

Michiel Sprik

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

134
papers

10,480
citations

56
h-index

101
g-index

140
ext. papers

11,156
ext. citations

4.7
avg, IF

6.44
L-index

#	Paper	IF	Citations
134	Computational Amperometry of Nanoscale Capacitors in Molecular Simulations. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4357-4361	6.4	5
133	Electric-field-based Poisson-Boltzmann theory: Treating mobile charge as polarization. <i>Physical Review E</i> , 2021 , 103, 022803	2.4	1
132	Chemomechanical equilibrium at the interface between a simple elastic solid and its liquid phase.. <i>Journal of Chemical Physics</i> , 2021 , 155, 244701	3.9	0
131	Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. <i>Journal of Chemical Physics</i> , 2020 , 152, 194706	3.9	1
130	Electromechanics of the liquid water vapour interface. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10676-10686	3.6	11
129	Modelling electrochemical systems with finite field molecular dynamics. <i>JPhys Energy</i> , 2020 , 2, 032005	4.9	32
128	Thermodynamic Investigation of Proton/Electron Interplay on the Pourbaix Diagram at the TiO ₂ /Electrolyte Interface. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 19003-19014	3.8	7
127	Computing Surface Acidity Constants of Proton Hopping Groups from Density Functional Theory-Based Molecular Dynamics: Application to the SnO(110)/HO Interface. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6520-6527	6.4	8
126	Coupling of Surface Chemistry and Electric Double Layer at TiO Electrochemical Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 3871-3876	6.4	36
125	Finite field formalism for bulk electrolyte solutions. <i>Journal of Chemical Physics</i> , 2019 , 151, 064506	3.9	10
124	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. <i>Physical Review Letters</i> , 2019 , 123, 195501	7.4	30
123	Finite electric displacement simulations of polar ionic solid-electrolyte interfaces: Application to NaCl(111)/aqueous NaCl solution. <i>Journal of Chemical Physics</i> , 2019 , 150, 041716	3.9	14
122	Finite Maxwell field and electric displacement Hamiltonians derived from a current dependent Lagrangian. <i>Molecular Physics</i> , 2018 , 116, 3114-3120	1.7	9
121	Effects of third-order susceptibility in sum frequency generation spectra: a molecular dynamics study in liquid water. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 3040-3053	3.6	53
120	Charge compensation at the interface between the polar NaCl(111) surface and a NaCl aqueous solution. <i>Journal of Chemical Physics</i> , 2017 , 147, 104702	3.9	15
119	Computing the dielectric constant of liquid water at constant dielectric displacement. <i>Physical Review B</i> , 2016 , 93,	3.3	33
118	Density Functional Theory Calculation of the Band Alignment of (101 0) In(x)Ga(1-x)N/Water Interfaces. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 1928-39	3.4	11

117	Computing the Kirkwood g-Factor by Combining Constant Maxwell Electric Field and Electric Displacement Simulations: Application to the Dielectric Constant of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2696-701	6.4	50
116	Finite field methods for the supercell modeling of charged insulator/electrolyte interfaces. <i>Physical Review B</i> , 2016 , 94,	3.3	30
115	Electronic Energy Levels and Band Alignment for Aqueous Phenol and Phenolate from First Principles. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 9651-60	3.4	15
114	Temperature dependence of interfacial structures and acidity of clay edge surfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 160, 91-99	5.5	20
113	Interfacial structures and acidity of edge surfaces of ferruginous smectites. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 168, 293-301	5.5	25
112	Aqueous transition-metal cations as impurities in a wide gap oxide: the Cu(2+)/Cu(+) and Ag(2+)/Ag(+) redox couples revisited. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 1152-63	3.4	22
111	Reductive Hydrogenation of the Aqueous Rutile TiO ₂ (110) Surface. <i>Electrochimica Acta</i> , 2015 , 179, 658-667	6.7	18
110	The temperature dependence of the symmetry factor for a model Fe ³⁺ (aq)/Fe ²⁺ (aq) redox half reaction. <i>Molecular Physics</i> , 2015 , 113, 2463-2475	1.7	2
109	Molecular simulation study of hydrated Na-rectorite. <i>Langmuir</i> , 2015 , 31, 2008-13	4	12
108	Modeling the Oxygen Evolution Reaction on Metal Oxides: The Influence of Unrestricted DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 4095-4102	3.8	81
107	Redox potentials and acidity constants from density functional theory based molecular dynamics. <i>Accounts of Chemical Research</i> , 2014 , 47, 3522-9	24.3	134
106	Identifying Trapped Electronic Holes at the Aqueous TiO ₂ Interface. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 5437-5444	3.8	72
105	Solute-Solvent Charge-Transfer Excitations and Optical Absorption of Hydrated Hydroxide from Time-Dependent Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2465-70	6.4	3
104	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2014 , 140, 410-417	5.5	63
103	Aligning Electronic and Protonic Energy Levels of Proton-Coupled Electron Transfer in Water Oxidation on Aqueous TiO ₂ . <i>Angewandte Chemie</i> , 2014 , 126, 12242-12246	3.6	13
102	The ionization potential of aqueous hydroxide computed using many-body perturbation theory. <i>Journal of Chemical Physics</i> , 2014 , 141, 034501	3.9	32
101	Aligning electronic and protonic energy levels of proton-coupled electron transfer in water oxidation on aqueous TiO ₂ . <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 12046-50	16.4	64
100	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2013 , 120, 487-495	5.5	46

99	Acidity of edge surface sites of montmorillonite and kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , 2013 , 117, 180-190	5.5	146
98	Hydration, acidity and metal complexing of polysulfide species: A first principles molecular dynamics study. <i>Chemical Physics Letters</i> , 2013 , 563, 9-14	2.5	12
97	Vibrational Sum Frequency Generation Spectroscopy of the Water Liquid-Vapor Interface from Density Functional Theory-Based Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 83-7	6.4	128
96	Solution Structures and Acidity Constants of Molybdic Acid. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2926-2930	6.4	33
95	Alignment of electronic energy levels at electrochemical interfaces. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 11245-67	3.6	185
94	Free energies of absorption of alkali ions onto beidellite and montmorillonite surfaces from constrained molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2012 , 91, 109-119	5.5	30
93	Absolute acidity of clay edge sites from ab-initio simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2012 , 94, 1-11	5.5	74
92	The Silica-Water Interface: How the Silanols Determine the Surface Acidity and Modulate the Water Properties. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1037-47	6.4	279
91	Oxide/water interfaces: how the surface chemistry modifies interfacial water properties. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 124106	1.8	90
90	Aqueous Redox Chemistry and the Electronic Band Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3411-5	6.4	67
89	Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO ₂ (110). <i>ChemCatChem</i> , 2012 , 4, 636-640	5.2	56
88	Activation energy for a model ferrous-ferric half reaction from transition path sampling. <i>Journal of Chemical Physics</i> , 2012 , 136, 034506	3.9	10
87	Absolute pKa Values and Solvation Structure of Amino Acids from Density Functional Based Molecular Dynamics Simulation. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1951-61	6.4	70
86	The oxidation of tyrosine and tryptophan studied by a molecular dynamics normal hydrogen electrode. <i>Journal of Chemical Physics</i> , 2011 , 134, 244508	3.9	98
85	Acidity constants from DFT-based molecular dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 284116	1.8	47
84	Aligning electronic energy levels at the TiO ₂ /H ₂ O interface. <i>Physical Review B</i> , 2010 , 82,	3.3	108
83	Acidity of the Aqueous Rutile TiO ₂ (110) Surface from Density Functional Theory Based Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 880-9	6.4	159
82	The electron attachment energy of the aqueous hydroxyl radical predicted from the detachment energy of the aqueous hydroxide anion. <i>Journal of the American Chemical Society</i> , 2009 , 131, 6046-7	16.4	45

81	Redox potentials and pKa for benzoquinone from density functional theory based molecular dynamics. <i>Journal of Chemical Physics</i> , 2009 , 131, 154504	3.9	138
80	Acidity constants from vertical energy gaps: density functional theory based molecular dynamics implementation. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 5238-49	3.6	113
79	A classical point charge model study of system size dependence of oxidation and reorganization free energies in aqueous solution. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 257-69	3.4	45
78	First Principles Study of Alkali-Tyrosine Complexes: Alkali Solvation and Redox Properties. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1049-56	6.4	12
77	Calculation of redox properties: understanding short- and long-range effects in rubredoxin. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 3969-76	3.4	81
76	Redox free energies and one-electron energy levels in density functional theory based ab initio molecular dynamics. <i>Journal of Electroanalytical Chemistry</i> , 2007 , 607, 113-120	4.1	35
75	Free energy calculation of water addition coupled to reduction of aqueous RuO ₄ ⁻ . <i>Journal of Chemical Physics</i> , 2007 , 126, 204506	3.9	25
74	Electron Transfer Properties from Atomistic Simulations and Density Functional Theory. <i>Chimia</i> , 2007 , 61, 155-158	1.3	6
73	From solvent fluctuations to quantitative redox properties of quinones in methanol and acetonitrile. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 1936-8	16.4	25
72	Diabatic free energy curves and coordination fluctuations for the aqueous Ag ⁺ /Ag ²⁺ redox couple: a biased Born-Oppenheimer molecular dynamics investigation. <i>Journal of Chemical Physics</i> , 2006 , 124, 64507	3.9	100
71	Ligand Field Effects on the Aqueous Ru(III)/Ru(II) Redox Couple from an All-Atom Density Functional Theory Perspective. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 1403-15	6.4	26
70	Density functional theory study of tetrathiafulvalene and thianthrene in acetonitrile: structure, dynamics, and redox properties. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3614-23	3.4	37
69	Long-range solvent effects on the orbital interaction mechanism of water acidity enhancement in metal ion solutions: a comparative study of the electronic structure of aqueous Mg and Zn dications. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 11444-53	3.4	41
68	A molecular dynamics study of the hydroxyl radical in solution applying self-interaction-corrected density functional methods. <i>Physical Chemistry Chemical Physics</i> , 2005 , 7, 1363-7	3.6	146
67	Ab initio molecular dynamics simulation of the aqueous Ru ²⁺ /Ru ³⁺ redox reaction: the Marcus perspective. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 6793-804	3.4	79
66	Time-dependent density functional theory description of on-site electron repulsion and ligand field effects in the optical spectrum of hexaaquoruthenium(II) in solution. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 12222-6	3.4	5
65	Ab initio molecular dynamics simulation of redox reactions in solution. <i>Computer Physics Communications</i> , 2005 , 169, 256-261	4.2	33
64	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. <i>Journal of Chemical Physics</i> , 2005 , 122, 14515	3.9	417

63	On the position of the highest occupied molecular orbital in aqueous solutions of simple ions. <i>ChemPhysChem</i> , 2005 , 6, 1805-8	3.2	30
62	Toward a Monte Carlo program for simulating vapor-liquid phase equilibria from first principles. <i>Computer Physics Communications</i> , 2005 , 169, 289-294	4.2	25
61	Density-functional molecular-dynamics study of the redox reactions of two anionic, aqueous transition-metal complexes. <i>Journal of Chemical Physics</i> , 2005 , 122, 234505	3.9	81
60	Density functional calculation of the electronic absorption spectrum of Cu ⁺ and Ag ⁺ aqua ions. <i>Journal of Chemical Physics</i> , 2004 , 121, 11885-99	3.9	40
59	Hartree-Fock exchange in time dependent density functional theory: application to charge transfer excitations in solvated molecular systems. <i>Chemical Physics Letters</i> , 2004 , 394, 141-146	2.5	49
58	Free Energy of Oxidation of Metal Aqua Ions by an Enforced Change of Coordination. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 6529-6535	3.4	41
57	Ab Initio Molecular Dynamics Study of Uracil in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 7458-7467	3.4	67
56	Electronic structure and solvation of copper and silver ions: a theoretical picture of a model aqueous redox reaction. <i>Journal of the American Chemical Society</i> , 2004 , 126, 3928-38	16.4	183
55	Liquid Water from First Principles: Investigation of Different Sampling Approaches. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 12990-12998	3.4	309
54	Time dependent density functional theory study of charge-transfer and intramolecular electronic excitations in acetone-water systems. <i>Journal of Chemical Physics</i> , 2003 , 119, 12417-12431	3.9	128
53	Thermal versus electronic broadening in the density of states of liquid water. <i>Chemical Physics Letters</i> , 2003 , 376, 68-74	2.5	56
52	Ab Initio Molecular Dynamics Computation of the Infrared Spectrum of Aqueous Uracil. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 10344-10358	3.4	227
51	Theoretical pKa estimates for solvated P(OH) ₅ from coordination constrained Car Parrinello molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2003 , 5, 2612-2618	3.6	38
50	Molecular dynamics study of electron gas models for liquid water. <i>Molecular Physics</i> , 2003 , 101, 1183-1198	1.7	11
49	Constrained reaction coordinate dynamics for systems with constraints. <i>Molecular Physics</i> , 2003 , 101, 2885-2894	1.7	29
48	Ab initio molecular dynamics for molecules with variable numbers of electrons. <i>Physical Review Letters</i> , 2002 , 88, 213002	7.4	77
47	Electronic properties of hard and soft ions in solution: Aqueous Na ⁺ and Ag ⁺ compared. <i>Journal of Chemical Physics</i> , 2001 , 115, 3454-3468	3.9	78
46	Computation of the pK of liquid water using coordination constraints. <i>Chemical Physics</i> , 2000 , 258, 139-150	1.7	141

45	Electronic excitation spectra from time-dependent density functional response theory using plane-wave methods. <i>Chemical Physics Letters</i> , 2000 , 330, 563-569	2.5	23
44	Ab initio molecular dynamics simulation of liquids and solutions. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, A161-A163	1.8	11
43	Key Steps of the cis-Platin-DNA Interaction: Density Functional Theory-Based Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 823-835	3.4	158
42	Hydrogen Elimination and Solid-State Reaction in Hydrogen-Bonded Systems under Pressure: The Case of HBr. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 11801-11804	3.4	6
41	New generalized gradient approximation functionals. <i>Journal of Chemical Physics</i> , 2000 , 112, 1670-1678	3.9	312
40	Pressure-induced structural changes of HBr. <i>Physica B: Condensed Matter</i> , 1999 , 265, 101-104	2.8	3
39	Pressure-induced structural and chemical changes of solid HBr. <i>Journal of Chemical Physics</i> , 1999 , 111, 1595-1607	3.9	18
38	Ab Initio Molecular Dynamics Study of the Reaction of Water with Formaldehyde in Sulfuric Acid Solution. <i>Journal of the American Chemical Society</i> , 1998 , 120, 6345-6355	16.4	81
37	Coordination numbers as reaction coordinates in constrained molecular dynamics. <i>Faraday Discussions</i> , 1998 , 110, 437-445	3.6	94
36	Living polymers. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998 , 94, 501-508		20
35	A Density Functional Study of the Addition of Water to SO ₃ in the Gas Phase and in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 2893-2898	2.8	70
34	Free energy from constrained molecular dynamics. <i>Journal of Chemical Physics</i> , 1998 , 109, 7737-7744	3.9	633
33	Pressure Effects on Hydrogen Bonding in the Disordered Phase of Solid HBr. <i>Physical Review Letters</i> , 1998 , 81, 4416-4419	7.4	18
32	Structure of Solid Poly(tetrafluoroethylene): A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 2745-2749	3.4	37
31	Density Functional Theory-Based Molecular Dynamics Simulation of Acid-Catalyzed Chemical Reactions in Liquid Trioxane. <i>Journal of the American Chemical Society</i> , 1997 , 119, 7218-7229	16.4	82
30	Ab initio molecular dynamics of ion solvation. The case of Be ²⁺ in water. <i>Chemical Physics Letters</i> , 1997 , 273, 360-366	2.5	144
29	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. <i>Journal of Chemical Physics</i> , 1996 , 105, 1142-1152	3.9	562
28	A density-functional study of the intermolecular interactions of benzene. <i>Journal of Chemical Physics</i> , 1996 , 105, 8684-8689	3.9	224

27	The torsional potential of perfluoro n-alkanes: A density functional study. <i>Journal of Chemical Physics</i> , 1996 , 104, 3692-3700	3.9	48
26	Ab initiomolecular dynamics simulation of liquids and solutions. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 9405-9409	1.8	23
25	Influence of surface topology and electrostatic potential on water/electrode systems. <i>Journal of Chemical Physics</i> , 1995 , 102, 511-524	3.9	268
24	Competing interactions in self-assembled monolayers containing peptide groups: molecular dynamics studies of long-chain perfluoro mercaptans on Au(111). <i>Journal of Materials Chemistry</i> , 1994 , 4, 793-803		7
23	Molecular dynamics simulation of an aqueous sodium octanoate micelle using polarizable surfactant molecules. <i>Langmuir</i> , 1993 , 9, 916-926	4	105
22	Orientalional ordering in solid C70: Predictions from computer simulation. <i>Physical Review Letters</i> , 1992 , 69, 1660-1663	7.4	90
21	Ordering of fractional monolayers of H2O on Ni(110). <i>Surface Science Letters</i> , 1992 , 279, L185-L190		
20	Folding of model heteropolymers by configurational-bias Monte Carlo. <i>Chemical Physics Letters</i> , 1992 , 199, 220-224	2.5	7
19	Hydrogen bonding and the static dielectric constant in liquid water. <i>Journal of Chemical Physics</i> , 1991 , 95, 6762-6769	3.9	135
18	Adiabatic dynamics of the solvated electron in liquid ammonia. <i>Journal of Chemical Physics</i> , 1989 , 91, 5665-5671	3.9	37
17	Application of path integral simulations to the study of electron solvation in polar fluids. <i>Computer Physics Reports</i> , 1988 , 7, 147-166		16
16	A polarizable model for water using distributed charge sites. <i>Journal of Chemical Physics</i> , 1988 , 89, 7556-7560	3.5	445
15	Molecular model for aqueous ferrous/ferric electron transfer. <i>Journal of Chemical Physics</i> , 1988 , 89, 3248-3257	3.9	386
14	Solvation of electrons, atoms and ions in liquid ammonia. <i>Faraday Discussions of the Chemical Society</i> , 1988 , 85, 373		23
13	Optimization of a distributed Gaussian basis set using simulated annealing: Application to the adiabatic dynamics of the solvated electron. <i>Journal of Chemical Physics</i> , 1988 , 89, 1592-1607	3.9	75
12	Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. <i>Journal of Chemical Physics</i> , 1988 , 89, 4918-4923	3.9	28
11	Ionic solvation in nonaqueous solvents: the structure of lithium ion and chloride in methanol, ammonia, and methylamine. <i>Journal of the American Chemical Society</i> , 1987 , 109, 5900-5904	16.4	76
10	Electron-ion interactions and ionization in a polar solvent. <i>Physical Review Letters</i> , 1986 , 56, 2326-2329	7.4	53

9	Staging: A sampling technique for the Monte Carlo evaluation of path integrals. <i>Physical Review B</i> , 1985 , 31, 4234-4244	3.3	168
8	Computer simulation of a quantum particle in a quenched disordered system: Direct observation of Lifshitz traps. <i>Physical Review B</i> , 1985 , 32, 545-547	3.3	42
7	Simulation of an excess electron in a hard sphere fluid. <i>Journal of Chemical Physics</i> , 1985 , 83, 3042-3049	3.9	61
6	Simulation of the cubic to orthorhombic phase transition in potassium cyanide. <i>Journal of Chemical Physics</i> , 1985 , 83, 3638-3644	3.9	21
5	Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations. <i>Journal of Chemical Physics</i> , 1985 , 83, 5802-5809	3.9	67
4	Computer simulation of muonium in water. <i>Journal of Chemical Physics</i> , 1984 , 80, 5719-5724	3.9	111
3	Orientalional ordering in solid parahydrogen and orthodeuterium. <i>Journal of Chemical Physics</i> , 1984 , 81, 6207-6213	3.9	11
2	A correlated variational wave function for the orientational ground state of solid methane. <i>Journal of Chemical Physics</i> , 1984 , 80, 1988-1999	3.9	7
1	Second-order elastic constants for the Lennard-Jones solid. <i>Physical Review B</i> , 1984 , 29, 4368-4374	3.3	76