Koichi Ohno

List of Publications by Year
in descending order

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267	7,133	70961	85405
papers	citations	41 h-index	71 g-index

270	270	270	4019
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Systematic exploration of the mechanism of chemical reactions: the global reaction route mapping (GRRM) strategy using the ADDF and AFIR methods. Physical Chemistry Chemical Physics, 2013, 15, 3683.	1.3	456
2	A scaled hypersphere search method for the topography of reaction pathways on the potential energy surface. Chemical Physics Letters, 2004, 384, 277-282.	1.2	360
3	Global Mapping of Equilibrium and Transition Structures on Potential Energy Surfaces by the Scaled Hypersphere Search Method:â€‰ Applications to ab Initio Surfaces of Formaldehyde and Propyne Molecules. Journal of Physical Chemistry A, 2005, 109, 5742-5753.	1.1	310
4	Global Reaction Route Mapping on Potential Energy Surfaces of Formaldehyde, Formic Acid, and Their Metal-Substituted Analogues. Journal of Physical Chemistry A, 2006, 110, 8933-8941.	1.1	270
5	Study of electron distributions of molecular orbitals by Penning ionization electron spectroscopy. Journal of the American Chemical Society, 1983, 105, 4555-4561.	6.6	187
6	Stateâ€resolved collision energy dependence of Penning ionization cross sections for N2and CO2by He*23S. Journal of Chemical Physics, 1991, 94, 2675-2687.	1.2	138
7	Updated Branching Plane for Finding Conical Intersections without Coupling Derivative Vectors. Journal of Chemical Theory and Computation, 2010, 6, 1538-1545.	2.3	137
8	Raman spectra of polycyclic aromatic hydrocarbons. Comparison of calculated Raman intensity distributions with observed spectra for naphthalene, anthracene, pyrene, and perylene. Journal of Molecular Structure, 1998, 442, 221-234.	1.8	130
9	Structures of Water Octamers (H2O)8:â€‰ Exploration on Ab Initio Potential Energy Surfaces by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 4527-4534.	1.1	118
10	Kinetic energy dependence of partial cross sections for the collisional ionization of H2O, H2S, O2, and Ar with He(2â€‰3S) metastable atoms. Journal of Chemical Physics, 1989, 91, 1618-1625.	1.2	111
11	Computational Study of Titanocene-Catalyzed Dehydrocoupling of the Adduct Me2NHÂ·BH3:Â An Intramolecular, Stepwise Mechanism. Organometallics, 2007, 26, 3597-3600.	1.1	106
12	Automated Global Mapping of Minimal Energy Points on Seams of Crossing by the Anharmonic Downward Distortion Following Method: A Case Study of H₂CO. Journal of Physical Chemistry A, 2009, 113, 1704-1710.	1.1	92
13	From Roaming Atoms to Hopping Surfaces: Mapping Out Global Reaction Routes in Photochemistry. Journal of the American Chemical Society, 2015, 137, 3433-3445.	6.6	91
14	Collisionâ€energy/electronâ€energy resolved twoâ€dimensional study of Penning ionization of Ar by He metastable atoms 23Sand 21S. Journal of Chemical Physics, 1996, 105, 7536-7542.	1.2	82
15	Exterior electron model for Penning ionization. Unsaturated hydrocarbons. Journal of Chemical Physics, 1984, 81, 4447-4454.	1.2	80
16	Penning ionization of (CH3)4C and (CH3)3CCl by collision with He*(2â€‰3S) metastable atoms. Journal of Chemical Physics, 1991, 95, 918-929.	1.2	80
17	Collision energyâ€resolved Penning ionization electron spectra of unsaturated hydrocarbons with He*(2â€‰3S) metastable atoms. Journal of Chemical Physics, 1992, 96, 6523-6530.	1.2	73
18	Penning Ionization of HCHO, CH2CH2, and CH2CHCHO by Collision with He(23S) Metastable Atoms. The Journal of Physical Chemistry, 1995, 99, 14247-14253.	2.9	73

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19	The Rise of Catalyst Informatics: Towards Catalyst Genomics. ChemCatChem, 2019, 11, 1146-1152.	1.8	72
20	A new approach for finding a transition state connecting a reactant and a product without initial guess: applications of the scaled hypersphere search method to isomerization reactions of HCN, (H2O)2, and alanine dipeptide. Chemical Physics Letters, 2005, 404, 95-99.	1.2	66
21	Quantum Chemistry Study of H⁺(H₂O)₈:â€‰ A Global Search for Its Isomers by the Scaled Hypersphere Search Method, and Its Thermal Behavior. Journal of Physical Chemistry A, 2007, 111, 10732-10737.	1.1	65
22	Water-catalyzed gas-phase reaction of formic acid with hydroxyl radical: A computational investigation. Chemical Physics Letters, 2009, 469, 57-61.	1.2	64
23	Collision-Energy-Resolved Penning Ionization Electron Spectroscopy of Nitriles:â€‰ Conjugation Effects on Interactions with He*(23S) Metastable Atoms. Journal of Physical Chemistry A, 1997, 101, 5038-5045.	1.1	60
24	An Automated and Systematic Transition Structure Explorer in Large Flexible Molecular Systems Based on Combined Global Reaction Route Mapping and Microiteration Methods. Journal of Chemical Theory and Computation, 2009, 5, 2734-2743.	2.3	60
25	A Theoretical Study on the Photodissociation of Acetone: Insight into the Slow Intersystem Crossing and Exploration of Nonadiabatic Pathways to the Ground State. Journal of Physical Chemistry Letters, 2010, 1, 1841-1845.	2.1	58
26	Defect-Induced Vibration Modes of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mi>Ar</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math>-Irradiated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Applied, 2017, 7, .	1.5	58
27	Global Investigation on the Potential Energy Surface of CH3CN:â€‰ Application of the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2005, 109, 7319-7328.	1.1	57
28	Systematic Search for Isomerization Pathways of Hexasilabenzene for Finding Its Kinetic Stability. Organometallics, 2009, 28, 2218-2224.	1.1	56
29	Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics. Chemical Science, 2015, 6, 2746-2753.	3.7	56
30	Synthesis and structure of stable base-free dialkylsilanimines. New Journal of Chemistry, 2010, 34, 1637.	1.4	55
31	Phonon dispersions of hydrogenated and dehydrogenated carbon nanoribbons. Physical Review B, 2008, 77, .	1.1	54
32	Penning Ionization of Thiophene, Furan, and Pyrrole by Collision with He*(23S) Metastable Atoms. The Journal of Physical Chemistry, 1996, 100, 8204-8211.	2.9	51
33	No activation barrier synthetic route of glycine from simple molecules (NH3, CH2, and CO2) via carboxylation of ammonium ylide: a theoretical study by the scaled hypersphere search method. Chemical Physics Letters, 2004, 398, 240-244.	1.2	50
34	Vibrational Analysis of Electronic Transition Bands of Coronene. Bulletin of the Chemical Society of Japan, 1972, 45, 996-1004.	2.0	48
35	Insight into Global Reaction Mechanism of [C2, H4, O] System from ab Initio Calculations by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 5099-5110.	1.1	48
36	Lowest Transition State for the Chirality-Determining Step in Ru((R)-BINAP)-Catalyzed Asymmetric Hydrogenation of Methyl-3-Oxobutanoate. Journal of the American Chemical Society, 2008, 130, 17228-17229.	6.6	48

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37	Normal coordinate calculations of benzenoid hydrocarbons. Journal of Molecular Spectroscopy, 1979, 77, 329-348.	0.4	47
38	Aromaticity of Giant Polycyclic Aromatic Hydrocarbons with Hollow Sites: Super Ring Currents in Super-Rings. Chemistry - A European Journal, 2006, 12, 5757-5769.	1.7	47
39	Penning ionization electron spectroscopy of nitriles. The Journal of Physical Chemistry, 1984, 88, 206-209.	2.9	44
40	A simple predictive model for planar vibrations of polycyclic benzenoid hydrocarbons. Journal of Chemical Physics, 1991, 95, 5524-5538.	1.2	44
41	Automated exploration of stable isomers of H⁺(H₂O)_n (n = 5â€“7) via ab initio calculations: An application of the anharmonic downward distortion following algorithm. Journal of Computational Chemistry, 2009, 30, 952-961.	1.5	44
42	Variations in reactivity of lone-pair electrons due to intramolecular hydrogen bonding as observed by Penning ionization electron spectroscopy. Journal of the American Chemical Society, 1985, 107, 8078-8082.	6.6	42
43	Classical trajectory calculations of collision energy dependence of total and partial Penning ionization cross sections for He*(23S)+N2â†'He+N2++eâ^'. Journal of Chemical Physics, 1999, 110, 3773-3780.	1.2	41
44	Anharmonic Downward Distortion Following for Automated Exploration of Quantum Chemical Potential Energy Surfaces. Bulletin of the Chemical Society of Japan, 2014, 87, 1315-1334.	2.0	41
45	Normal coordinate calculations of benzenoid hydrocarbons. Journal of Molecular Spectroscopy, 1978, 72, 238-251.	0.4	39
46	Penning Ionization of CH3OH, (CH3)2O, and (CH3CH2)2O by Collision with He(23S) Metastable Atoms. The Journal of Physical Chemistry, 1995, 99, 17093-17099.	2.9	36
47	Collision Energy Resolved Penning Ionization Electron Spectroscopy of Azines:â€‰Anisotropic Interaction of Azines with He*(23S) Atoms and Assignments of Ionic States. Journal of Physical Chemistry A, 2000, 104, 6940-6950.	1.1	35
48	Conversion pathways between a fullerene and a ring among C20 clusters by a sphere contracting walk method: Remarkable difference in local potential energy landscapes around the fullerene and the ring. Journal of Chemical Physics, 2006, 124, 174306.	1.2	35
49	Intramolecular vibrational frequencies of water clusters (H2O)nâ€^(n=2â€“5): Anharmonic analyses using potential functions based on the scaled hypersphere search method. Journal of Chemical Physics, 2008, 129, 074315.	1.2	35
50	Study of stereochemical properties of molecular orbitals by Penning ionization electron spectroscopy. Effects of through-space/through-bond interactions on electron distributions. Journal of the American Chemical Society, 1985, 107, 8082-8086.	6.6	34
51	Two-Dimensional Penning Ionization Electron Spectroscopy of NNO, HCNO, and HNNN:Â Electronic Structure and the Interaction Potential with He*(23S) Metastable and Li(22S) Ground State Atoms. Journal of Physical Chemistry A, 1999, 103, 6746-6756.	1.1	34
52	Exterior Characteristics of Molecular Orbitals and Molecular Surfaces as Studied by Atomic Probes. Bulletin of the Chemical Society of Japan, 2004, 77, 887-908.	2.0	32
53	Global analysis of reaction pathways on the potential energy surface of cyanoacetylene by the scaled hypersphere search method. Chemical Physics Letters, 2006, 418, 208-216.	1.2	32
54	Molecular vibrations of [n]oligoacenes (n=2â^'5 and 10) and phonon dispersion relations of polyacene. Journal of Chemical Physics, 2007, 126, 064904.	1.2	32

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55	Global reaction route mapping on potential energy surfaces of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/. Chemical Physics Letters, 2007, 447, 21-26.	1.2	32
56	A new global reaction route map on the potential energy surface of H2CO with unrestricted level. Chemical Physics Letters, 2008, 460, 55-58.	1.2	32
57	Penning Ionization of CH3CN and CH3NC by Collision with He(23S) Metastable Atoms. The Journal of Physical Chemistry, 1995, 99, 14678-14685.	2.9	31
58	A highly sensitive electron spectrometer for crossed-beam collisional ionization: A retarding-type magnetic bottle analyzer and its application to collision-energy resolved Penning ionization electron spectroscopy. Review of Scientific Instruments, 2000, 71, 3042-3049.	0.6	31
59	Microsolvation of Hydrogen Sulfide:â€‰ Exploration of H₂SÂ·(H₂O)_n and SH⁻Â·H₃O⁺Â·(H₂O)_n₋₁ (n = 5â^7) Cluster Structures on Ab Initio Potential Energy Surfaces by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2008, 112, 2962-2968.	1.1	31
60	Finding important anharmonic terms in the sixth-order potential energy function by the scaled hypersphere search method: An application to vibrational analyses of molecules and clusters. Journal of Chemical Physics, 2008, 128, 144111.	1.2	31
61	On the asymptotic behavior of Hartree-Fock orbitals. Theoretica Chimica Acta, 1992, 81, 355-364.	0.9	30
62	Collision energy resolved Penning ionization electron spectra of polycyclic aromatic hydrocarbons. Journal of Electron Spectroscopy and Related Phenomena, 1998, 88-91, 155-161.	0.8	30
63	A new method for constructing multidimensional potential energy surfaces by a polar coordinate interpolation technique. Chemical Physics Letters, 2003, 381, 177-186.	1.2	30
64	Anthryl-Substituted 3-Silylene-2-silaaziridine Obtained by Isomerization of Disilacyclopropanimine: An Exocyclic Silene Showing a Distinct Intramolecular Charge Transfer Transition. Journal of the American Chemical Society, 2013, 135, 10606-10609.	6.6	30
65	Assignment of photoelectro bands for naphthalene and anthracene by penning ionization electron spectroscopy. Chemical Physics Letters, 1981, 83, 243-245.	1.2	29
66	Penning ionization of [2,2]-paracyclophane by collision with metastable He*(23S) atoms. Chemical Physics Letters, 2000, 322, 189-198.	1.2	29
67	Exploring Multiple Potential Energy Surfaces: Photochemistry of Small Carbonyl Compounds. Advances in Physical Chemistry, 2012, 2012, 1-13.	2.0	29
68	Observation of structural change in organic monolayer film by penning ionization electron spectroscopy: Fe-phthalocyanine on graphite. Surface Science, 1984, 147, 356-360.	0.8	28
69	Penning ionization of substituted benzenes (aniline, phenol and thiophenol) by collision with He*(23S) metastable atoms. Journal of Electron Spectroscopy and Related Phenomena, 2000, 113, 35-48.	0.8	28
70	Two-Dimensional Penning Ionization Electron Spectroscopy of Monohalogenobenzenes by He*(23S):â€‰ C6H5X (X = F, Cl, Br, I). Journal of Physical Chemistry A, 2001, 105, 4189-4199.	1.1	28
71	Probing the Shape and Stereochemistry of Molecular Orbitals in Locally Flexible Aromatic Chains:â€‰ A Penning Ionization Electron Spectroscopy and Green's Function Study of the Electronic Structure of Biphenyl. Journal of Physical Chemistry A, 2005, 109, 10535-10546.	1.1	28
72	Two-dimensional penning ionization electron spectrum of N2 by collision with He*(23S) metastable atoms. Journal of Electron Spectroscopy and Related Phenomena, 1998, 88-91, 143-147.	0.8	26

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73	Photoionization and density functional study of clusters of alkali metal atoms solvated with acetonitrile molecules, M(CH3CN) (M=Li and Na). Chemical Physics Letters, 1999, 301, 356-364.	1.2	26
74	Ab initio Studies on Synthetic Routes of Glycine from Simple Molecules via Ammonolysis of Acetolactone: Applications of the Scaled Hypersphere Search Method. Chemistry Letters, 2004, 33, 1372-1373.	0.7	26
75	Penning electron spectrum of ferrocene. evidence for steric effect on the electronic interaction causing penning ionization. Chemical Physics Letters, 1981, 84, 6-8.	1.2	25
76	Penning ionization electron spectroscopy of molecules containing the C = O group. Aldehydes and carboxylic acids. The Journal of Physical Chemistry, 1986, 90, 2015-2019.	2.9	25
77	Penning ionization of thiocyanatomethane, isocyanatomethane, and isothiocyanatomethane by collision with helium*(23S) metastable atoms. The Journal of Physical Chemistry, 1993, 97, 12718-12724.	2.9	25
78	Penning Ionization of CH3SCH3, CH3SSCH3, and CH3CH2SH by Collision with He*(23S) Metastable Atoms. Journal of Physical Chemistry A, 1997, 101, 3284-3292.	1.1	25
79	Two-Dimensional Penning Ionization Electron Spectroscopy of Adamantanes and Cyclohexanes:â€‰ Electronic Structure of Adamantane, 1-Chloroadamantane, Cyclohexane, and Chlorocyclohexane and Interaction Potential with He*(23S). Journal of Physical Chemistry A, 2002, 106, 6541-6553.	1.1	25
80	A scaled hypersphere interpolation technique for efficient construction of multidimensional potential energy surfaces. Chemical Physics Letters, 2005, 414, 265-270.	1.2	25
81	Automated Exploration of Adsorption Structures of an Organic Molecule on RuH₂â^'BINAP by the ONIOM Method and the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 13168-13171.	1.1	25
82	Orientation of benzene molecules adsorbed on graphite as studied by penning ionization electron spectroscopy. Chemical Physics, 1984, 87, 399-403.	0.9	24
83	Large Raman-scattering activities for the low-frequency modes of substituted benzenes: Induced polarizability and stereo-specific ring-substituent interactions. Journal of Chemical Physics, 2006, 124, 104301.	1.2	24
84	Polarized absorption, fluorescence and phosphorescence spectra of coronene in triphenylene matrix at 4.2 Â°K. Chemical Physics Letters, 1973, 23, 561-566.	1.2	23
85	Electronic Spectra of Perylene and Coronene Evaporated Films as a Function of Their Crystallinity. Bulletin of the Chemical Society of Japan, 1976, 49, 418-422.	2.0	23
86	A study of excited state molecular vibrations of aromatic hydrocarbons. Chemical Physics Letters, 1979, 64, 560-566.	1.2	23
87	Penning Ionization of Dichloroethylenes by Collision with He*(23S) Metastable Atoms. The Journal of Physical Chemistry, 1995, 99, 9687-9693.	2.9	23
88	Classical Trajectory Calculations of Collision Energy Dependence of Partial Penning Ionization Cross Sections for He*(23S) + CH3CN â†' He + CH3CN++ e-. Journal of Physical Chemistry A, 1999, 103, 9925-9930.	1.1	23
89	Novel series of giant polycyclic aromatic hydrocarbons: electronic structure and aromaticity. Chemical Physics Letters, 2004, 385, 512-518.	1.2	23
90	Simple calculations of Franck-Condon factors for electronic transition bands of polyacenes. Chemical Physics Letters, 1978, 53, 571-577.	1.2	22

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91	Highly disordered amorphous selenium studied by ultraviolet photoemission spectroscopy. Physical Review B, 1980, 21, 3399-3404.	1.1	22
92	Penning Ionization of Cyclic Ethers by Collision with He*(23S) Metastable Atoms. Journal of Physical Chemistry A, 1997, 101, 6184-6194.	1.1	22
93	Classical trajectory calculations for collision-energy/electron-energy resolved two-dimensional Penning ionization electron spectra of N2, CO, and CH3CN with metastable He*(2â€Š3S) atoms. Journal of Chemical Physics, 2002, 117, 5707-5721.	1.2	22
94	Study of radiative properties of the phosphorescent coronene in n-octane by microwave induced delayed phosphorescence. Chemical Physics Letters, 1975, 33, 293-297.	1.2	21
95	Penning Ionization of (NH2)2CX (X = O, S) with He*(23S) Metastable Atoms. Difference of Anisotropic Interaction around N, O, and S Atoms. Journal of Physical Chemistry A, 2000, 104, 1393-1399.	1.1	21
96	Intracluster multiple trimeric cyclization of acrylonitrile clusters initiated by electron transfer from a potassium atom: Size-dependent pathways in metastable dissociation of K+(CH2=CHCN)n photoions. Journal of Chemical Physics, 2002, 117, 5209-5220.	1.2	21
97	Long-Range Migration of a Water Molecule To Catalyze a Tautomerization in Photoionization of the Hydrated Formamide Cluster. Journal of Physical Chemistry A, 2010, 114, 11896-11899.	1.1	21
98	Vibronic calculations in aromatic hydrocarbons. Chemical Physics Letters, 1980, 70, 526-531.	1.2	20
99	Application of Penning ionization electron spectroscopy to stereochemistry. Steric shielding effect of methyl groups on Penning ionization in substituted anilines. The Journal of Physical Chemistry, 1982, 86, 440-441.	2.9	20
100	Penning ionization electron spectroscopy of C2H5X (X = NH2, OH, SH, Cl, I). Relative reactivity of orbitals localizing on functional groups upon electrophilic attack by metastable helium atoms. The Journal of Physical Chemistry, 1983, 87, 4346-4348.	2.9	20
101	Penning ionization electron spectroscopy of Group IVB tetramethyl compounds: (CH3)4M (M = C, Si,) Tj ETQq1 1 0.784314 rgBT /Ov	2.9	20
102	Determination of outer molecular orbitals by collisional ionization experiments and comparison with Hartree-Fock, Kohn-Sham, and Dyson orbitals. Physical Review A, 2007, 75, .	1.0	20
103	Observation of anisotropic interactions between metastable atoms and target molecules by two-dimensional collisional ionization electron spectroscopy. International Reviews in Physical Chemistry, 2007, 26, 93-138.	0.9	20
104	Potential Energy Surface-Based Automatic Deduction of Conformational Transition Networks and Its Application on Quantum Mechanical Landscapes of<scp>d</scp>-Glucose Conformers. Journal of Chemical Theory and Computation, 2016, 12, 5293-5308.	2.3	20
105	Study of wave function tails and reactivity from exterior electron model. Journal of Chemical Physics, 1984, 81, 2183-2184.	1.2	19
106	Basis-Set dependence of exterior electron distributions of molecular orbitals. International Journal of Quantum Chemistry, 1986, 29, 677-688.	1.0	19
107	An overlap expansion method for improvingab initiomodel potentials: Anisotropic intermolecular potentials of N2, CO, and C2H2 with He*(2â€Š3S). Journal of Chemical Physics, 2004, 120, 781-790.	1.2	19
108	Application of Penning ionization electron spectroscopy to the study of chemical reactions on the solid surface; Photooxidation of naphthacene and rubrene. Surface Science, 1982, 115, L128-L132.	0.8	18

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109	Angular distributions of electrons emitted by collisional ionization of hydrogen sulfide and argon with helium metastable atom. The Journal of Physical Chemistry, 1989, 93, 3062-3068.	2.9	18
110	Dâ€“L Conversion Pathways between Optical Isomers of Alanine: Applications of the Scaled Hypersphere Search Method to Explore Unknown Reaction Routes in a Chiral System. Chemistry Letters, 2006, 35, 492-493.	0.7	18
111	Isolable 2,3â€Disilaâ€1,3â€butadiene from a Double Silaâ€Peterson Reaction. Chemistry - A European Journal, 2014, 20, 9424-9430.	1.7	18
112	Reply to the â€˜Comment on â€œTheoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamicsâ€â€™ by E. M. Cabaleiro-Lago, J. Rodriguez-Otero and A. Gil, Chem. Sci., 2016, 7, DOI: 10.1039/C5SC04676A. Chemical Science, 2016, 7, 2929-2932.	3.7	17
113	Application of Penning ionization electron spectroscopy to assignments of electron spectroscopic bands of anthracene. Journal of the Chemical Society Perkin Transactions II, 1988, , 507.	0.9	16
114	Penning ionization of vinyl chloride and vinyl iodide by collision with He*(23S) metastable atoms. Journal of Electron Spectroscopy and Related Phenomena, 1999, 104, 145-154.	0.8	16
115	Strong Raman activities of low frequency vibrational modes in alkylbenzenes: conformation specific Ïƒâ€“Ï€ interactions between alkyl chain and benzene ring. Chemical Physics Letters, 2001, 342, 207-219.	1.2	16
116	A study of Franckâ€”Condon envelopes of the photoelectron bands of polycyclic aromatic hydrocarbons. Chemical Physics, 1979, 37, 63-74.	0.9	15
117	Theoretical synthesis of vibrational spectra of polycyclic aromatic hydrocarbons. Infrared spectra of coronene. Journal of Molecular Structure, 1995, 352-353, 475-479.	1.8	15
118	Penning Ionization of Cyclopropanes by Collision with He*(23S) Metastable Atoms. Journal of Physical Chemistry A, 1997, 101, 3887-3894.	1.1	15
119	Penning ionization of amides by collision with He*(23S) metastable atoms. Journal of Electron Spectroscopy and Related Phenomena, 2001, 114-116, 183-190.	0.8	15
120	Penning ionization electron spectroscopy of C6H6 by collision with He*(2â€Š3S) metastable atoms and classical trajectory calculations: Optimization ofab initiomodel potentials. Journal of Chemical Physics, 2005, 122, 044303.	1.2	15
121	Photodissociation of Mg+â€“XCH3 (X=F, Cl, Br, and I) complexes. I. Electronic spectra and dissociation pathways. Journal of Chemical Physics, 2006, 125, 094309.	1.2	15
122	Global exploration of isomers and isomerization channels on the quantum chemical potential energy surface of H₃CNO₃. Journal of Computational Chemistry, 2017, 38, 669-687.	1.5	15
123	Penning ionization electron spectroscopy of diphenyl chalcogenides: PhOPh, PhSPh, and PhSePh. Journal of Organic Chemistry, 1989, 54, 540-544.	1.7	14
124	Penning Ionization Electron Spectroscopic and Ab Initio Study of the Interaction and Ionization of HNCO and HNCS with He*(23S) Metastable and Li(22S) Ground State Atoms. Journal of Physical Chemistry A, 1999, 103, 9195-9203.	1.1	14
125	Collision-energy-resolved Penning ionization electron spectroscopy of OCS with He*(23S) metastable atoms. Chemical Physics Letters, 2003, 379, 332-339.	1.2	14
126	A systematic study on the RuHClâ€“BINAP-catalyzed asymmetric hydrogenation mechanism by the global reaction route mapping methodâ€ . Journal of Molecular Catalysis A, 2010, 324, 133-140.	4.8	14

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127	Prism-C2n carbon dimer, trimer, and nano-sheets: A quantum chemical study. Chemical Physics Letters, 2015, 633, 120-125.	1.2	14
128	Absorption Spectra of Gaseous Benzo[g,h,i]perylene and Coronene. Bulletin of the Chemical Society of Japan, 1970, 43, 2435-2439.	2.0	13
129	Photoelectron and penning ionization electron spectroscopic investigation of trimethylsilyl- and t-butyl-thiophenes. Journal of Organometallic Chemistry, 1983, 252, 121-125.	0.8	13
130	Outer Shape of Molecules as Probed by Ground-State Atoms from H to Ar. Journal of the American Chemical Society, 1997, 119, 8276-8284.	6.6	13
131	Anisotropic Interaction of Halogen Atom in C2H5X (X = Cl, F) with He*(23S) As Probed by Two-Dimensional Penning Ionization Electron Spectroscopy. Journal of Physical Chemistry A, 2001, 105, 6378-6385.	1.1	13
132	Penning Ionization â€" The Outer Shape of Molecules. , 1991, , 199-233.		13
133	Effect of HOMO Levels on Chemiionization of Substituted Ethylenes by Metastable Helium Atoms. Chemistry Letters, 1997, 26, 269-270.	0.7	12
134	Trajectory calculations of two-dimensional Penning ionization electron spectra of N2 in collision with metastable He*23S atoms. Chemical Physics Letters, 2000, 332, 167-174.	1.2	12
135	Photoionization and density functional theory study of clusters of acetone containing an alkali metal atom, M((CH3)2CO)n (M=Li, Na): intracluster electron transfer from metal to acetone in 1:1 complexes. Chemical Physics Letters, 2000, 316, 442-448.	1.2	12
136	Intracluster Anionic Oligomerization of Acrylic Ester Molecules Initiated by Electron Transfer from an Alkali Metal Atom. Journal of the American Chemical Society, 2001, 123, 683-690.	6.6	12
137	Spinâ^'Orbit Coupling Effect and Intramolecular Orbital Interactions:Â Penning Ionization of CH2BrCl, CHBrCl2, and CH2BrCN by Collision with He*(23S) Metastable Atoms. Journal of Physical Chemistry A, 2003, 107, 2137-2147.	1.1	12
138	Two-Dimensional Penning Ionization Electron Spectroscopy of 2-Aminoethanol and Related Molecules by He*(23S) Atoms:â€‰ Influence of Intramolecular Hydrogen Bonding on Collisional Ionization. Journal of Physical Chemistry A, 2004, 108, 4211-4218.	1.1	12
139	DFT Study on Isomerization and Decomposition of Cuprous Dialkyldithiophosphate and Its Reaction with Alkylperoxy Radical. Journal of Physical Chemistry A, 2008, 112, 5720-5726.	1.1	12
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