Masahiko Hada

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190 papers	3,982 citations	36 h-index	50 g-index
201 ext. papers	4,314 ext. citations	3.9 avg, IF	5.37 L-index

#	Paper	IF	Citations
190	Excited and ionized states of free base porphin studied by the symmetry adapted cluster-configuration interaction (SAC-CI) method. *Journal of Chemical Physics*, **1996**, 104, 2321-2329	3.9	157
189	Quasirelativistic theory for the magnetic shielding constant. I. Formulation of Douglas□Kroll□Hess transformation for the magnetic field and its application to atomic systems. *Journal of Chemical Physics*, **2003**, 118, 1015-1026	3.9	100
188	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method. *Chemical Physics Letters*, **1995**, 233, 95-101	2.5	98
187	Dilithioplumbole: a lead-bearing aromatic cyclopentadienyl analog. *Science*, **2010**, 328, 339-42	33.3	95
186	Quasirelativistic theory for magnetic shielding constants. II. Gauge-including atomic orbitals and applications to molecules. *Journal of Chemical Physics*, **2003**, 118, 1027-1035	3.9	95
185	Theoretical Study of the Excited States of Chlorin, Bacteriochlorin, Pheophytin a, and Chlorophyll a by the SAC/SAC□CI Method. *Journal of Physical Chemistry B*, **1998**, 102, 1320-1326	3.4	89
184	Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster□configuration interaction method. *Journal of Chemical Physics*, **2000**, 113, 7853-7866	3.9	82
183	Relativistic study of nuclear magnetic shielding constants: hydrogen halides. *Chemical Physics Letters*, **1996**, 254, 170-178	2.5	76
182	Effect of the axial ligand on the reactivity of the oxoiron(IV) porphyrin □-cation radical complex: higher stabilization of the product state relative to the reactant state. *Inorganic Chemistry*, **2012**, 51, 7296-305	5.1	66
181	An ab initio molecular orbital study of the nuclear volume effects in uranium isotope fractionations. *Journal of Chemical Physics*, **2008**, 129, 164309	3.9	66
180	Unique properties and reactivity of high-valent manganese-oxo versus manganese-hydroxo in the salen platform. *Inorganic Chemistry*, **2010**, 49, 6664-72	5.1	63
179	Relativistic study of nuclear magnetic shielding constants: mercury dihalides. *Chemical Physics Letters*, **1996**, 255, 195-202	2.5	60
178	Excited and Ionized States of p-Benzoquinone and Its Anion Radical: SAC□CI Theoretical Study. *Journal of Physical Chemistry A*, **2002**, 106, 3838-3849	2.8	55
177	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method: tin tetrahalides. *Chemical Physics Letters*, **1996**, 261, 1-6	2.5	55
176	Ground and excited states of Mg porphin studied by the SAC/SAC-CI method. *Chemical Physics Letters*, **1996**, 250, 159-164	2.5	54
175	Relativistic study of nuclear magnetic shielding constants: tungsten hexahalides and tetraoxide. *Chemical Physics Letters*, **1996**, 261, 7-12	2.5	52
174	Theoretical Study of the Chemisorption and Surface Reaction of HCOOH on a ZnO(101 0) Surface. *The Journal of Physical Chemistry*, **1996**, 100, 694-700		51

173	Theoretical study on the chemisorption of a hydrogen molecule on palladium. *Journal of the American Chemical Society*, **1987**, 109, 1902-1912	16.4	50
172	Examination of accuracy of electron□electron Coulomb interactions in two-component relativistic methods. *Chemical Physics Letters*, **2008**, 461, 327-331	2.5	49
171	Electronic excitation spectrum of thiophene studied by symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 842	3.9	49
170	Theoretical Study on the Reaction Mechanism and Regioselectivity of Silastannation of Acetylenes with a Palladium Catalyst. *Journal of the American Chemical Society*, **1994**, 116, 8754-8765	16.4	49
169	Effect of a tridentate ligand on the structure, electronic structure, and reactivity of the copper(I) nitrite complex: role of the conserved three-histidine ligand environment of the type-2 copper site in copper-containing nitrite reductases. *Journal of the American Chemical Society*, **2008**, 130, 6088-98	16.4	48
168	Interaction of a hydrogen molecule with palladium. *Journal of the American Chemical Society*, **1985**, 107, 8264-8266	16.4	48
167	Relativistic theory of the magnetic shielding constant:. *Chemical Physics Letters*, **1998**, 283, 119-124	2.5	47
166	Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study. *Journal of Chemical Physics*, **2002**, 117, 2045-2052	3.9	46
165	Application of relativistic coupled-cluster theory to the effective electric field in YbF. *Physical Review A*, **2014**, 90,	2.6	45
164	Critical role of external axial ligands in chirality amplification of trans-cyclohexane-1,2-diamine in salen complexes. *Journal of the American Chemical Society*, **2009**, 131, 12394-405	16.4	45
163	Electronic excitation and ionization spectra of azabenzenes: Pyridine revisited by the symmetry-adapted cluster configuration interaction method. *Journal of Chemical Physics*, **2001**, 114, 5117-5123	3.9	44
162	Test of mp/me changes using vibrational transitions in N2+. *Physical Review A*, **2014**, 89,	2.6	40
161	Theoretical Study on the Decomposition of HCOOH on a ZnO(1010) Surface. *Journal of Catalysis*, **1998**, 173, 53-63	7.3	38
160	Dirac□ock calculations of the magnetic shielding constants of protons and heavy nuclei in XH2 (X=O, S, Se, and Te): a comparison with quasi-relativistic calculations. *Chemical Physics Letters*, **2000**, 321, 452-458	2.5	38
159	Ground and excited states of oxyheme: SAC/SAC-CI study. *Chemical Physics Letters*, **1996**, 250, 379-386	2.5	38
158	Elimination of the Stark shift from the vibrational transition frequency of optically trapped 174Yb6Li molecules. *Physical Review A*, **2011**, 84,	2.6	37
157	Orientational effect of aryl groups on 77Se NMR chemical shifts: experimental and theoretical investigations. *Chemistry - A European Journal*, **2006**, 12, 3829-46	4.8	37
156	Relativistic calculations of ground and excited states of LiYb molecule for ultracold photoassociation spectroscopy studies. *Journal of Chemical Physics*, **2010**, 133, 124317	3.9	36

155	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method. Electronic mechanism in the aluminum compounds, A1X4□(X = H, F, Cl, Br and I). *Chemical Physics Letters*, **1996**, 249, 284-289	2.5	36
154	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method: silicon tetrahalides. *Chemical Physics Letters*, **1995**, 247, 418-424	2.5	36
153	Oxygen-atom transfer from iodosylarene adducts of a manganese(IV) salen complex: effect of arenes and anions on I(III) of the coordinated iodosylarene. *Inorganic Chemistry*, **2013**, 52, 9557-66	5.1	34
152	Relativistic effects and the halogen dependencies in the 13C chemical shifts of CH4□In, CH4□Brn, CCl4□In, and CBr4□In (n=0□4). *Journal of Computational Chemistry*, **2001**, 22, 528-536	3.5	33
151	Electronic excitation and ionization spectra of cyclopentadiene: Revisit by the symmetry-adapted cluster□onfiguration interaction method. *Journal of Chemical Physics*, **2000**, 113, 5245	3.9	32
150	Ab initio study of permanent electric dipole moment and radiative lifetimes of alkaline-earth-metal--Li molecules. *Physical Review A*, **2011**, 84,	2.6	31
149	Force in SCF theories. MC SCF and open-shell RHF theories. *Chemical Physics Letters*, **1981**, 80, 94-100	2.5	31
148	Ab initiostudy on vibrational dipole moments of XH+molecular ions: X =24Mg,40Ca,64Zn,88Sr,114Cd,138Ba,174Yb and202Hg. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2010**, 43, 245102	1.3	30
147	Ionized and excited states of ferrocene: Symmetry adapted cluster□onfiguration□nteraction study. *Journal of Chemical Physics*, **2002**, 117, 6533-6537	3.9	30
146	Theoretical study on the chemisorption and the surface reaction of HCOOH on a MgO(001) surface. *Surface Science*, **1995**, 336, 232-244	1.8	30
145	Spin-orbit effect on the magnetic shielding constant using the ab initio UHF method: gallium and indium tetrahalides. *Chemical Physics Letters*, **1995**, 235, 13-16	2.5	30
144	Electronic structures of dative metal-metal bonds; Ab initio molecular orbital calculations of (OC)5Os-M(CO)5 (M = tungsten, chromium) in comparison with (OC)5M-M(CO)5 (M = rhenium, manganese). *Inorganic Chemistry*, **1992**, 31, 1740-1744	5.1	30
143	Magnetic shielding constants calculated by the infinite-order Douglas-Kroll-Hess method with electron-electron relativistic corrections. *Journal of Chemical Physics*, **2010**, 132, 174105	3.9	29
142	Estimated accuracies of pure XH+(X: even isotopes of group II atoms) vibrational transition frequencies: towards the test of the variance inmp/me. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2011**, 44, 025402	1.3	29
141	Theoretical studies on magnetic circular dichroism by the finite perturbation method with relativistic corrections. *Journal of Chemical Physics*, **2005**, 123, 164113	3.9	29
140	Force in SCF theories. Test of the new method. *Journal of Chemical Physics*, **1982**, 77, 3109-3122	3.9	29
139	Sensitivity of vibrational spectroscopy of optically trapped SrLi and CaLi molecules to variations inmp/me. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2013**, 46, 025001	1.3	28
138	Self-Condensation Reaction of Lithium (Alkoxy)silylenoid: A Model Study by ab Initio Calculation. *Organometallics*, **1998**, 17, 4573-4577	3.8	28

137	Dirac–Hock calculations of magnetic shielding constants: hydrogen molecule and hydrogen halides. *Chemical Physics Letters*, **1999**, 310, 342-346	2.5	28
136	Expectation values in two-component relativistic theories. *Journal of Chemical Physics*, **2010**, 132, 164108	3.9	27
135	Relativistic configuration interaction and coupled cluster methods using four-component spinors: Magnetic shielding constants of HX and CH3X (X=F, Cl, Br, I). *Chemical Physics Letters*, **2005**, 408, 150-156	2.5	27
134	CO and NO adsorption on copper-containing zeolite. A theoretical ab initio study. *Catalysis Letters*, **1996**, 42, 173-176	2.8	27
133	Theoretical study on the catalytic activity of palladium for the hydrogenation of acetylene. *Surface Science*, **1987**, 185, 319-342	1.8	27
132	Synthesis, structure, and reactivity of Lewis base stabilized plumbacyclopentadienylidenes. *Chemistry - A European Journal*, **2013**, 19, 16946-53	4.8	26
131	Theoretical Study on the Molecular and Dissociative Adsorptions of H2 on a ZrO2 Surface. *The Journal of Physical Chemistry*, **1994**, 98, 11840-11845		26
130	Relativistic coupled-cluster calculation of the electron-nucleus scalar-pseudoscalar interaction constant Ws in YbF. *Physical Review A*, **2016**, 93,	2.6	25
129	Dipole polarizability of alkali-metal (Na, K, Rb)-alkaline-earth-metal (Ca, Sr) polar molecules: prospects for alignment. *Journal of Chemical Physics*, **2014**, 140, 224303	3.9	25
128	Ligand effect on uranium isotope fractionations caused by nuclear volume effects: An ab initio relativistic molecular orbital study. *Journal of Chemical Physics*, **2010**, 133, 044309	3.9	25
127	Quasirelativistic study of 125Te nuclear magnetic shielding constants and chemical shifts. *Journal of Computational Chemistry*, **2001**, 22, 1502-1508	3.5	24
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125	Topology of density difference and force analysis. *Theoretica Chimica Acta*, **1996**, 93, 67-78		24
124	Theoretical study on the ground and excited states of the chromate anion CrO_4^{2-}. *Journal of Chemical Physics*, **1994**, 101, 1029-1036	3.9	24
123	An ab initio study based on a finite nucleus model for isotope fractionation in the U(III)-U(IV) exchange reaction system. *Journal of Chemical Physics*, **2008**, 128, 144309	3.9	23
122	Experimental and Theoretical Investigation of the Role of Bismuth in Promoting the Selective Oxidation of Glycerol over Supported PtBi Catalyst under Mild Conditions. *ACS Catalysis*, **2020**, 10, 6071-6083	13.1	22
121	Chromosome aberrations induced by dual exposure of protons and iron ions. *Radiation and Environmental Biophysics*, **2007**, 46, 125-9	2	22
120	Induction of micronuclei in human fibroblasts across the Bragg curve of energetic heavy ions. *Radiation Research*, **2006**, 166, 583-9	3.1	22

119	Theoretical study on the excitation spectrum and the photofragmentation reaction of Ni(CO)4. *Journal of Chemical Physics*, **1995**, 103, 6993-6998	3.9	22
118	Relativistic effects on magnetic circular dichroism studied by GUHF/SECI method. *Chemical Physics Letters*, **2002**, 355, 219-225	2.5	21
117	Comprehensive Understanding of Structure-Controlling Factors of a Zinc Tetraphenylporphyrin Thin Film Using pMAIRS and GIXD Techniques. *Chemistry - A European Journal*, **2016**, 22, 16539-16546	4.8	20
116	Rotational Energy Barriers and Relaxation Times of the Organic Cation in Cubic Methylammonium Lead/Tin Halide Perovskites from First Principles. *Journal of Physical Chemistry C*, **2017**, 121, 14051-14059	3.8	19
115	Basis set dependence of magnetic shielding constant calculated by the Hartree-Fock/finite perturbation method. *Chemical Physics*, **1996**, 203, 159-175	2.3	19
114	Accuracy estimations of overtone vibrational transition frequencies of optically trapped 174Yb6Li molecules. *Physical Review A*, **2012**, 85,	2.6	18
113	SAC and SAC-CI calculations of excitation and circular dichroism spectra of straight-chain and cyclic dichalcogens. *Journal of Physical Chemistry A*, **2006**, 110, 10053-62	2.8	18
112	Theoretical Study on Metal NMR Chemical Shifts. Electronic Mechanism of the Xe Chemical Shift. *Bulletin of the Chemical Society of Japan*, **1996**, 69, 953-959	5.1	18
111	Anomalous Dielectric Behavior of a Pb/Sn Perovskite: Effect of Trapped Charges on Complex Photoconductivity. *ACS Photonics*, **2018**, 5, 3189-3197	6.3	17
110	Automatic High-Throughput Screening Scheme for Organic Photovoltaics: Estimating the Orbital Energies of Polymers from Oligomers and Evaluating the Photovoltaic Characteristics. *Journal of Physical Chemistry C*, **2017**, 121, 28275-28286	3.8	17
109	Synthesis and reactivity of a ruthenocene-type complex bearing an aromatic ligand with the heaviest group 14 element. *Chemical Science*, **2017**, 8, 3092-3097	9.4	16
108	Ab initio study on potential energy curves of electronic ground and excited states of 40CaH+ molecule. *Chemical Physics Letters*, **2012**, 521, 31-35	2.5	16
107	Ab initio study of ground and excited states of 6Li40Ca and 6Li88Sr molecules. *Journal of Chemical Physics*, **2013**, 138, 194307	3.9	16
106	Relativistic effect on 77Se NMR chemical shifts of various selenium species in the framework of zeroth-order regular approximation. *Journal of Physical Chemistry A*, **2011**, 115, 8721-30	2.8	16
105	Ground and excited states of singlet, cation doublet, and anion doublet states of o-benzoquinone: a theoretical study. *Journal of Physical Chemistry A*, **2007**, 111, 2634-9	2.8	16
104	Ground and excited states of carboxyheme: a SAC/SAC-CI study. *Chemical Physics Letters*, **1996**, 256, 220-228	2.3	16
103	Ab Initio MO Study of the Reaction of Pentacoordinate Allylsilicates with Aldehydes. *Chemistry Letters*, **1991**, 20, 387-390	1.7	16
102	The functional role of the structure of the dioxo-isobacteriochlorin in the catalytic site of cytochrome cd for the reduction of nitrite. *Chemical Science*, **2016**, 7, 2896-2906	9.4	16

101	Experimental and theoretical studies of the porphyrin ligand effect on the electronic structure and reactivity of oxoiron(iv) porphyrin π-cation-radical complexes. *Journal of Biological Inorganic Chemistry*, **2019**, 24, 483-494	3.7	15
100	Calculations of nuclear magnetic shielding constants based on the exact two-component relativistic method. *Journal of Chemical Physics*, **2017**, 147, 154104	3.9	14
99	Di-μ-oxo dimetal core of Mn(IV) and Ti(IV) as a linker between two chiral salen complexes leading to the stereoselective formation of different M- and P-helical structures. *Inorganic Chemistry*, **2014**, 53, 1070-9	5.1	14
98	Theoretical Study on Rotational Controllability of Organic Cations in Organic–Inorganic Hybrid Perovskites: Hydrogen Bonds and Halogen Substitution. *Journal of Physical Chemistry C*, **2017**, 121, 26188-26195	3.8	14
97	Quasi-Relativistic Study of 199Hg Nuclear Magnetic Shielding Constants of Dimethylmercury, Disilylmercury and Digermylmercury. *Journal of Physical Chemistry A*, **2001**, 105, 128-133	2.8	14
96	Characterizing of variation in the proton-to-electron mass ratio via precise measurements of molecular vibrational transition frequencies. *Journal of Molecular Spectroscopy*, **2014**, 300, 99-107	1.3	13
95	Effects of ambient pressure on Cu Kα X-ray radiation with millijoule and high-repetition-rate femtosecond laser. *Applied Physics B: Lasers and Optics*, **2010**, 99, 173-179	1.9	13
94	Applicability of the lowest-order two-electron Breit–Pauli relativistic correction in many-electron heavy and super-heavy elements. *Chemical Physics Letters*, **2007**, 442, 134-139	2.5	13
93	Quantum-chemical calculations for paramagnetic 13C NMR chemical shifts of iron-bound cyanide ions of iron porphyrins in ground and low-lying excited states containing ferric (dxy)2(dxz,yz)3 and (dxy)1(dxz,yz)4 configurations. *Journal of the American Chemical Society*, **2004**, 126, 486-7	16.4	13
92	Does the Schrock-type metallasilylene complex exist?. *Chemical Physics Letters*, **1992**, 196, 404-409	2.5	13
91	Theoretical study on the methane activation reactions by Pt, Pt+, and Pt− atoms. *Computational and Theoretical Chemistry*, **1993**, 281, 207-212		13
90	Exploring the Relationship between Effective Mass, Transient Photoconductivity, and Photocatalytic Activity of SrxPb1−xBiO2Cl (x = 0−1) Oxyhalides. *Chemistry of Materials*, **2020**, 32, 4166-4173	9.6	12
89	Theoretical Insights into the Electronic Structures and Stability of Dimetallofullerenes M2@Ih-C80. *Journal of Physical Chemistry C*, **2017**, 121, 18169-18177	3.8	12
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87	Enhancement factors of parity- and time-reversal-violating effects for monofluorides. *Physical Review A*, **2018**, 98,	2.6	12
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84	Magnetic-field effects in transitions of X Li molecules (X: even isotopes of group II atoms). *Physical Review A*, **2011**, 84,	2.6	11

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82	Theoretical Study on Metal NMR Chemical Shifts. Arsenic and Antimony Compounds. *The Journal of Physical Chemistry*, **1995**, 99, 7951-7957		11
81	Analysis of large effective electric fields of weakly polar molecules for electron electric-dipole-moment searches. *Physical Review A*, **2017**, 95,	2.6	10
80	Relativistic quantum-chemical calculations of magnetizabilities of noble gas atoms using the Douglas□Kroll□Hess method. *Chemical Physics Letters*, **2008**, 458, 223-226	2.5	10
79	Theoretical Study of the Transition Energies of the Visible Absorption Spectra of [RhCl6]3□and [RhCl5(H2O)]2□Complexes in Aqueous Solution. *Bulletin of the Chemical Society of Japan*, **1995**, 68, 1601-1605	5.1	10
78	First-Principles Calculations of the Rotational Motion and Hydrogen Bond Capability of Large Organic Cations in Hybrid Perovskites. *Journal of Physical Chemistry C*, **2018**, 122, 15966-15972	3.8	9
77	Inverted Sandwich Rh Complex Bearing a Plumbole Ligand and Its Catalytic Activity. *Organometallics*, **2019**, 38, 3099-3103	3.8	9
76	Infrared spectra and chemical abundance of methyl propionate in icy astrochemical conditions. *Monthly Notices of the Royal Astronomical Society*, **2015**, 448, 1372-1377	4.3	9
75	Excited states of four hemes in a c-type cytochrome subunit of the photosynthetic reaction center of Rhodopseudomonas viridis: SAC-CI calculations. *Journal of Porphyrins and Phthalocyanines*, **2001**, 05, 256-266	1.8	9
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73	Time-dependent DFT study of the K-edge spectra of vanadium and titanium complexes: effects of chloride ligands on pre-edge features. *Physical Chemistry Chemical Physics*, **2020**, 22, 674-682	3.6	9
72	Merits of heavy-heavy diatomic molecules for electron electric-dipole-moment searches. *Physical Review A*, **2019**, 99,	2.6	8
71	Correlating Magnetic Exchange in Dinuclear Bis(phenolate)-Bridged Complexes: A Computational Perspective. *Bulletin of the Chemical Society of Japan*, **2016**, 89, 657-665	5.1	8
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69	Substitution effects on olefin epoxidation catalyzed by Oxoiron(IV) porphyrin □cation radical complexes: A dft study. *Journal of Computational Chemistry*, **2019**, 40, 1780-1788	3.5	7
68	Quantum-chemical analyses of aromaticity, UV spectra, and NMR chemical shifts in plumbacyclopentadienylidenes stabilized by Lewis bases. *Journal of Computational Chemistry*, **2014**, 35, 847-53	3.5	7
67	The Electronic Spectra of Ethylene. *Bulletin of the Chemical Society of Japan*, **1996**, 69, 1901-1906	5.1	7
66	High coordinate germanium and tin complexes in the allylation reactions of aldehydes. *Organometallics*, **1993**, 12, 3398-3404	3.8	7

65	Alternative materials for perovskite solar cells from materials informatics. *Physical Review Materials*, **2019**, 3,	3.2	7
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61	An ab initio study of nuclear volume effects for isotope fractionations using two-component relativistic methods. *Journal of Computational Chemistry*, **2015**, 36, 816-20	3.5	6
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59	The Douglas–Kroll–Hess method based on vector-potential-including Foldy–Wouthuysen transformation: Application to NMR shielding tensor. *Chemical Physics Letters*, **2013**, 580, 145-151	2.5	6
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50	A theoretical study on the size-dependence of ground-state proton transfer in phenol-ammonia clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 3265-3276	3.6	5
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48	Gauge-origin dependence of NMR shielding constants in the Douglas–Kroll–Hess method. *Chemical Physics Letters*, **2015**, 618, 132-141	2.5	4

47	Spin□orbit effect on the magnetic shielding constant using the ab initio UHF method: silicon tetrahalides. *Chemical Physics Letters*, **1995**, 247, 418-424	2.5	4
46	Reply to □omment on □orce in SCF theories□□*Journal of Chemical Physics*, **1983**, 79, 2493-2495	3.9	4
45	Catalytic Reactions of Transition Metal Clusters and Surfaces From Ab-Initio Theory **1992**, 251-285		4
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