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	Metal-ligand bonding in bispidine chelate complexes for radiopharmaceutical applications. Structural Chemistry, 2023, 34, 5-15.	2.0	3
2	A terminal neptunium(V)â€“mono(oxo) complex. Nature Chemistry, 2022, 14, 342-349.	13.6	19
3	Theoretical study of heptadentate bispidine ligands for radiopharmaceutic applications. Computational and Theoretical Chemistry, 2022, 1212, 113716.	2.5	1
4	Competing Metalâ€“Ligand Interactions in Tris(cyclopentadienyl)-cyclohexylisonitrile Complexes of Trivalent Actinides and Lanthanides. Molecules, 2022, 27, 3811.	3.8	4
5	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
6	Modelling the Impacts of Climate Change on Shallow Groundwater Conditions in Hungary. Water (Switzerland), 2021, 13, 668.	2.7	9
7	Theoretical Study of Actinide(III)-DOTA Complexes. ACS Omega, 2021, 6, 13321-13330.	3.5	13
8	Tris-{Hydridotris(1-pyrazolyl)borato}lanthanide Complexes: Synthesis, Spectroscopy, Crystal Structure and Bonding Properties. Inorganics, 2021, 9, 44.	2.7	6
9	Metalâ€“ligand interactions in complexes of cyclen-based ligands with Bi and Ac. Structural Chemistry, 2021, 32, 1719-1731.	2.0	3
10	Structure and bonding of lanthanide dinitrogen complexes, Ln(N 2) 1â€8. International Journal of Quantum Chemistry, 2020, 120, e26051.	2.0	2
11	Theoretical Study of Actinide Complexes with Macropa. ACS Omega, 2020, 5, 26431-26440.	3.5	22
12	Molecular oxides of high-valent actinides. Structural Chemistry, 2020, 31, 1247-1271.	2.0	8
13	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
14	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
15	Solidâ€Sstate Structure of Trisâ€Cyclopentadienide Uranium(III) and Plutonium(III). Chemistry - A European Journal, 2018, 24, 2841-2844.	3.3	18
16	Electronic structure of mixed caesium actinide oxides Cs2AnO4 (Anâ€¯=â€¯U, Np, Pu, Am). Chemical Physics Letters, 2018, 692, 202-207.	2.6	0
17	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
18	Coordination of N2 ligands to lanthanum: the complexes La (N2)1â€8. Structural Chemistry, 2018, 29, 1825-1837.	2.0	6

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19	Pentavalent Curium, Berkelium, and Californium in Nitrate Complexes: Extending Actinide Chemistry and Oxidation States. Inorganic Chemistry, 2018, 57, 9453-9467.	4.0	15
20	Benchmarking density functionals in conjunction with <scp>G</scp>rimme's dispersion correction for noble gas dimers (Ne₂, Ar₂, Kr₂, Xe₂,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 697	2.0	32
21	Modelling the matrix shift on the vibrational frequency of ThO by DFT-D3 calculations. Journal of Chemical Physics, 2017, 146, 124301.	3.0	0
22	A Uranyl Peroxide Dimer in the Gas Phase. Inorganic Chemistry, 2017, 56, 4186-4196.	4.0	9
23	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
24	The thermodynamic properties of gaseous UO 2 (OH) 2. Journal of Nuclear Materials, 2017, 496, 163-165.	2.7	2
25	Electronic structure and spectroscopic properties of mixed sodium actinide oxides Na2AnO4 (AnÂ= U,) Tj ETQq1 1 0.784314 rgBT /Ov	3.6	4
26	Theoretical study of actinide monocarbides (ThC, UC, PuC, and AmC). Journal of Chemical Physics, 2016, 145, 244310.	3.0	15
27	Molecular data of mixed metal oxides with importance in nuclear safety. Journal of Nuclear Materials, 2016, 477, 134-138.	2.7	8
28	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
29	â€˜Lanthanide contractionâ€™ in [Ln(BTP)3](CF3SO3)3 complexes. Structural Chemistry, 2015, 26, 1287-1295.	2.0	13
30	Quantum Chemical Calculations and Experimental Investigations of Molecular Actinide Oxides. Chemical Reviews, 2015, 115, 1725-1759.	47.7	103
31	Theoretical investigation of NpC, NpC2 and NpC4 molecules. Structural Chemistry, 2015, 26, 1309-1322.	2.0	7
32	Theoretical study of the electronic spectra of neutral and cationic NpO and NpO2. Journal of Chemical Physics, 2015, 143, 074305.	3.0	6
33	Theoretical Study of Thorium and Uranium Tetracarbide Molecules. European Journal of Inorganic Chemistry, 2014, 2014, 1062-1071.	2.0	11
34	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
35	Theoretical study of Pu and Am tetracarbide molecules. International Journal of Quantum Chemistry, 2014, 114, 587-597.	2.0	9
36	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

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37	Study of the Anâ€“Cl bond contraction in actinide trichlorides. Structural Chemistry, 2014, 25, 991-996.	2.0	8
38	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
39	Theoretic study of the electronic spectra of neutral and cationic PaO and PaO2. Structural Chemistry, 2013, 24, 917-925.	2.0	8
40	Structure and Other Molecular Properties of Actinide Trichlorides AnCl₃ (An = Thâ€“Cm). Journal of Physical Chemistry A, 2013, 117, 11357-11363.	2.5	17
41	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
42	Theoretical Study of Bond Distances and Dissociation Energies of Actinide Oxides AnO and AnO₂. Inorganic Chemistry, 2012, 51, 4841-4849.	4.0	39
43	Theoretical Study of the Structure and Bonding in ThC₂ and UC₂. Journal of Physical Chemistry A, 2012, 116, 747-755.	2.5	28
44	Theoretical study of the Pu and Am dicarbide molecules. Structural Chemistry, 2012, 23, 1281-1289.	2.0	12
45	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
46	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
47	How accurate are electronic structure methods for actinoid chemistry?. Theoretical Chemistry Accounts, 2011, 129, 657-666.	1.4	65
48	Theoretical study of hyaluronan oligosaccharides. Structural Chemistry, 2010, 21, 1185-1194.	2.0	4
49	ANFIS regulated type 1diabetic model for different glucose absorption scenarios. , 2010, , .		2
50	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
51	Comparative spectral and thermal studies of [Pt(DioxH)₂] chelates. Journal of Coordination Chemistry, 2009, 62, 2429-2437.	2.2	3
52	Phosphorus retention patterns along the Tisza River, Hungary. Water Science and Technology, 2009, 59, 391-397.	2.5	2
53	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
54	The twentieth year in Structural Chemistry. Structural Chemistry, 2009, 20, 1-10.	2.0	3

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55	Vibrational Analysis of Î±-<scp>d</scp>-Glucose Trapped in Ar Matrix. Journal of Physical Chemistry B, 2009, 113, 2151-2159.	2.6	29
56	MÃ¶ssbauer study of [Fe(Dioximato) n L2] mixed coordination compounds. Hyperfine Interactions, 2008, 185, 159-165.	0.5	4
57	Molecular structure and thermodynamic properties of the gaseous ThC2 and ThC4 species. Journal of Nuclear Materials, 2008, 372, 391-393.	2.7	15
58	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
59	A theoretical study of AmO_nand CmO_n(n = 1, 2). Physical Chemistry Chemical Physics, 2008, 10, 1114-1117.	2.8	17
60	Spectroscopic and thermal studies of [Fe(dioximato)2(amine)2] mixed chelates. Journal of Coordination Chemistry, 2007, 60, 379-392.	2.2	9
61	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
62	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
63	Comparative study of two watershed scale models to calculate diffuse phosphorus pollution. Water Science and Technology, 2006, 53, 281-288.	2.5	10
64	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
65	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
66	Hydrogen bonding in peptide secondary structures. International Journal of Quantum Chemistry, 2005, 105, 302-312.	2.0	11
67	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
68	Structural, spectroscopic and computational studies of the HgL2Cl2 complex (L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 Td (3,5-dim 2005, 29, 833.	2.8	26
69	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
70	Pyridine-type complexes of transition-metal halides. Journal of Thermal Analysis and Calorimetry, 2004, 75, 965-974.	3.6	1
71	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
72	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

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73	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
74	Structural Characteristics of Intramolecular Hydrogen Bonding in Benzene Derivatives. Accounts of Chemical Research, 2002, 35, 887-894.	15.6	72
75	Analytical Calculation of Sensitivity for Capacitive Pressure Transducers. Proceedings in Applied Mathematics and Mechanics, 2002, 1, 135.	0.2	3
76	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 2001, 63, 723-732.	1.4	29
77	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 2001, 66, 573-581.	1.4	26
78	Title is missing!. Structural Chemistry, 2000, 11, 193-201.	2.0	29
79	Title is missing!. Magyar AprÃ³vad KÃ¶zlemÃ©nyek, 1999, 56, 493-501.	1.4	16
80	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
81	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
82	Comparison ofab initio and density functional methods for vibrational analysis of TeCl4. Journal of Computational Chemistry, 1998, 19, 308-318.	3.3	9
83	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
84	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
85	Modeling and Optimization of Runway Traffic Flow Using Coloured Petri Nets. , 0, , .		7