

ValÃ©rie Vallet

List of Publications by Year in descending order

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107
papers

3,389
citations

185998

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161609

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118
all docs

118
docs citations

118
times ranked

2363
citing authors

#	ARTICLE	IF	CITATIONS
1	Reactivity of Ru oxides with air radiolysis products investigated by theoretical calculations. Journal of Nuclear Materials, 2022, 558, 153395.	1.3	3
2	Environment Effects on X-Ray Absorption Spectra With Quantum Embedded Real-Time Time-Dependent Density Functional Theory Approaches. Frontiers in Chemistry, 2022, 10, 823246.	1.8	3
3	Influence of the First Coordination of Uranyl on Its Luminescence Properties: A Study of Uranyl Binitrate with N,N -Dialkyl Amide DEHBA and Water. Inorganic Chemistry, 2022, 61, 890-901.	1.9	9
4	NaCl Salts in Finite Aqueous Environments at the Fine Particle Marine Aerosol Scale. ACS Earth and Space Chemistry, 2022, 6, 1612-1626.	1.2	2
5	Structural and thermodynamics properties of pure phase alkanes, monoamides and alkane/monoamide mixtures with an ab initio based force-field model. Journal of Molecular Liquids, 2022, 363, 119797.	2.3	0
6	Insights from quantum chemical calculations into inner and outer-sphere complexation of plutonium(iv) by monoamide and carbamide extractants. Physical Chemistry Chemical Physics, 2021, 23, 2229-2237.	1.3	2
7	Revisiting the Complexation of Cm(III) with Aqueous Phosphates: What Can We Learn from the Complex Structures Using Luminescence Spectroscopy and Ab Initio Simulations?. Inorganic Chemistry, 2021, 60, 10656-10673.	1.9	3
8	Structure-Property Relationships in Photoluminescent Bismuth Halide Organic Hybrid Materials. Inorganic Chemistry, 2021, 60, 9727-9744.	1.9	12
9	Synthesis and photoluminescence of three bismuth(III)-organic compounds bearing heterocyclic N-donor ligands. Dalton Transactions, 2020, 49, 11756-11771.	1.6	13
10	Cover Image, Volume 120, Issue 21. International Journal of Quantum Chemistry, 2020, 120, e26496.	1.0	0
11	Conformational Landscape of Oxygen-Containing Naphthalene Derivatives. Journal of Physical Chemistry A, 2020, 124, 4484-4495.	1.1	5
12	Investigating solvent effects on the magnetic properties of molybdate ions (MoO_4^{2-}) with relativistic embedding. International Journal of Quantum Chemistry, 2020, 120, e26207.	1.0	7
13	Properties of the tetravalent actinide series in aqueous phase from a microscopic simulation self-consistent engine. Physical Chemistry Chemical Physics, 2020, 22, 2343-2350.	1.3	6
14	Carbon-sulfur bond strength in methanesulfinate and benzenesulfinate ligands directs decomposition of Np(V) and Pu(V) coordination complexes. Dalton Transactions, 2020, 49, 3293-3303.	1.6	1
15	Investigation of the Luminescence of $[\text{UO}_2\text{X}_4]^{2+}$ ($\text{X} = \text{Cl}, \text{Br}$) Complexes in the Organic Phase Using Time-Resolved Laser-Induced Fluorescence Spectroscopy and Quantum Chemical Simulations. Inorganic Chemistry, 2020, 59, 5896-5906.	1.9	15
16	Influence of Alkaline Earth Metal Ions on Structures and Luminescent Properties of $\text{NaMnUO}_2(\text{CO}_3)_3$ ($\text{M} = \text{Mg}, \text{Ca}$; $\text{Mn} = \text{O}^{2+}$): Time-Resolved Fluorescence Spectroscopy and Ab Initio Studies. Inorganic Chemistry, 2020, 59, 15036-15049.	1.9	16
17	Accurate Predictions of Volatile Plutonium Thermodynamic Properties. Inorganic Chemistry, 2019, 58, 14507-14521.	1.9	11
18	Ion hydration free energies and water surface potential in water nano drops: The cluster pair approximation and the proton hydration Gibbs free energy in solution. Journal of Chemical Physics, 2019, 151, 174504.	1.2	9

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19	Improving the description of solvent pairwise interactions using local solute/solvent three-body functions. The case of halides and carboxylates in aqueous environment. <i>Journal of Computational Chemistry</i> , 2019, 40, 1209-1218.	1.5	7
20	Global 15-Meter Mosaic Derived from Simulated True-Color ASTER Imagery. <i>Remote Sensing</i> , 2019, 11, 441.	1.8	3
21	Protactinium and the intersection of actinide and transition metal chemistry. <i>Nature Communications</i> , 2018, 9, 622.	5.8	27
22	Predictive Simulations of Ionization Energies of Solvated Halide Ions with Relativistic Embedded Equation of Motion Coupled Cluster Theory. <i>Physical Review Letters</i> , 2018, 121, 266001.	2.9	19
23	Unraveling the Ground State and Excited State Structures and Dynamics of Hydrated Ce ³⁺ Ions by Experiment and Theory. <i>Inorganic Chemistry</i> , 2018, 57, 10111-10121.	1.9	11
24	On the multi-reference nature of plutonium oxides: PuO ₂ ²⁺ , PuO ₂ , PuO ₃ and PuO ₂ (OH) ₂ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4317-4329.	1.3	27
25	Linking Solution Structures and Energetics: Thorium Nitrate Complexes. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8577-8584.	1.2	9
26	Organic ion association in aqueous phase and <i>ab initio</i> -based force fields: The case of carboxylate/ammonium salts. <i>Journal of Chemical Physics</i> , 2017, 147, 161720.	1.2	9
27	Aqueous chemistry of Ce(IV): estimations using actinide analogues. <i>Dalton Transactions</i> , 2017, 46, 13553-13561.	1.6	34
28	Structure and Bonding in Uranyl(VI) Peroxide and Crown Ether Complexes; Comparison of Quantum Chemical and Experimental Data. <i>Inorganic Chemistry</i> , 2017, 56, 15231-15240.	1.9	5
29	Facing the challenge of predicting the standard formation enthalpies of <i>n</i> -butyl-phosphate species with <i>ab initio</i> methods. <i>Journal of Chemical Physics</i> , 2017, 146, 244312.	1.2	4
30	Measurement of double differential cross-section of light water at high temperature and pressure to generate S($\hat{1}, \hat{1}^2$). <i>EPJ Web of Conferences</i> , 2017, 146, 13006.	0.1	5
31	Structural and Electronic Properties of Fluoride Complexes of Nb V, Ta V, and Pa V: The Influence of Relativistic Effects on Group V Elements. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5467-5476.	1.0	8
32	Structural, dynamical, and transport properties of the hydrated halides: How do At ⁺ bulk properties compare with those of the other halides, from F ⁻ to I ⁻ ? <i>Journal of Chemical Physics</i> , 2016, 144, 124513.	1.2	27
33	Thermochemistry of Ruthenium Oxyhydroxide Species and Their Impact on Volatile Speciations in Severe Nuclear Accident Conditions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 606-614.	1.1	7
34	First structural characterization of Pa(IV) in aqueous solution and quantum chemical investigations of the tetravalent actinides up to Bk(IV): the evidence of a curium break. <i>Dalton Transactions</i> , 2016, 45, 453-457.	1.6	28
35	Benchmark binding energies of ammonium and alkyl-ammonium ions interacting with water. Are ammonium-water hydrogen bonds strong?. <i>Chemical Physics Letters</i> , 2015, 618, 168-173.	1.2	9
36	Alkali-metal ion coordination in uranyl(VI) poly-peroxo complexes in solution, inorganic analogues to crown-ethers. Part 2. Complex formation in the tetramethyl ammonium-, Li ⁺ -, Na ⁺ - and K ⁺ -uranyl(VI)-peroxide-carbonate systems. <i>Dalton Transactions</i> , 2015, 44, 16565-16572.	1.6	8

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37	Alkali-metal ion coordination in uranyl(UO_2^{2+}) poly-peroxide complexes in solution. Part 1: the Li^+ , Na^+ and K^+ "peroxide" hydroxide systems. Dalton Transactions, 2015, 44, 1549-1556.	1.6	13
38	Effective bond orders from two-step spin-orbit coupling approaches: The I_2 , At_2 , IO^+ , and AtO^+ case studies. Journal of Chemical Physics, 2015, 142, 094305.	1.2	29
39	Thermodynamic Properties of Gaseous Ruthenium Species. Journal of Physical Chemistry A, 2015, 119, 4961-4971.	1.1	17
40	Theoretical Study of Plutonium(IV) Complexes Formed within the PUREX Process: A Proposal of a Plutonium Surrogate in Fire Conditions. Journal of Physical Chemistry A, 2014, 118, 10073-10080.	1.1	29
41	Electronic structure investigation of the evanescent AtO^+ ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	1.3	25
42	Activation of Gas-Phase Uranyl: From an Oxo to a Nitrido Complex. Journal of Physical Chemistry A, 2014, 118, 325-330.	1.1	25
43	How to build accurate macroscopic models of actinide ions in aqueous solvents?. , 2014, , .		0
44	Towards systematically improvable models for actinides in condensed phase: the electronic spectrum of uranyl in $\text{Cs}_2\text{UO}_2\text{Cl}_4$ as a test case. Physical Chemistry Chemical Physics, 2013, 15, 15153.	1.3	44
45	Further insights in the ability of classical nonadditive potentials to model actinide ion-water interactions. Journal of Computational Chemistry, 2013, 34, 707-719.	1.5	29
46	Can Quantum Chemical Methods be used to Predict Gibbs Energies for Reactions in Solution? A Case Study using Binary and Ternary Lanthanide(III) and Actinide(III) - Tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) "Tributyl/Trimethyl phosphate (TBP/TMP) Complexes. Solvent Extraction and Ion Exchange, 2013, 31, 358-369.	0.8	5
47	Revisiting a many-body model for water based on a single polarizable site: From gas phase clusters to liquid and air/liquid water systems. Journal of Chemical Physics, 2013, 139, 114502.	1.2	27
48	Probing the Nature of Chemical Bonding in Uranyl(VI) Complexes with Quantum Chemical Methods. Journal of Physical Chemistry A, 2012, 116, 12373-12380.	1.1	113
49	Modeling the hydration of mono-atomic anions from the gas phase to the bulk phase: The case of the halide ions F^- , Cl^- , and Br^- . Journal of Chemical Physics, 2012, 136, 044509.	1.2	36
50	Structure and dynamics of binary and ternary lanthanide(III) and actinide(III) tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) "tributylphosphate (TBP) complexes. Part 3, the structure, thermodynamics and reaction mechanisms of 8- and 9-coordinated binary and ternary Y-TTA-TBP complexes studied by quantum chemical methods. Dalton Transactions, 2011, 40, 3154.	1.6	7
51	Quantum Chemical and Molecular Dynamics Study of the Coordination of Th(IV) in Aqueous Solvent. Journal of Physical Chemistry B, 2010, 114, 15913-15924.	1.2	48
52	The structure and bonding of Y, Eu, U, Am and Cm complexes as studied by quantum chemical methods and X-ray crystallography. Dalton Transactions, 2010, 39, 7666.	1.6	21
53	Structure and dynamics of binary and ternary lanthanide(III) and actinide(III) tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) complexes. Part 2, the structure and dynamics of binary and ternary complexes in the Y(III)/Eu(III) "TTA" tributylphosphate (TBP) system in chloroform as studied by NMR spectroscopy. Dalton Transactions, 2010, 39, 10944.	1.6	8
54	Effects of the first hydration sphere and the bulk solvent on the spectra of the f2isoelectronic actinide compounds: U^{4+} , NpO_2^{2+} , and PuO_2^{2+} . Physical Chemistry Chemical Physics, 2010, 12, 1116-1130.	1.3	26

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55	On the combined use of discrete solvent models and continuum descriptions of solvent effects in ligand exchange reactions: a case study of the uranyl(VI) aquo ion. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 377-384.	0.5	22
56	Water Exchange Mechanism in the First Excited State of Hydrated Uranyl(VI). <i>Inorganic Chemistry</i> , 2009, 48, 11310-11313.	1.9	14
57	An ab Initio Theoretical Study of the Electronic Structure of UO_2^{2+} and $[\text{UO}_2(\text{CO}_3)_3]^{5-}$. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1420-1428.	1.1	42
58	Benchmarking Electronic Structure Calculations on the Bare UO_2^{2+} Ion: How Different are Single and Multireference Electron Correlation Methods?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12504-12511.	1.1	62
59	Multiconfiguration Dirac-Hartree-Fock Adjusted Energy-Consistent Pseudopotential for Uranium: Spin-Orbit Configuration Interaction and Fock-Space Coupled-Cluster Study of U^{4+} and U^{5+} . <i>Journal of Physical Chemistry A</i> , 2009, 113, 11509-11516.	1.1	20
60	Improvement of the ab initio embedded cluster method for luminescence properties of doped materials by taking into account impurity induced distortions: The example of $\text{Y}[\text{O}]_2[\text{O}]_3:\text{Bi}^{3+}$. <i>Journal of Chemical Physics</i> , 2009, 131, 194501.	1.2	20
61	An Investigation of the Accuracy of Different DFT Functionals on the Water Exchange Reaction in Hydrated Uranyl(VI) in the Ground State and the First Excited State. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 569-577.	2.3	64
62	Ground- and Excited-State Properties of the Mixed-Valence Complex $[(\text{NH}_3)_5(\text{H}_2\text{O})\text{Ru}^{\text{III}}\text{NCRu}^{\text{II}}(\text{CN})_5]^{3+}$. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5467-5477.	1.1	10
63	Ab Initio Study of the Mechanism for Photoinduced Yl-Oxygen Exchange in Uranyl(VI) in Acidic Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2008, 130, 11742-11751.	6.6	28
64	Spin-orbit configuration interaction study of the electronic structure of the 5f ₂ manifold of U^{4+} and the 5f manifold of U^{5+} . <i>Journal of Chemical Physics</i> , 2008, 128, 154310.	1.2	12
65	In silico prediction of atomic static electric-dipole polarizabilities of the early tetravalent actinide ions: $\text{Th}^{4+}(5f_0)$, $\text{Pa}^{4+}(5f_1)$, and $\text{U}^{4+}(5f_2)$. <i>Physical Review A</i> , 2008, 78, .	1.0	16
66	Ab initio embedded cluster study of the excitation spectrum and Stokes shifts of Bi^{3+} -doped Y_2O_3 . <i>Journal of Chemical Physics</i> , 2007, 127, 104705.	1.2	17
67	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: A comparison between wave-function theory and density functional theory. <i>Journal of Chemical Physics</i> , 2007, 127, 214302.	1.2	75
68	Comment on "The Water Exchange Mechanism of the $[\text{UO}_2(\text{OH})_2]^{2+}$ Ion Revisited: The Importance of a Proper Treatment of Electron Correlation" [F. P. Rotzinger <i>Chem. Eur. J.</i> , 2007, 13, 800]. <i>Chemistry - A European Journal</i> , 2007, 13, 10294-10297.	1.7	11
69	Photoinduced multi-mode quantum dynamics of pyrrole at the conical intersections. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 177-189.	2.0	44
70	The luminescence spectrum of in 2GeF_6 crystals: A quantum chemical study. <i>Journal of Luminescence</i> , 2007, 126, 779-783.	1.5	18
71	On the structure and relative stability of uranyl(VI) sulfate complexes in solution. <i>Comptes Rendus Chimie</i> , 2007, 10, 905-915.	0.2	28
72	Ab initio study of a Bi^{3+} impurity in $\text{Cs}_2\text{NaYCl}_6$ and Y_2O_3 : Comparison of perturbative and variational electron correlation methods. <i>Journal of Chemical Physics</i> , 2006, 125, 174709.	1.2	10

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73	Investigation of the dynamics of two coupled oscillators with mixed quantum-classical methods. <i>Journal of Chemical Physics</i> , 2006, 124, 184105.	1.2	6
74	Solution coordination chemistry of actinides: Thermodynamics, structure and reaction mechanisms. <i>Coordination Chemistry Reviews</i> , 2006, 250, 784-815.	9.5	177
75	Actinide Chemistry in Solution, Quantum Chemical Methods and Models. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 145-160.	0.5	114
76	Importance of Spin-Orbit Coupling for the Assignment of the Photodetachment Spectra of AuX ₂ ⁻ (X=Cl, Br, and I). <i>ChemPhysChem</i> , 2006, 7, 723-727.	1.0	15
77	Calculation of the vibronic structure of the photodetachment spectra of CCl ₄ ⁻ and CBr ₄ ⁻ . <i>Journal of Chemical Physics</i> , 2006, 125, 164327.	1.2	8
78	Calculation of the vibronic structure of the X ₁ ¹ photoelectron spectra of XCN, X=F, Cl, and Br. <i>Journal of Chemical Physics</i> , 2006, 124, 044317.	1.2	18
79	The importance of electron correlation and intermediate coupling in the spectroscopy of actinides molecules. , 2006, , 1302-1305.		0
80	Spin-orbit effects on the electronic spectroscopy of transition metal dihydrides H ₂ M(CO) ₄ (M=Fe,) <i>J. Chem. Phys.</i> 2005, 123, 231103.	0.9	23
81	Experimental and Quantum Chemical Studies of Structure and Reaction Mechanisms of Dioxouranium(VI) Complexes in Solution. <i>ChemInform</i> , 2005, 36, no.	0.1	0
82	Remarkable impact of intermode couplings on multimode vibronic dynamics: the photoelectron spectrum of CH ₃ F. <i>Journal of Chemical Physics</i> , 2005, 123, 231103.	1.2	20
83	Photochemistry of pyrrole: Time-dependent quantum wave-packet description of the dynamics at the $\tilde{1}^1\Sigma^+ - \tilde{1}^1\Sigma^+$ conical intersections. <i>Journal of Chemical Physics</i> , 2005, 123, 144307.	1.2	120
84	Spectroscopic effects of first-order relativistic vibronic coupling in linear triatomic molecules. <i>Journal of Chemical Physics</i> , 2005, 123, 124104.	1.2	20
85	Time-dependent quantum wave-packet description of the $\tilde{1}^1\Sigma^+$ photochemistry of phenol. <i>Journal of Chemical Physics</i> , 2005, 122, 224315.	1.2	177
86	Spin-Orbit Effects in Electron Transfer in Neptunyl(VI)~Neptunyl(V) Complexes in Solution. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4957-4960.	1.1	14
87	Can density functional methods be used for open-shell actinide molecules? Comparison with multiconfigurational spin-orbit studies. <i>Journal of Chemical Physics</i> , 2004, 121, 5312-5321.	1.2	81
88	Relativistic Pseudopotential Calculations for Electronic Excited States. <i>Theoretical and Computational Chemistry</i> , 2004, 14, 476-551.	0.2	8
89	The Mechanism of Water Exchange in AmO ₂ (H ₂ O) ₅ ²⁺ and in the Isoelectronic UO ₂ (H ₂ O) ₅ ²⁺ and NpO ₂ (H ₂ O) ₅ ²⁺ Complexes as Studied by Quantum Chemical Methods. <i>Journal of the American Chemical Society</i> , 2004, 126, 7766-7767.	6.6	63
90	The Mechanism of Water Exchange in AmO ₂ (H ₂ O) ₅ ²⁺ and in the Isoelectronic UO ₂ (H ₂ O) ₅ ²⁺ and NpO ₂ (H ₂ O) ₅ ²⁺ Complexes as Studied by Quantum Chemical Methods.. <i>ChemInform</i> , 2004, 35, no.	0.1	0

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91	Multimode Jahn-Teller and pseudo-Jahn-Teller coupling effects in the photoelectron spectrum of CH ₃ F. <i>Chemical Physics</i> , 2004, 304, 17-34.	0.9	41
92	Time-dependent quantum wave-packet description of the $1\tilde{E}^*_1$ photochemistry of pyrrole. <i>Faraday Discussions</i> , 2004, 127, 283-293.	1.6	78
93	Experimental and quantum chemical studies of structure and reaction mechanisms of dioxouranium(vi) complexes in solution. <i>Dalton Transactions</i> , 2004, , 3799-3807.	1.6	26
94	Structure and Bonding in Solution of Dioxouranium(VI) Oxalate Complexes: Isomers and Intramolecular Ligand Exchange. <i>Inorganic Chemistry</i> , 2003, 42, 1982-1993.	1.9	68
95	The electronic spectroscopy of transition metal di-hydrides H ₂ M(CO) ₄ (M = Fe, Os): a theoretical study based on CASSCF/MS-CASPT2 and TD-DFT. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2948-2953.	1.3	15
96	Chelate Effect and Thermodynamics of Metal Complex Formation in Solution: A Quantum Chemical Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 14941-14950.	6.6	78
97	Rates and Mechanism of Fluoride and Water Exchange in UO ₂ F ₃ - and [UO ₂ F ₄ (H ₂ O)] ₂ - Studied by NMR Spectroscopy and Wave Function Based Methods. <i>Inorganic Chemistry</i> , 2002, 41, 5626-5633.	1.9	37
98	Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry. <i>Inorganic Chemistry</i> , 2001, 40, 3516-3525.	1.9	138
99	The Mechanism for Water Exchange in [UO ₂ (H ₂ O) ₅] ²⁺ and [UO ₂ (oxalate) ₂ (H ₂ O)] ²⁻ , as Studied by Quantum Chemical Methods. <i>Journal of the American Chemical Society</i> , 2001, 123, 11999-12008.	6.6	123
100	Ab initio study of the ground-state potential of XH ⁻ anions (X=He,Ne,Ar). <i>Chemical Physics</i> , 2001, 263, 33-40.	0.9	21
101	Accurate ab initio study on the spectroscopy of Ag and Ag ⁺ including spin-orbit couplings aimed at molecular calculations. <i>Journal of Chemical Physics</i> , 2001, 115, 3201-3207.	1.2	19
102	A two-step uncontracted determinantal effective Hamiltonian-based SO-CI method. <i>Journal of Chemical Physics</i> , 2000, 113, 1391-1402.	1.2	140
103	Theoretical spectroscopy of molecular iodine. 1. Ab initio study on the B ⁰ _u and A ¹ _g and B ² _u X ⁰ _u and X ⁰ _g radiative transition intensities. <i>Molecular Physics</i> , 2000, 98, 1973-1979.	0.8	9
104	Reduction of uranyl by hydrogen: an ab initio study. <i>Chemical Physics</i> , 1999, 244, 185-193.	0.9	81
105	Investigation of the low-lying excited states of PuO ₂ ²⁺ . <i>Chemical Physics</i> , 1999, 244, 195-201.	0.9	42
106	Reduction Behavior of the Early Actinyl Ions in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9285-9289.	1.1	54
107	Structure of Uranium(VI) in Strong Alkaline Solutions. A Combined Theoretical and Experimental Investigation. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8257-8264.	1.1	169