermodynamic investigation of the enthalpy of formation. Journal of Chemical Thermodynamics, 2013, 60, 132-141.	2.0	9
50	Theoretical study of Pu and Am tetracarbide molecules. International Journal of Quantum Chemistry, 2014, 114, 587-597.	2.0	9
51	A Uranyl Peroxide Dimer in the Gas Phase. Inorganic Chemistry, 2017, 56, 4186-4196.	4.0	9
52	Modelling the Impacts of Climate Change on Shallow Groundwater Conditions in Hungary. Water (Switzerland), 2021, 13, 668.	2.7	9
53	Theoretic study of the electronic spectra of neutral and cationic PaO and PaO2. Structural Chemistry, 2013, 24, 917-925.	2.0	8
54	A DFT investigation of the interactions of Pd, Ag, Sn, and Cs with silicon carbide. International Journal of Quantum Chemistry, 2014, 114, 1534-1545.	2.0	8

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55	Study of the Anâ€“Cl bond contraction in actinide trichlorides. Structural Chemistry, 2014, 25, 991-996.	2.0	8
56	Molecular data of mixed metal oxides with importance in nuclear safety. Journal of Nuclear Materials, 2016, 477, 134-138.	2.7	8
57	Molecular oxides of high-valent actinides. Structural Chemistry, 2020, 31, 1247-1271.	2.0	8
58	Modeling and Optimization of Runway Traffic Flow Using Coloured Petri Nets. , 0, , .		7
59	Theoretical investigation of NpC, NpC2 and NpC4 molecules. Structural Chemistry, 2015, 26, 1309-1322.	2.0	7
60	THE FORMATION OF THE BENZO[f]-3-PHOSPHABICYCLO[3.3.0]OCT-6-ENE RING SYSTEM IN THE FRIEDEL-CRAFTS REACTION OF THE ADDUCTS OF 2,5-DIHYDRO-1H-PHOSPHOLE 1-OXIDES WITH DICHLOROCARBENE. Phosphorus, Sulfur and Silicon and the Related Elements, 1991, 63, 131-141.	1.6	6
61	Theoretical study of the electronic spectra of neutral and cationic NpO and NpO2. Journal of Chemical Physics, 2015, 143, 074305.	3.0	6
62	Coordination of N2 ligands to lanthanum: the complexes La (N2)1â€“8. Structural Chemistry, 2018, 29, 1825-1837.	2.0	6
63	Tris-{Hydridotris(1-pyrazolyl)borato}lanthanide Complexes: Synthesis, Spectroscopy, Crystal Structure and Bonding Properties. Inorganics, 2021, 9, 44.	2.7	6
64	Synthesis, structure and thermokinetic studies on perchlorate salts of metal complexes containing a formamidine-type ligand. Journal of Coordination Chemistry, 2013, 66, 453-463.	2.2	5
65	MÃ¶ssbauer study of [Fe(Dioximato) n L2] mixed coordination compounds. Hyperfine Interactions, 2008, 185, 159-165.	0.5	4
66	Theoretical study of hyaluronan oligosaccharides. Structural Chemistry, 2010, 21, 1185-1194.	2.0	4
67	Electronic structure and spectroscopic properties of mixed sodium actinide oxides Na2AnO4 (AnÂ= U,) Tj ETQq1 1 0.784314 rgBT /Ov	3.6	4
68	Competing Metalâ€“Ligand Interactions in Tris(cyclopentadienyl)-cyclohexylisonitrile Complexes of Trivalent Actinides and Lanthanides. Molecules, 2022, 27, 3811.	3.8	4
69	Analytical Calculation of Sensitivity for Capacitive Pressure Transducers. Proceedings in Applied Mathematics and Mechanics, 2002, 1, 135.	0.2	3
70	A theoretical study on the mechanism of the baeyerâ€“villiger type oxidation of 7â€phosphanorbornene 7â€Oxides. Heteroatom Chemistry, 2007, 18, 759-766.	0.7	3
71	Comparative spectral and thermal studies of [Pt(DioxH)₂] chelates. Journal of Coordination Chemistry, 2009, 62, 2429-2437.	2.2	3
72	The twentieth year in Structural Chemistry. Structural Chemistry, 2009, 20, 1-10.	2.0	3

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73	Metalâ€“ligand interactions in complexes of cyclen-based ligands with Bi and Ac. Structural Chemistry, 2021, 32, 1719-1731.	2.0	3
74	Metal-ligand bonding in bispidine chelate complexes for radiopharmaceutical applications. Structural Chemistry, 2023, 34, 5-15.	2.0	3
75	Unexpected condensation reaction of two units of 1,2-dihydrophosphinine 1-oxides in the presence of tetracyanoethylene. Heteroatom Chemistry, 2003, 14, 29-35.	0.7	2
76	Phosphorus retention patterns along the Tisza River, Hungary. Water Science and Technology, 2009, 59, 391-397.	2.5	2
77	ANFIS regulated type 1diabetic model for different glucose absorption scenarios. , 2010, , .		2
78	The geometry of the nitroguanyl fragment in the simplest nitroguanidine derivatives in the absence of intermolecular interactions: The gas electron diffraction data on 1,1,3,3-tetramethyl-2-nitroguanidine. Russian Journal of Physical Chemistry A, 2011, 85, 441-446.	0.6	2
79	The thermodynamic properties of gaseous UO 2 (OH) 2. Journal of Nuclear Materials, 2017, 496, 163-165.	2.7	2
80	Structure and bonding of lanthanide dinitrogen complexes, Ln(N 2) 1â€8. International Journal of Quantum Chemistry, 2020, 120, e26051.	2.0	2
81	H2O coordination in macropa complexes of f elements (Ac, La, Lu): feasibility of the 11th coordination site. Structural Chemistry, 2021, 32, 643-653.	2.0	2
82	Pyridine-type complexes of transition-metal halides. Journal of Thermal Analysis and Calorimetry, 2004, 75, 965-974.	3.6	1
83	Theoretical study of heptadentate bispidine ligands for radiopharmaceutic applications. Computational and Theoretical Chemistry, 2022, 1212, 113716.	2.5	1
84	Modelling the matrix shift on the vibrational frequency of ThO by DFT-D3 calculations. Journal of Chemical Physics, 2017, 146, 124301.	3.0	0
85	Electronic structure of mixed caesium actinide oxides Cs2AnO4 (Anâ€¯=â€¯U, Np, Pu, Am). Chemical Physics Letters, 2018, 692, 202-207.	2.6	0