Majdi Hochlaf

List of Publications by Year
in descending order

278	3,815	172457	276875
papers	citations	29 h-index	41 g-index

282	282	282	2505
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Carbon dioxide adsorption and activation on ionic liquid decorated Au(111) surface: A DFT study. Chemosphere, 2022, 286, 131612.	8.2	13
2	Identification of a Grotthuss proton hopping mechanism at protonated polyhedral oligomeric silsesquioxane (POSS) â€“ water interface. Journal of Colloid and Interface Science, 2022, 605, 701-709.	9.4	9
3	Corrosion inhibition of mild steel by aminobenzoic acid isomers in hydrochloric acid solution: Efficiency and adsorption mechanisms. Applied Surface Science, 2022, 576, 151780.	6.1	19
4	Collisional Excitation and Non-LTE Modeling of Interstellar Chiral Propylene Oxide. Astrophysical Journal, 2022, 926, 3.	4.5	4
5	Theoretical treatment of IOâ€“X (X = N₂, CO, CO₂, H₂O) complexes. Physical Chemistry Chemical Physics, 2022, 24, 7203-7213.	2.8	0
6	A Computational Approach to Nontraditional Intrinsic Luminescence: Vibrationally Resolved Absorption and Fluorescence Spectra of DABCO. Journal of Physical Chemistry A, 2022, 126, 1094-1102.	2.5	0
7	Editorial: Theoretical Characterization of Astrophysical Species. Frontiers in Astronomy and Space Sciences, 2022, 9, .	2.8	0
8	Accounting for molecular flexibility in photoionization: case of tert-butyl hydroperoxide. Physical Chemistry Chemical Physics, 2022, 24, 10826-10837.	2.8	3
9	Ultrafast CO₂ photodissociation in the energy region of the lowest Rydberg series. Physical Chemistry Chemical Physics, 2022, 24, 14072-14084.	2.8	3
10	Chemistry deriving from OOQOOH radicals in alkane low-temperature oxidation: A first combined theoretical and electron-ion coincidence mass spectrometry study. Proceedings of the Combustion Institute, 2021, 38, 309-319.	3.9	16
11	Structural, QSAR, machine learning and molecular docking studies of 5-thiophen-2-yl pyrazole derivatives as potent and selective cannabinoid-1 receptor antagonists. New Journal of Chemistry, 2021, 45, 17796-17807.	2.8	5
12	S₂O₂^{q+} (q = 0, 1, and 2) Molecular Systems: Characterization and Atmospheric Planetary Implications. Journal of Physical Chemistry A, 2021, 125, 1958-1971.	2.5	2
13	Collisional (de-)excitation of protonated cyanoacetylene (HC3NH+) by helium at low and moderate temperatures. Monthly Notices of the Royal Astronomical Society, 2021, 503, 2902-2912.	4.4	0
14	Explicitly correlated potential energy surface of the CH3Clâ€“He van der Waals complex and applications. Journal of Chemical Physics, 2021, 154, 094304.	3.0	2
15	Thionitroxyl Radical (H2NS) Isomers: Structures, Vibrational Spectroscopy, Electronic States and Photochemistry. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	0
16	State selective fragmentation of doubly ionized sulphur dioxide. Scientific Reports, 2021, 11, 17137.	3.3	3
17	Tribute to Cheuk-Yiu Ng. Journal of Physical Chemistry A, 2021, 125, 7353-7355.	2.5	0
18	In silico design of a new Znâ€“triazole based metalâ€“organic framework for CO2 and H2O adsorption. Journal of Chemical Physics, 2021, 154, 024303.	3.0	5

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19	Sodium isocyanideâ€“Helium potential energy surface and astrophysical applications. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
20	Threshold photoelectron spectroscopy of 9-methyladenine: theory and experiment. Physical Chemistry Chemical Physics, 2021, , .	2.8	4
21	Unimolecular Double Photoionization-Induced Processes in Iron Pentacarbonyl. Inorganic Chemistry, 2021, 60, 17966-17975.	4.0	3
22	Identification of DNA Bases and Their Cations in Astrochemical Environments: Computational Spectroscopy of Thymine as a Test Case. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	0
23	Jet-Stirred Reactor Study of Low-Temperature Neopentane Oxidation: A Combined Theoretical, Chromatographic, Mass Spectrometric, and PEPICO Analysis. Energy & Fuels, 2021, 35, 19689-19704.	5.1	12
24	Pyrazolo[1,5-a][1,3,5]triazin-2-thioxo-4-ones derivatives as thymidine phosphorylase inhibitors: Structure, drug-like calculations and quantitative structure-activity relationships (QSAR) modeling. Journal of Molecular Structure, 2020, 1199, 127027.	3.6	9
25	In-silico astrochemistry of life's building blocks. Physics of Life Reviews, 2020, 32, 101-103.	2.8	5
26	Mechanistic study of the [2+2] cycloaddition reaction of cyclohexenone and its derivatives with vinyl acetate. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	7
27	IO(X2Î)â€“Ar cluster: ab initio potential energy surface and dynamical computations. Physical Chemistry Chemical Physics, 2020, 22, 740-747.	2.8	2
28	Isomer-sensitive characterization of low temperature oxidation reaction products by coupling a jet-stirred reactor to an electron/ion coincidence spectrometer: case of n-pentane. Physical Chemistry Chemical Physics, 2020, 22, 1222-1241.	2.8	28
29	Three-phenyl transfer in palladium-catalyzed C C coupling reactions by triarylbismuths: A mechanistic study. Molecular Catalysis, 2020, 482, 110649.	2.0	0
30	Neutral and Multicharged Ions of Small Aluminum Oxides: Structures, Spectroscopy, and Energetics. Journal of Physical Chemistry A, 2020, 124, 9021-9034.	2.5	1
31	State-to-state dissociative photoionization of molecular nitrogen: the full story. Advances in Physics: X, 2020, 5, 1831955.	4.1	4
32	Characterization of the simplest sulfenyl thiocyanate: isomers, spectroscopy and implications of astrophysical and biological relevance. Physical Chemistry Chemical Physics, 2020, 22, 17052-17061.	2.8	3
33	Identifying isomers of peroxy radicals in the gas phase: 1-C₃H₇O₂vs. 2-C₃H₇O₂. Chemical Communications, 2020, 56, 15525-15528.	4.1	12
34	Carbazole derivatives containing chalcone analogues targeting topoisomerase II inhibition: First principles characterization and QSAR modelling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118724.	3.9	6
35	Insights into the mechanism and regiochemistry of the 1,3-dipolar cycloaddition reaction between benzaldehyde and diazomethane. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	18
36	State-to-state inelastic rate coefficients of phosphine in collision with He at low to moderate temperature. Monthly Notices of the Royal Astronomical Society, 2020, 499, 1578-1586.	4.4	5

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37	Electronic structure and magnetic properties of naphthalene- and stilbene-diimide-bridged diuranium(V) complexes: a theoretical study. Journal of Molecular Modeling, 2020, 26, 282.	1.8	2
38	Unimolecular decomposition of methyl ketene and its dimer in the gas phase: theory and experiment. Physical Chemistry Chemical Physics, 2020, 22, 20394-20408.	2.8	9
39	Theoretical Characterization of the Structure and Spectroscopy of HCNO2 Isomers and Applications. Journal of Physical Chemistry A, 2020, 124, 11061-11071.	2.5	2
40	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
41	Hâ€“He collision-induced satellite in the LymanÂÎ± profile of DBA white dwarf stars. Monthly Notices of the Royal Astronomical Society, 2020, 494, 868-875.	4.4	6
42	QSAR investigations and structure-based virtual screening on a series of nitrobenzoxadiazole derivatives targeting human glutathione-S-transferases. Journal of Molecular Structure, 2020, 1211, 128015.	3.6	11
43	Electronic states of monocesium monoxide and its ions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 250, 107000.	2.3	0
44	Gold with +4 oxidation state compounds: mass spectrometric and theoretical characterization of AuO²⁺. Physical Chemistry Chemical Physics, 2019, 21, 16120-16126.	2.8	1
45	Collision excitation of sodium cyanide molecule by helium at low temperature. Monthly Notices of the Royal Astronomical Society, 2019, 489, 4322-4328.	4.4	2
46	Photoionization and dissociative photoionization of propynal in the gas phase: theory and experiment. Physical Chemistry Chemical Physics, 2019, 21, 14053-14062.	2.8	11
47	Copperâ€“Chalcogen Bonds in Olfaction: Accurate ab Initio Characterization of CuSH and CuOH. Journal of Physical Chemistry A, 2019, 123, 1177-1185.	2.5	0
48	Explicitly correlated potential energy surface of the CO2â€“CO van der Waals dimer and applications. Physical Chemistry Chemical Physics, 2019, 21, 15871-15878.	2.8	9
49	Energetics and ionization dynamics of two diarylketone molecules: benzophenone and fluorenone. Physical Chemistry Chemical Physics, 2019, 21, 14453-14464.	2.8	4
50	Alkyl Methyl Imidazolium-Based Ionic Liquids at the Au(111) Surface: Anions and Alkyl Chain Cations Induced Interfacial Effects. Journal of Physical Chemistry C, 2019, 123, 15087-15098.	3.1	30
51	Complexes of Zn(II)â€“Triazoles with CO₂ and H₂O: Structures, Energetics, and Applications. Journal of Physical Chemistry A, 2019, 123, 5555-5565.	2.5	5
52	A novel nanocomposite with superior electrocatalytic activity: A magnetic property based ZnFe2O4 nanocubes embellished with reduced graphene oxide by facile ultrasonic approach. Ultrasonics Sonochemistry, 2019, 57, 116-124.	8.2	14
53	Facile synthesis of copper(II) oxide nanospheres covered on functionalized multiwalled carbon nanotubes modified electrode as rapid electrochemical sensing platform for super-sensitive detection of antibiotic. Ultrasonics Sonochemistry, 2019, 58, 104596.	8.2	25
54	Interaction of Chiral Propylene Oxide (CH₃CHCH₂O) with Helium: Potential Energy Surface and Scattering Calculations. ACS Earth and Space Chemistry, 2019, 3, 964-972.	2.7	18

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55	Formation of H₃⁺ through Chloromethane Dication Fragmentation. ACS Earth and Space Chemistry, 2019, 3, 980-985.	2.7	7
56	Exploration of large amplitude motions in the Ca⁺Ar₂ complex. Molecular Physics, 2019, 117, 1673-1681.	1.7	4
57	Spectroscopy and characterization of AlNX (X = O and S): Triatomic circumstellar molecules. Journal of Chemical Physics, 2019, 150, 124306.	3.0	7
58	QSAR Modeling and Drug-Likeness Screening for Antioxidant Activity of Benzofuran Derivatives. Journal of Molecular Structure, 2019, 1189, 307-314.	3.6	19
59	Encapsulation of anticancer drug doxorubicin inside dendritic macromolecular cavities: First-principles benchmarks. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 217, 278-287.	3.9	4
60	Single photon ionization of methyl isocyanide and the subsequent unimolecular decomposition of its cation: experiment and theory. Physical Chemistry Chemical Physics, 2019, 21, 26017-26026.	2.8	5
61	Quantum tunneling dynamical behaviour on weakly bound complexes: the case of a CO₂â€“N₂ dimer. Physical Chemistry Chemical Physics, 2019, 21, 3550-3557.	2.8	13
62	Electronic and vibrational spectroscopy of the low-lying states of potassium mono-sulphide KS, and comparison in the series of MS (Mâ€‰=â€‰Li, Na, K, Rb, Cs). Molecular Physics, 2019, 117, 1653-1662.	1.7	5
63	Structural, energetic and spectroscopic characterisation of 5-fluorouracil anticarcinogenic drug isomers, tautomers and ions. Molecular Physics, 2019, 117, 1589-1603.	1.7	8
64	Spectroscopy and Stability of AlOP: A Possible Progenitor of Interstellar Metal. Journal of Physical Chemistry A, 2019, 123, 463-470.	2.5	10
65	Multi reference studies of gas phase vanadium nitride di- and trications. Chemical Physics, 2019, 517, 113-118.	1.9	1
66	Spinâ€“Orbit Effects in the Spectroscopy of the X²Î and a⁴Î£^{â€“} Electronic States of Carbon Iodide, CI. Journal of Physical Chemistry A, 2018, 122, 2353-2360.	2.5	4
67	Identification of Key Intermediates during the NO and H₂S Crosstalk Signaling Pathways. Journal of Physical Chemistry A, 2018, 122, 2877-2883.	2.5	6
68	Imidazole derivatives as angiotensin II AT1 receptor blockers: Benchmarks, drug-like calculations and quantitative structure-activity relationships modeling. Chemical Physics Letters, 2018, 696, 70-78.	2.6	6
69	Insights into the bonding between tributylphosphine chalcogenides and zinc(II). Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
70	Electronic and spectroscopic characterizations of SNP isomers. Journal of Chemical Physics, 2018, 148, 054305.	3.0	6
71	Rotational relaxation of AlO+(1Î£+) in collision with He. Monthly Notices of the Royal Astronomical Society, 2018, 475, 783-787.	4.4	7
72	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44

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73	Structural and energetic properties of tautomeric forms of phosphonyl thioamides. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
74	A combined experimental and theoretical study on <scp>pâ€‹s</scp>ulfonatocalix[4]arene encapsulated 7â€‹<scp>m</scp>ethoxycoumarin. Journal of Physical Organic Chemistry, 2018, 31, e3788.	1.9	8
75	Insights on the interaction of Zn2+ cation with triazoles: Structures, bonding, electronic excitation and applications. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 193, 375-384.	3.9	6
76	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	3.2	1
77	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	3.2	0
78	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	3.2	4
79	Molecules in confinement in liquid solvents: general discussion. Faraday Discussions, 2018, 212, 383-397.	3.2	1
80	Adsorption of Hydrophobic and Hydrophilic Ionic Liquids at the Au(111) Surface. ACS Omega, 2018, 3, 18039-18051.	3.5	37
81	Spectroscopy of the electronic excited states of thioxophosphane, HPS, and of its deuterated species. Journal of Chemical Physics, 2018, 149, 164303.	3.0	2
82	Electronic and Vibrational Spectroscopy of CsS. Journal of Physical Chemistry A, 2018, 122, 5354-5360.	2.5	3
83	Toward the detection of the triatomic negative ion SPNâ¯: Spectroscopy and potential energy surfaces. Journal of Chemical Physics, 2018, 148, 164305.	3.0	1
84	On the gas-phase formation of the HCO^{â¯} anion: accurate quantum study of the H^{â¯} + CO radiative association and HCO radiative electron attachment. Faraday Discussions, 2018, 212, 101-116.	3.2	3
85	Unveiling the complex vibronic structure of the canonical adenine cation. Physical Chemistry Chemical Physics, 2018, 20, 20756-20765.	2.8	14
86	Rotational (de-)excitation of NS+(X1Î£+) by collision with He at low temperature. Monthly Notices of the Royal Astronomical Society, 2018, 480, 4259-4264.	4.4	2
87	Rotational (de-)excitation of isocyanogen by collision with helium at low energies. Journal of Chemical Physics, 2018, 149, 064305.	3.0	9
88	Mechanistic study of the photoexcitation, photoconversion, and photodissociation of CS2. Journal of Chemical Physics, 2018, 149, 064304.	3.0	19
89	Disentangling the complex spectrum of the ethynyl cation. Faraday Discussions, 2018, 212, 51-64.	3.2	2
90	Characterization of the electronic states of the biological relevant SSNO molecule. Journal of Chemical Physics, 2017, 146, 074301.	3.0	1

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91	Complex rovibrational dynamics of the ArÂ·NO⁺ complex. Physical Chemistry Chemical Physics, 2017, 19, 8152-8160.	2.8	19
92	Prediction of metastable <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi mathvariant="bold">AlS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup dications in the gas phase. Physical Review A, 2017, 95, .	2.5	1
93	Benchmark study of the structural and spectroscopic parameters of the hydroxymethyl peroxy (HOCH2OO) radical and its decomposition reaction to HO2 and H2CO. Journal of Chemical Physics, 2017, 146, 144303.	3.0	5
94	Full-Dimensional Theory of Pair-Correlated HNCO Photofragmentation. Journal of Physical Chemistry Letters, 2017, 8, 2420-2424.	4.6	11
95	One-electron pseudo-potential investigation of NO(X2Î)â€“Arn clusters (n = 1,2,3,4). Molecular Physics, 2017, 115, 2586-2596.	1.7	1
96	Periodic Dispersion-Corrected Approach for Isolation Spectroscopy of N₂ in an Argon Environment: Clusters, Surfaces, and Matrices. Journal of Physical Chemistry A, 2017, 121, 4093-4102.	2.5	4
97	Rotational excitation of HNCO by He: potential energy surface, collisional cross-sections and rate coefficients. Monthly Notices of the Royal Astronomical Society, 2017, 471, 80-88.	4.4	7
98	Cold collisions of SHâ¯ with He: Potential energy surface and rate coefficients. Journal of Chemical Physics, 2017, 147, 124301.	3.0	7
99	Advances in spectroscopy and dynamics of small and medium sized molecules and clusters. Physical Chemistry Chemical Physics, 2017, 19, 21236-21261.	2.8	50
100	Abâ€...Initio and DFT Studies on CO₂ Interacting with Zn^{q+}â€“Imidazole (q=0, 1, 2) Complexes: Prediction of Charge Transfer through Ïƒâ€•or Ï€â€Type Models. ChemPhysChem, 2016, 17, 994-1005.	2.1	22
101	First principle investigations of organobismuth palladium-catalyzed Câ€“C coupling reaction: mechanism, chemoselectivity and solvent effects. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
102	Explanation of efficient quenching of molecular ion vibrational motion by ultracold atoms. Nature Communications, 2016, 7, 11234.	12.8	30
103	Stereoisomers of hydroxymethanes: Probing structural and spectroscopic features upon substitution. Journal of Chemical Physics, 2016, 145, 244305.	3.0	2
104	Toward the laboratory identification of [O,N,S,S] isomers: Implications for biological NO chemistry. Journal of Chemical Physics, 2016, 144, 234316.	3.0	6
105	HNS+ and HSN+ cations: Electronic states, spin-rovibronic spectroscopy with planetary and biological implications. Journal of Chemical Physics, 2016, 145, 084307.	3.0	11
106	Identifying Cytosine-Specific Isomers via High-Accuracy Single Photon Ionization. Journal of the American Chemical Society, 2016, 138, 16596-16599.	13.7	25
107	Electronic, structural and vibrational induced effects upon ionization of 2-quinolinone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 164, 1-7.	3.9	3
108	SPECTROSCOPIC CONSTANTS OF THE X¹Î£⁺ AND 1³Î STATES OF AlO⁺. Astrophysical Journal, 2016, 826, 163.	4.5	16

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109	Theoretical investigation of the long-lived metastable AlO2+ dication in gas phase. Chemical Physics, 2016, 477, 32-38.	1.9	4
110	Vibrational memory in quantum localized states. Physical Review A, 2016, 93, .	2.5	14
111	Explicitly correlated three-dimensional potential-energy surface of the thiazyl-hydrideâ€“helium weakly bound system and implications for HSN detection. Physical Review A, 2016, 94, .	2.5	10
112	Energetic Diagrams and Structural Properties of Monohaloacetylenes HCâ‰¡CX (X = F, Cl, Br). Journal of Physical Chemistry A, 2016, 120, 5985-5992.	2.5	4
113	Microscopic investigations of site and functional selectivity of triazole for CO₂ capture and catalytic applications. Physical Chemistry Chemical Physics, 2016, 18, 29709-29720.	2.8	20
114	Mechanistic study of bismuth-catalyzed direct benzylation of 2,4-pentanediones: the case of BiCl3 and generalization. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	1
115	QUANTUM-STATE DEPENDENCE OF PRODUCT BRANCHING RATIOS IN VACUUM ULTRAVIOLET PHOTODISSOCIATION OF N₂. Astrophysical Journal, 2016, 819, 23.	4.5	24
116	Rotational (de-)excitation of HNS by He: three-dimensional potential energy surface and collision rate coefficients. Monthly Notices of the Royal Astronomical Society, 2016, 458, 1581-1589.	4.4	10
117	Spectroscopy and Dynamics of Medium-Sized Molecules and Clusters: Theory, Experiment, and Applications. Journal of Physical Chemistry A, 2016, 120, 475-476.	2.5	1
118	Theoretical characterization of vanadyl and VO3+ cations in gas phase. Chemical Physics Letters, 2016, 646, 142-147.	2.6	4
119	Structure, Reactivity, and Fragmentation of Small Multi-Charged Methane Clusters. Journal of Physical Chemistry A, 2016, 120, 1669-1676.	2.5	8
120	Mapping the Dissociative Ionization Dynamics of Molecular Nitrogen with Attosecond Time Resolution. Physical Review X, 2015, 5, .	8.9	25
121	Electronic structure of NSOâ^' and SNOâ^' anions: Stability, electron affinity, and spectroscopic properties. Journal of Chemical Physics, 2015, 143, 164301.	3.0	12
122	Accurate structural and spectroscopic characterization of prebiotic molecules: The neutral and cationic acetyl cyanide and their related species. Journal of Chemical Physics, 2015, 143, 184314.	3.0	10
123	On the role of HNS and HSN as light-sensitive NO-donors for delivery in biological media. Journal of Chemical Physics, 2015, 143, 134301.	3.0	8
124	Mapping the dissociative ionization dynamics of molecular nitrogen with attosecond resolution. Journal of Physics: Conference Series, 2015, 635, 112101.	0.4	0
125	Photoionization of Benzophenone in the Gas Phase: Theory and Experiment. Journal of Physical Chemistry A, 2015, 119, 6148-6154.	2.5	7
126	Understanding of matrix embedding: a theoretical spectroscopic study of CO interacting with Ar clusters, surfaces and matrices. Physical Chemistry Chemical Physics, 2015, 17, 17159-17168.	2.8	6

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127	Potential energy surface of the CO2â€“N2 van der Waals complex. Journal of Chemical Physics, 2015, 142, 174301.	3.0	41
128	Structure, Spectroscopy, and Bonding within the Zn^{q+}â€“Imidazole_n (q = 0, 1, 2; n = 1â€“4) Clusters and Implications for Zeolitic Imidazolate Frameworks and Znâ€“Enzymes. Journal of Physical Chemistry A, 2015, 119, 11928-11940.	2.5	13
129	Vibrationally Resolved Photoelectron Spectroscopy of Electronic Excited States of DNA Bases: Application to the Ãƒ State of Thymine Cation. Journal of Physical Chemistry A, 2015, 119, 1146-1153.	2.5	13
130	Towards the computations of accurate spectroscopic parameters and vibrational spectra for organic compounds. Molecular Physics, 2015, 113, 1661-1673.	1.7	16
131	Collisional excitation of MgO by He. Monthly Notices of the Royal Astronomical Society, 2015, 452, 1561-1566.	4.4	4
132	Structural single and multiple molecular adsorption of CO 2 and H 2 O in zeolitic imidazolate framework (ZIF) crystals. Microporous and Mesoporous Materials, 2015, 218, 33-41.	4.4	24
133	VUV photoionization and dissociative photoionization spectroscopy of the interstellar molecule aminoacetonitrile: Theory and experiment. Journal of Molecular Spectroscopy, 2015, 315, 196-205.	1.2	7
134	Explicitly correlated interaction potential energy profile of imidazoleÂ+ÂCO2 complex. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
135	Characterization of Zn^{q+}â€“imidazole (q = 0, 1, 2) organometallic complexes: DFT methods vs. standard and explicitly correlated post-Hartreeâ€“Fock methods. Physical Chemistry Chemical Physics, 2015, 17, 14417-14426.	2.8	23
136	State-to-state vacuum ultraviolet photodissociation study of CO₂ on the formation of state-correlated CO(X¹Î£⁺; v) with O(¹D) and O(¹S) photoproducts at 11.95â€“12.22 eV. Physical Chemistry Chemical Physics, 2015, 17, 11752-11762.	2.8	20
137	Microsolvation of NO+ in Arn clusters: A theoretical treatment. Journal of Chemical Physics, 2015, 142, 204309.	3.0	9
138	Characterization and reactivity of the weakly bound complexes of the [H, N, S]â^' anionic system with astrophysical and biological implications. Journal of Chemical Physics, 2015, 143, 034303.	3.0	11
139	Rotational Excitation of the OH⁺ Radical by Collision with H at Low Temperature. Journal of Physical Chemistry A, 2015, 119, 12599-12606.	2.5	6
140	Theoretical and Experimental Photoelectron Spectroscopy Characterization of the Ground State of Thymine Cation. Journal of Physical Chemistry A, 2015, 119, 5951-5958.	2.5	24
141	Ab initio treatment of gas phase GeO2+ doubly charged ion. Chemical Physics, 2015, 446, 13-17.	1.9	3
142	Photoionization Spectroscopy of Nucleobases and Analogues in the Gas Phase Using Synchrotron Radiation as Excitation Light Source. Topics in Current Chemistry, 2014, 355, 155-208.	4.0	25
143	Role of size and shape selectivity in interaction between gold nanoclusters and imidazole: a theoretical study. Journal of Molecular Modeling, 2014, 20, 2534.	1.8	19
144	Accurate global potential energy surface for the H + OH+ collision. Journal of Chemical Physics, 2014, 140, 184306.	3.0	7

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145	VUV photoionization and dissociative photoionization of the prebiotic molecule acetyl cyanide: Theory and experiment. Journal of Chemical Physics, 2014, 141, 134311.	3.0	8
146	Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate. Journal of Chemical Physics, 2014, 141, 104303.	3.0	10
147	On the use of explicitly correlated treatment methods for the generation of accurate polyatomic â€"He/H2 interaction potential energy surfaces: The case of C3â€"He complex and generalization. Journal of Chemical Physics, 2014, 141, 044308.	3.0	26
148	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF ETHYL MERCAPTAN AND DIMETHYL SULFIDE ISOTOPOLOGUES: A ROUTE TOWARD THEIR ASTROPHYSICAL DETECTION. Astrophysical Journal, 2014, 796, 50.	4.5	16
149	Time resolved observation of the solvation dynamics of a Rydberg excited molecule deposited on an argon cluster-I: DABCO^{â˜†}at short times. Physical Chemistry Chemical Physics, 2014, 16, 516-526.	2.8	19
150	A roaming wavepacket in the dynamics of electronically excited 2-hydroxypyridine. Physical Chemistry Chemical Physics, 2014, 16, 581-587.	2.8	24
151	Ab initio study of the structures and electronic states of small neutral and ionic DABCO â€" Arn clusters. Journal of Molecular Modeling, 2014, 20, 2135.	1.8	3
152	Theoretical spectroscopic characterization at low temperatures of detectable sulfur-organic compounds: Ethyl mercaptan and dimethyl sulfide. Journal of Chemical Physics, 2014, 140, 124302.	3.0	23
153	Explicit correlation treatment of the potential energy surface of CO2 dimer. Journal of Chemical Physics, 2014, 140, 234310.	3.0	53
154	Theoretical spectroscopic investigations of HNSq and HSNq (q = 0, +1, â¯1) in the gas phase. Journal of Chemical Physics, 2014, 140, 244309.	3.0	23
155	Theoretical spectroscopic characterization of the ArBeO complex. Journal of Chemical Physics, 2014, 141, 174305.	3.0	7
156	Carbon dioxide interaction with isolated imidazole or attached on gold clusters and surface: competition between Ïƒ H-bond and Ï€ stacking interaction. Physical Chemistry Chemical Physics, 2014, 16, 12503-12509.	2.8	39
157	Characterization of gas phase WC²⁺: a thermodynamically stable carbide dication. Physical Chemistry Chemical Physics, 2014, 16, 21356-21362.	2.8	5
158	Theoretical investigations of the IO,q+ (q = 2, 3, 4) multi-charged ions: Metastability, characterization and spectroscopy. Journal of Chemical Physics, 2014, 141, 014302.	3.0	9
159	Theoretical studies of 2-quinolinol: Geometries, vibrational frequencies, isomerization, tautomerism, and excited states. Chemical Physics Letters, 2014, 613, 29-33.	2.6	11
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