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	Photoionization of 2-pyridone and 2-hydroxypyridine. Physical Chemistry Chemical Physics, 2010, 12, 3566.	2.8	123
2	A study of the mode-selective transâ€“cis isomerization in HONO using ab initio methodology. Journal of Chemical Physics, 2004, 120, 1306-1317.	3.0	96
3	On the accuracy of explicitly correlated methods to generate potential energy surfaces for scattering calculations and clustering: application to the HClâ€“He complex. Physical Chemistry Chemical Physics, 2013, 15, 10062.	2.8	70
4	Benchmarks for the generation of interaction potentials for scattering calculations: applications to rotationally inelastic collisions of C4 (X3Î£â¯g) with He. Physical Chemistry Chemical Physics, 2010, 12, 15672.	2.8	69
5	Threshold photoelectrons coincidence spectroscopy of N22+ and CO2+ ions. Chemical Physics, 1996, 207, 159-165.	1.9	68
6	Explicit correlation treatment of the potential energy surface of CO2 dimer. Journal of Chemical Physics, 2014, 140, 234310.	3.0	53
7	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ar</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Photoelectron Spectroscopy Mediated by Autoionizing States. Physical Review Letters, 2012, 109, 193401.	7.8	50
8	Advances in spectroscopy and dynamics of small and medium sized molecules and clusters. Physical Chemistry Chemical Physics, 2017, 19, 21236-21261.	2.8	50
9	Photo double ionization spectra of CO: comparison of theory with experiment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 3197-3214.	1.5	48
10	Oxygen-containing gas-phase diatomic trications and tetracations: ReOz+, NbOz+ and HfOz+ (z = 3, 4). Physical Chemistry Chemical Physics, 2011, 13, 15233.	2.8	48
11	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
12	Valenceâ€“Rydberg electronic states of N₂: spectroscopy and spinâ€“orbit couplings. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 245101.	1.5	43
13	Pulsed field ionizationâ€“photoelectron bands for CO2+(Aâ€Š2Îuâ€,andâ€,Bâ€Š2Î£u+) in the energy range of 17.2â€“19.0 eV: An experimental and theoretical study. Journal of Chemical Physics, 2000, 113, 7988-7999.	3.0	42
14	Explicitly correlated treatment of the Arâ€“NO+ cation. Journal of Chemical Physics, 2011, 135, 044312.	3.0	42
15	Potential energy surface of the CO2â€“N2 van der Waals complex. Journal of Chemical Physics, 2015, 142, 174301.	3.0	41
16	Reactivity of Xenon with Ice at Planetary Conditions. Physical Review Letters, 2013, 110, 265501.	7.8	40
17	Electronic structure calculations on the C4 cluster. Journal of Chemical Physics, 2006, 124, 234304.	3.0	39
18	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

#	Article	IF	Citations
19	High resolution pulsed field ionizationâ€“photoelectron study of CO2+(Xâ€Š2Îg) in the energy range of 13.6â€“14.7 eV. Journal of Chemical Physics, 2000, 112, 10767-10777.	3.0	38
20	Sign reversal of the spin-orbit constant for the Câ€‰Î3u state of N2. Journal of Chemical Physics, 2008, 129, 164307.	3.0	37
21	Adsorption of Hydrophobic and Hydrophilic Ionic Liquids at the Au(111) Surface. ACS Omega, 2018, 3, 18039-18051.	3.5	37
22	Titanâ€™s Ionic Species: Theoretical Treatment of N₂H⁺ and Related Ions. Journal of Physical Chemistry A, 2009, 113, 11107-11111.	2.5	34
23	Characterization of the MgO²⁺dication in the gas phase: electronic states, spectroscopy and atmospheric implications. Physical Chemistry Chemical Physics, 2013, 15, 824-831.	2.8	32
24	Accurateab initiospinâ€“orbit predissociation lifetimes of the A states of SH and SH⁺. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 045101.	1.5	31
25	Spectroscopy, Metastability, and Single and Double Ionization of AlCl. Journal of Physical Chemistry A, 2008, 112, 13419-13426.	2.5	30
26	Autoionization and ultrafast relaxation dynamics of highly excited states in N2. Physical Review A, 2012, 86, .	2.5	30
27	VUV photoionization of gas phase adenine and cytosine: A comparison between oven and aerosol vaporization. Journal of Chemical Physics, 2013, 138, 094203.	3.0	30
28	Explanation of efficient quenching of molecular ion vibrational motion by ultracold atoms. Nature Communications, 2016, 7, 11234.	12.8	30
29	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
30	Potential energy function and vibrational states of N2CO+. Journal of Chemical Physics, 1999, 111, 4948-4955.	3.0	29
31	AB INITIO CHARACTERIZATION OF C^{â€“}₄, C₄H, AND C₄H^{â€“}. Astrophysical Journal, 2010, 708, 1452-1458.	4.5	29
32	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
33	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
34	Electronic states of MgO: Spectroscopy, predissociation, and cold atomic Mg and O production. Journal of Chemical Physics, 2010, 133, 144302.	3.0	27
35	Systematic theoretical studies of the interaction of 1,4-diazabicyclo [2.2.2]octane (DABCO) with rare gases. Journal of Chemical Physics, 2013, 139, 164306.	3.0	27
36	Theoretical investigations of the SH+ and LiS+ cations. Journal of Molecular Spectroscopy, 2006, 237, 232-240.	1.2	26

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37	OCS2+ dication spectroscopy and electronic states. Chemical Physics, 2008, 346, 23-33.	1.9	26
38	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
39	Quartet states in the radical cation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 4509-4514.	1.5	25
40	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
41	Mapping the Dissociative Ionization Dynamics of Molecular Nitrogen with Attosecond Time Resolution. Physical Review X, 2015, 5, .	8.9	25
42	Identifying Cytosine-Specific Isomers via High-Accuracy Single Photon Ionization. Journal of the American Chemical Society, 2016, 138, 16596-16599.	13.7	25
43	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
44	Vacuum ultraviolet pulsed-field ionization-photoelectron study of H2S in the energy range of 10â€“17 eV. Journal of Chemical Physics, 2004, 120, 6944-6956.	3.0	24
45	Lowâ€Temperature Rate Constants for Rotational Excitation and Deâ€excitation of C₃(XÂ¹Î£$^{+}_{g}$) by Collisions with He (¹S). Astrophysical Journal, 2008, 686, 379-383.	4.5	24
46	Rotational excitation and de-excitation of C2(Xâ€‰Î£1g+) by para-H2(j=). Journal of Chemical Physics, 2009, 130, 204305.	3.0	24
47	A roaming wavepacket in the dynamics of electronically excited 2-hydroxypyridine. Physical Chemistry Chemical Physics, 2014, 16, 581-587.	2.8	24
48	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
49	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
50	QUANTUM-STATE DEPENDENCE OF PRODUCT BRANCHING RATIOS IN VACUUM ULTRAVIOLET PHOTODISSOCIATION OF N₂. Astrophysical Journal, 2016, 819, 23.	4.5	24
51	Theoretical study of the electronic states of CS2++. Journal of Chemical Physics, 1998, 108, 4047-4053.	3.0	23
52	Quartet and sextet states of CSâ^'. Journal of Chemical Physics, 1999, 110, 11835-11840.	3.0	23
53	Theoretical investigation of the SO2+ dication and the photo-double ionization spectrum of SO. Journal of Chemical Physics, 2005, 122, 054303.	3.0	23
54	REACTIVITY OF ANIONS IN INTERSTELLAR MEDIA: DETECTABILITY AND APPLICATIONS. Astrophysical Journal, 2013, 768, 59.	4.5	23

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55	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
56	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
57	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
58	Unusual Quantum Interference in the S₁ State of DABCO and Observation of Intramolecular Vibrational Redistribution. Journal of Physical Chemistry A, 2010, 114, 3313-3319.	2.5	22
59	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 Ïâ€Type Models. ChemPhysChem, 2016, 17, 994-1005.	2.1	22
60	A theoretical and experimental study of the SO22+ dication. Journal of Chemical Physics, 2004, 120, 6449-6460.	3.0	21
61	Triple ionization spectra by coincidence measurements of double Auger decay: The case of OCS. Journal of Chemical Physics, 2010, 132, 014311.	3.0	21
62	High Resolution Pulsed Field Ionizationâ˜'Photoelectron Bands for CS2+(Ãƒ2Îu):Â An Experimental and Theoretical Studyâ€. Journal of Physical Chemistry A, 2001, 105, 2183-2191.	2.5	20
63	Spectroscopy and metastability of BeO⁺. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 205101.	1.5	20
64	Solvation effects and stabilization of multicharged ions: a case study of ArmBeOq+ complexes. Physical Chemistry Chemical Physics, 2012, 14, 4236.	2.8	20
65	On the role of the simplest S-nitrosothiol, HSNO, in atmospheric and biological processes. Journal of Chemical Physics, 2013, 139, 234304.	3.0	20
66	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
67	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
68	Stable and metastable states of SNâ˜'. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 3395-3403.	1.5	19
69	Quintet electronic states of N2. Journal of Chemical Physics, 2010, 132, 104310.	3.0	19
70	Ab initio structural and spectroscopic study of HPSx and HSPx (x = 0,+1,â˜'1) in the gas phase. Journal of Chemical Physics, 2013, 139, 174313.	3.0	19
71	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
72	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

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73	Complex rovibrational dynamics of the ArÂ·NO⁺ complex. Physical Chemistry Chemical Physics, 2017, 19, 8152-8160.	2.8	19
74	Mechanistic study of the photoexcitation, photoconversion, and photodissociation of CS2. Journal of Chemical Physics, 2018, 149, 064304.	3.0	19
75	QSAR Modeling and Drug-Likeness Screening for Antioxidant Activity of Benzofuran Derivatives. Journal of Molecular Structure, 2019, 1189, 307-314.	3.6	19
76	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
77	Spectroscopic and spin-orbit calculations on the SO+ radical cation. Journal of Chemical Physics, 2006, 124, 054313.	3.0	18
78	Slow Photoelectron Spectroscopy of Î´â€Valerolactam and Its Dimer. ChemPhysChem, 2011, 12, 1822-1832.	2.1	18
79	Slow Photoelectron Spectroscopy of 3-Hydroxyisoquinoline. Journal of Physical Chemistry A, 2013, 117, 8095-8102.	2.5	18
80	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
81	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
82	Two spectrometers for threshold photoelectron coincidence studies of double photoionization. Canadian Journal of Physics, 1996, 74, 856-860.	1.1	17
83	Electronic states, conical intersections, and spin-rovibronic spectroscopy of the nitrogen oxide sulfide radical. Journal of Chemical Physics, 2013, 138, 104318.	3.0	17
84	The potential energy surface and vibrational structure of C3Hâ˜. Journal of Chemical Physics, 2001, 115, 3664-3672.	3.0	16
85	Anharmonic Spectroscopic Study of the Ground Electronic State of Various C₄Radical Isotopomers. Astrophysical Journal, 2007, 670, 1510-1517.	4.5	16
86	Identification and theoretical investigation of the SiO2+ dication. Chemical Physics Letters, 2010, 486, 16-20.	2.6	16
87	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF ETHYL MERCAPTAN AND DIMETHYL SULFIDE ISOTOPOLOGUES: A ROUTE TOWARD THEIR ASTROPHYSICAL DETECTION. Astrophysical Journal, 2014, 796, 50.	4.5	16
88	Towards the computations of accurate spectroscopic parameters and vibrational spectra for organic compounds. Molecular Physics, 2015, 113, 1661-1673.	1.7	16
89	SPECTROSCOPIC CONSTANTS OF THE X¹Î£⁺ AND 1³Î STATES OF AlO⁺. Astrophysical Journal, 2016, 826, 163.	4.5	16
90	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

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91	A new theoretical method for calculating the radiative association cross section of a triatomic molecule: application to N2â€“Hâ^. Physical Chemistry Chemical Physics, 2013, 15, 13818.	2.8	15
92	A vacuum ultraviolet pulsed field ionization-photoelectron study of cyanogen cation in the energy range of 13.2â€“15.9 eV. Journal of Chemical Physics, 2005, 123, 144302.	3.0	14
93	Theoretical study of the spectroscopy and the metastability of the NS⁺cation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 015101.	1.5	14
94	Accurate theoretical study of PSq (q = 0,+1,â^'1) in the gas phase. Journal of Chemical Physics, 2012, 136, 244309.	3.0	14
95	Vibrational memory in quantum localized states. Physical Review A, 2016, 93, .	2.5	14
96	Unveiling the complex vibronic structure of the canonical adenine cation. Physical Chemistry Chemical Physics, 2018, 20, 20756-20765.	2.8	14
97	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
98	Ionospheric chemistry: Theoretical treatment of ONOO+ and of NO3+. Journal of Chemical Physics, 2009, 130, 204301.	3.0	13
99	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
100	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
101	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
102	Carbon dioxide adsorption and activation on ionic liquid decorated Au(111) surface: A DFT study. Chemosphere, 2022, 286, 131612.	8.2	13
103	Electronic and infrared absorption spectra of NCCN+. International Journal of Mass Spectrometry, 2003, 223-224, 107-114.	1.5	12
104	Theoretical study of the C3S molecule. Theoretical Chemistry Accounts, 2005, 114, 341-349.	1.4	12
105	Electronic structure of NSOâ^' and SNOâ^' anions: Stability, electron affinity, and spectroscopic properties. Journal of Chemical Physics, 2015, 143, 164301.	3.0	12
106	Identifying isomers of peroxy radicals in the gas phase: 1-C₃H₇O₂vs. 2-C₃H₇O₂. Chemical Communications, 2020, 56, 15525-15528.	4.1	12
107	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
108	Accurate Rovibrational Spectroscopic Properties of Cyanogen and Its Isotopomers. Journal of Molecular Spectroscopy, 2001, 207, 269-275.	1.2	11

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109	Fluorescence from the dication: Theory and experiment. Chemical Physics, 2006, 330, 16-25.	1.9	11
110	Theoretical investigations of the MgO⁺cation: spectroscopy, spinâ€“orbit coupling and single ionization spectrum. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 225101.	1.5	11
111	Prediction of the existence of the N2Hâ^' molecular anion. Journal of Chemical Physics, 2012, 136, 244302.	3.0	11
112	Generation of full dimensional potential energy surfaces for atmospherically important charge transfer tetratomic complexes: the case of the OMgOO+ radical cation. Physical Chemistry Chemical Physics, 2013, 15, 10158.	2.8	11
113	Theoretical studies of 2-quinolinol: Geometries, vibrational frequencies, isomerization, tautomerism, and excited states. Chemical Physics Letters, 2014, 613, 29-33.	2.6	11
114	Accurate theoretical spectroscopy of the lowest electronic states of CP radical. Molecular Physics, 2014, 112, 2633-2645.	1.7	11
115	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
116	HNS+ and HSN+ cations: Electronic states, spin-rovibronic spectroscopy with planetary and biological implications. Journal of Chemical Physics, 2016, 145, 084307.	3.0	11
117	Full-Dimensional Theory of Pair-Correlated HNCO Photofragmentation. Journal of Physical Chemistry Letters, 2017, 8, 2420-2424.	4.6	11
118	Photoionization and dissociative photoionization of propynal in the gas phase: theory and experiment. Physical Chemistry Chemical Physics, 2019, 21, 14053-14062.	2.8	11
119	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
120	Ab initio investigation of the diaza-dicarbon CCNN molecule. Journal of Chemical Physics, 2000, 113, 5763-5769.	3.0	10
121	Ab Initio Calculations on the Tricarbon Monoxide Molecule C3O. Journal of Molecular Spectroscopy, 2001, 210, 284-289.	1.2	10
122	Spectroscopy and metastability of the HSSâ^'anionÂ§. Molecular Physics, 2007, 105, 1115-1122.	1.7	10
123	Photoionization of C4 molecular beam: Ab initio calculations. Journal of Chemical Physics, 2007, 127, 014310.	3.0	10
124	Ab initio characterization of linear C₃Si isomers. Astronomy and Astrophysics, 2008, 486, 1047-1052.	5.1	10
125	Double photoionization and dication fragmentation of CF3I: Experiment and theory. Journal of Chemical Physics, 2008, 128, 234303.	3.0	10
126	Theoretical investigations of the cyanogen anion. Chemical Physics, 2009, 355, 164-168.	1.9	10

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127	Theoretical spectroscopy and metastability of BeS and its cation. Chemical Physics, 2010, 373, 193-202.	1.9	10
128	Theoretical investigations of the electronic states of NaXe: A comparative study. Journal of Chemical Physics, 2012, 137, 224310.	3.0	10
129	State-Selected Unimolecular Decomposition of Î´-Valerolactam⁺ and Î´-Valerolactam₂⁺ Cations: Theory and Experiment. Journal of Physical Chemistry A, 2012, 116, 8706-8712.	2.5	10
130	Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate. Journal of Chemical Physics, 2014, 141, 104303.	3.0	10
131	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
132	Explicitly correlated interaction potential energy profile of imidazoleÂ+ÂCO2 complex. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
133	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
134	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
135	Spectroscopy and Stability of AlOP: A Possible Progenitor of Interstellar Metal. Journal of Physical Chemistry A, 2019, 123, 463-470.	2.5	10
136	Ion-pair formation observed in a pulsed-field ionization photoelectron spectroscopic study of HF. Faraday Discussions, 2000, 115, 355-362.	3.2	9
137	The A1Î(u)â†X1Î£ Electronic Transition of CCN+ and CNC+. Helvetica Chimica Acta, 2001, 84, 1432-1440.	1.6	9
138	Single and double photoionizations of methanal (formaldehyde). Journal of Chemical Physics, 2005, 123, 164314.	3.0	9
139	O O C O + cation I: Characterization of its isomers and lowest electronic states. Journal of Chemical Physics, 2007, 127, 064312.	3.0	9
140	O O C O + cation. II. Its role during the atmospheric ion-molecule reactions. Journal of Chemical Physics, 2007, 127, 064313.	3.0	9
141	Electronic spectrum of 2â€pyridone⁺: Ab initio and timeâ€dependent density functional calculations. International Journal of Quantum Chemistry, 2010, 110, 498-504.	2.0	9
142	Explicitly correlated treatment of H2NSi and H2SiN radicals: Electronic structure calculations and rovibrational spectra. Journal of Chemical Physics, 2011, 135, 074301.	3.0	9
143	Metastable ClO2+ and ClO3+ ions in the gas phase: a combined theoretical and mass spectrometric investigation. Physical Chemistry Chemical Physics, 2011, 13, 18315.	2.8	9
144	Theoretical study of the spectroscopy of methyl substituted 2-Pyridones, tautomers and ions. Computational and Theoretical Chemistry, 2012, 990, 94-99.	2.5	9

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145	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
146	Microsolvation of NO+ in Arn clusters: A theoretical treatment. Journal of Chemical Physics, 2015, 142, 204309.	3.0	9
147	Rotational (de-)excitation of isocyanogen by collision with helium at low energies. Journal of Chemical Physics, 2018, 149, 064305.	3.0	9
148	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
149	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
150	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
151	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
152	Theoretical calculations on the NaS and NaS+ radicals: electronic structure, spectroscopy and spin-orbit couplings. European Physical Journal D, 2012, 66, 1.	1.3	8
153	VUV photoionization and dissociative photoionization of the prebiotic molecule acetyl cyanide: Theory and experiment. Journal of Chemical Physics, 2014, 141, 134311.	3.0	8
154	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
155	Structure, Reactivity, and Fragmentation of Small Multi-Charged Methane Clusters. Journal of Physical Chemistry A, 2016, 120, 1669-1676.	2.5	8
156	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
157	Structural, energetic and spectroscopic characterisation of 5-fluorouracil anticarcinogenic drug isomers, tautomers and ions. Molecular Physics, 2019, 117, 1589-1603.	1.7	8
158	Theoretical investigations of the N2H2+ cation and of its reactivity. Journal of Chemical Physics, 2004, 121, 1782-1789.	3.0	7
159	Ionâ^'Molecule Reactions:Â Theoretical Studies of the [N2+ CO]+System. Journal of Physical Chemistry A, 2004, 108, 4978-4982.	2.5	7
160	A G3 Study of the Structure of Carbonâ^'Nitrogen Nanoclusters. Journal of Physical Chemistry A, 2010, 114, 12258-12268.	2.5	7
161	Theoretical study of the spectroscopically relevant parameters for the detection of HNPq and HPNq (q = 0, +1, â^'1) in the gas phase. Journal of Chemical Physics, 2012, 136, 244311.	3.0	7
162	Accurate global potential energy surface for the H + OH+ collision. Journal of Chemical Physics, 2014, 140, 184306.	3.0	7

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163	Theoretical spectroscopic characterization of the ArBeO complex. Journal of Chemical Physics, 2014, 141, 174305.	3.0	7
164	Photoionization of Benzophenone in the Gas Phase: Theory and Experiment. Journal of Physical Chemistry A, 2015, 119, 6148-6154.	2.5	7
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