

Ryan C Fortenberry

List of Publications by Year in descending order

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papers

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1107
citing authors

#	ARTICLE	IF	CITATIONS
1	The <i>trans</i> -HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. <i>Journal of Chemical Physics</i> , 2011, 135, 134301.	1.2	116
2	Quartic force field predictions of the fundamental vibrational frequencies and spectroscopic constants of the cations HOCO ⁺ and DOCO ⁺ . <i>Journal of Chemical Physics</i> , 2012, 136, 234309.	1.2	105
3	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN ⁺ . <i>Journal of Physical Chemistry A</i> , 2015, 119, 11623-11631.	1.1	81
4	Protonated nitrous oxide, NNOH ⁺ : Fundamental vibrational frequencies and spectroscopic constants from quartic force fields. <i>Journal of Chemical Physics</i> , 2013, 139, 084313.	1.2	80
5	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C ₂ H ₃ ⁺ , and Its Isotopologues. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7034-7043.	1.1	75
6	Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS ⁺ , HSCO ⁺ , and Isotopologues via Quartic Force Fields. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9582-9590.	1.1	70
7	On the use of quartic force fields in variational calculations. <i>Chemical Physics Letters</i> , 2013, 574, 1-12.	1.2	66
8	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF ¹ Al ²⁺ -C ₃ H ⁺ : A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. <i>Astrophysical Journal</i> , 2013, 772, 39.	1.6	63
9	The rovibrational nature of closed-shell third-row triatomics: HOX and HXO, X = Si ⁺ , P, S ⁺ , and Cl. <i>Chemical Physics</i> , 2016, 472, 119-127.	0.9	63
10	Quantum astrochemical spectroscopy. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 81-91.	1.0	63
11	Vibrational frequencies and spectroscopic constants from quartic force fields for <i>cis</i> -HOCO: The radical and the anion. <i>Journal of Chemical Physics</i> , 2011, 135, 214303.	1.2	62
12	Excited vibrational level rotational constants for SiC ₂ : A sensitive molecular diagnostic for astrophysical conditions. <i>Molecular Astrophysics</i> , 2015, 1, 13-19.	1.7	60
13	Computational vibrational spectroscopy for the detection of molecules in space. <i>Annual Reports in Computational Chemistry</i> , 2019, 15, 173-202.	0.9	59
14	SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES FOR ¹ Al-C ₃ H ⁺ AND ISOTOPOLOGUES FROM HIGHLY ACCURATE QUARTIC FORCE FIELDS: THE DETECTION OF ¹ Al-C ₃ H ⁺ IN THE HORSEHEAD NEBULA PDR QUESTIONED. <i>Astrophysical Journal Letters</i> , 2013, 768, L25.	3.0	54
15	Highly-accurate quartic force fields for the prediction of anharmonic rotational constants and fundamental vibrational frequencies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 248, 119184.	2.0	50
16	Theoretical prediction of new dipole-bound singlet states for anions of interstellar interest. <i>Journal of Chemical Physics</i> , 2011, 134, 154304.	1.2	48
17	Interstellar Anions: The Role of Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9941-9953.	1.1	47
18	The performance of explicitly correlated methods for the computation of anharmonic vibrational frequencies. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25899.	1.0	43

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19	Communication: Spectroscopic consequences of proton delocalization in OCHCO ⁺ . Journal of Chemical Physics, 2015, 143, 071102.	1.2	42
20	The performance of explicitly correlated wavefunctions [CCSD(T)-F12b] in the computation of anharmonic vibrational frequencies. Chemical Physics Letters, 2019, 734, 136720.	1.2	42
21	A spectroscopic case for SPSi detection: The third-row in a single molecule. Journal of Chemical Physics, 2016, 145, 124311.	1.2	41
22	A benchmark study of the vertical electronic spectra of the linear chain radicals C ₂ H and C ₄ H. Journal of Chemical Physics, 2010, 132, 144303.	1.2	40
23	Potential interstellar noble gas molecules. ArOH^+ and NeOH^+ and ArOH^+ and NeOH^+ rovibrational analysis from quantum chemical quartic force fields. Molecular Astrophysics, 2016, 2,	1.7	39
24	THE POSSIBLE INTERSTELLAR ANION CH ₂ ⁻ CN ⁺ : SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. Astrophysical Journal, 2013, 762, 121.	1.6	38
25	A Small Molecule with PAH Vibrational Properties and a Detectable Rotational Spectrum: c-(C) ₃ H ₂ , Cyclopropenylidene Carbene. Astrophysical Journal, 2019, 871, 236.	1.6	37
26	On the Detectability of the HSS, HSO, and HOS Radicals in the Interstellar Medium. Astrophysical Journal, 2017, 835, 243.	1.6	36
27	Theoretical Rovibronic Treatment of the X ¹ _g ⁻ and \tilde{A}^1 States of C ₂ H and the X ¹ _g ⁻ State of C ₂ H ⁺ from Quartic Force Fields. Journal of Physical Chemistry A, 2015, 119, 7013-7025.	1.1	34
28	Trihydrogen Cation with Neon and Argon: Structural, Energetic, and Spectroscopic Data from Quartic Force Fields. Journal of Physical Chemistry A, 2015, 119, 4915-4922.	1.1	34
29	Counter Anion Effect on the Photophysical Properties of Emissive Indolizine-Cyanine Dyes in Solution and Solid State. Molecules, 2018, 23, 3051.	1.7	34
30	Overcoming the Failure of Correlation for Out-of-Plane Motions in a Simple Aromatic: Rovibrational Quantum Chemical Analysis of <i>cis</i> -C ₃ H ₂ . Journal of Chemical Theory and Computation, 2018, 14, 2155-2164.	2.3	33
31	F12-TZ-cCR: A Methodology for Faster and Still Highly Accurate Quartic Force Fields. Journal of Physical Chemistry A, 2021, 125, 10532-10540.	1.1	32
32	ArH ₂ ⁺ and NeH ₂ ⁺ as global minima in the Ar ⁺ /Ne ⁺ +AH ₂ reactions: energetic, spectroscopic, and structural data. Monthly Notices of the Royal Astronomical Society, 2015, 446, 195-204.	1.6	31
33	and 1 ArHAr^+ and NeHNe^+ and ArHNe^+ complexes: Spectroscopic Data, Part A: Molecular and		
34	Rovibrational Characterization and Interstellar Implications of the Proton-Bound, Noble Gas Complexes: ArHAr^+ , NeHNe^+ , and ArHNe^+ . ACS Earth and Space Chemistry, 2017, 1, 60-69.	1.2	31
35	Dipole Surface and Infrared Intensities for the <i>cis</i> - and <i>trans</i> -HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939.	1.1	30
36	Accurate determination of the onset wavelength (λ_{onset}) of the Ar^+ and Ne^+ ions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 265, 107544.	1.1	30

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37	Singlet Excited States of Silicon-Containing Anions Relevant to Interstellar Chemistry. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8119-8124.	1.1	28
38	Singlet excited states of anions with higher main group elements. <i>Molecular Physics</i> , 2013, 111, 3265-3275.	0.8	26
39	Additional diffuse functions in basis sets for dipole-bound excited states of anions. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	26
40	Anharmonic Frequencies of (MO) ₂ and Related Hydrides for M = Mg, Al, Si, P, S, Ca, and Ti and Heuristics for Predicting Anharmonic Corrections of Inorganic Oxides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3191-3204.	1.1	26
41	Limited rotational and rovibrational line lists computed with highly accurate quartic force fields and ab initio dipole surfaces. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 119, 76-83.	2.0	25
42	Spectroscopic investigation of [Al,N,C,O] refractory molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 244303.	1.2	25
43	The interstellar formation and spectra of the noble gas, proton-bound HeHHe ⁺ , HeHNe ⁺ and HeHAr ⁺ complexes. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017, 469, 339-346.	1.6	24
44	Untangling the Formation of Methoxymethanol (CH ₃ OCH ₂ OH) and Dimethyl Peroxide (CH ₃ OOCH ₃) in Star-forming Regions. <i>Astrophysical Journal</i> , 2019, 881, 156.	1.6	24
45	The 1 ³ HCN and 1 ³ HCO ⁺ Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9324-9330.	1.1	23
46	Electronically excited states of PANH anions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14761-14772.	1.3	23
47	An Experimental and Theoretical Investigation into the Formation of Ketene (H ₂ CCO) and Ethynol (HCCOH) in Interstellar Analog Ices. <i>Astrophysical Journal</i> , 2020, 896, 88.	1.6	23
48	Symmetry breaking and spectral considerations of the surprisingly floppy <i>c</i> -C ₃ H radical and the related dipole-bound excited state of <i>c</i> -C ₃ H [*] . <i>Journal of Chemical Physics</i> , 2017, 146, 224303.	1.2	22
49	Synthesis of methanediol [CH ₂ (OH) ₂]: The simplest geminal diol. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	22
50	Quartic force field-derived vibrational frequencies and spectroscopic constants for the isomeric pair SNO and OSN and isotopologues. <i>Journal of Chemical Physics</i> , 2015, 143, 084308.	1.2	21
51	Communication: The failure of correlation to describe carbon-carbon bonding in out-of-plane bends. <i>Journal of Chemical Physics</i> , 2017, 147, 221101.	1.2	20
52	Copper-based redox shuttles supported by preorganized tetradentate ligands for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2020, 49, 343-355.	1.6	19
53	Coincidence between Bond Strength, Atomic Abundance, and the Composition of Rocky Materials. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 812-817.	1.2	19
54	The performance of low-cost commercial cloud computing as an alternative in computational chemistry. <i>Journal of Computational Chemistry</i> , 2015, 36, 926-933.	1.5	18

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55	Enstatite (MgSiO ₃) and forsterite (Mg ₂ SiO ₄) monomers and dimers: highly detectable infrared and radioastronomical molecular building blocks. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 492, 276-282.	1.6	18
56	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OF <i>cis</i> -C ₃ H ⁺ . <i>Astrophysical Journal</i> , 2014, 796, 139.	1.6	17
57	PSI4Education: Computational Chemistry Labs Using Free Software. <i>ACS Symposium Series</i> , 2015, , 85-98.	0.5	17
58	Theoretical rovibrational analysis of the covalent noble gas compound ArNH ⁺ . <i>Journal of Molecular Spectroscopy</i> , 2016, 322, 29-32.	0.4	17
59	The case for gas-phase astrochemistry without carbon. <i>Molecular Astrophysics</i> , 2020, 18, 100062.	1.7	17
60	Fundamental Vibrational Frequencies and Spectroscopic Constants of <i>cis</i> - and <i>trans</i> -HOCS, HSCO, and Isotopologues via Quartic Force Fields. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6498-6510.	1.2	16
61	Optimal cloud use of quartic force fields: The first purely commercial cloud computing based study for rovibrational analysis of SiCH ⁺ . <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1650-1657.	1.0	16
62	Vibrational frequencies and spectroscopic constants of three, stable noble gas molecules: NeCCH ⁺ , ArCCH ⁺ , and ArCN ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5230-5238.	1.3	16
63	Towards a quantum chemical protocol for the prediction of rovibrational spectroscopic data for transition metal molecules: Exploration of CuCN, CuOH, and CuCCH. <i>Journal of Chemical Physics</i> , 2017, 147, 234303.	1.2	16
64	Gas-phase spectra of MgO molecules: a possible connection from gas-phase molecules to planet formation. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 474, 2055-2063.	1.6	16
65	Hydrogen Sulfide as a Scavenger of Sulfur Atomic Cation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4983-4987.	1.1	16
66	Pathways to Detection of Strongly-Bound Inorganic Species: The Vibrational and Rotational Spectral Data of AlH ₂ OH, HMgOH, AlH ₂ NH ₂ , and HMgNH ₂ . <i>Frontiers in Astronomy and Space Sciences</i> , 2021, 8, .	1.1	16
67	Anharmonic vibrational frequencies of ammonia borane (BH ₃ NH ₃). <i>Journal of Chemical Physics</i> , 2021, 154, 041104.	1.2	15
68	Experimental identification of aminomethanol (NH ₂ CH ₂ OH) as the key intermediate in the Strecker Synthesis. <i>Nature Communications</i> , 2022, 13, 375.	5.8	15
69	Optical spectra of the silicon-terminated carbon chain radicals SiC _n H (<i>n</i> = 3,4,5). <i>Journal of Chemical Physics</i> , 2014, 141, 044310.	1.2	14
70	Formation of Potential Interstellar Noble Gas Molecules in Gas and Adsorbed Phases. <i>ACS Omega</i> , 2016, 1, 765-772.	1.6	14
71	TOWARD THE ASTRONOMICAL DETECTION OF THE PROTON-BOUND COMPLEX NN ⁺ HCO ⁺ : IMPLICATIONS FOR THE SPECTRA OF PROTOPLANETARY DISKS. <i>Astrophysical Journal</i> , 2016, 819, 141.	1.6	14
72	Quantum Chemical Rovibrational Analysis of the HOSO Radical. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8108-8114.	1.1	14

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73	Rovibrational Considerations for the Monomers and Dimers of Magnesium Hydride and Magnesium Fluoride. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7079-7088.	1.1	14
74	Vibrational and Rovibrational Spectroscopy Applied to Astrochemistry. , 2022, , 235-295.		14
75	ROVIBRATIONAL SPECTROSCOPIC CONSTANTS AND FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR ISOTOPOLOGUES OF CYCLIC AND BENT SINGLET HC ₂ N ISOMERS. <i>Astrophysical Journal</i> , 2013, 778, 160.	1.6	13
76	Predictable Valence Excited States of Anions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10763-10769.	1.1	13
77	Energetics, structure, and rovibrational spectroscopic properties of the sulfurous anions SNO ⁻ and OSN ⁻ . <i>Journal of Chemical Physics</i> , 2015, 143, 184301.	1.2	13
78	Electronic and rovibrational quantum chemical analysis of C ₃ P ⁺ : the next interstellar anion?. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 453, 2825-2830.	1.6	13
79	Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 13048-13054.	1.1	13
80	Inclusion of ¹³ C and D in protonated acetylene. <i>Chemical Physics Letters</i> , 2016, 650, 126-129.	1.2	13
81	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E11072-E11081.	3.3	13
82	An efficient algorithm for the determination of force constants and displacements in numerical definitions of a large, general order Taylor series expansion. <i>Journal of Mathematical Chemistry</i> , 2018, 56, 103-119.	0.7	13
83	A Photoionization Reflectron Time-of-Flight Mass Spectrometric Study on the Detection of Ethynamine (HCCNH ₂) and 2H ₂ Azidine (c ⁻ H ₂ CCHN). <i>ChemPhysChem</i> , 2021, 22, 985-994.	1.0	13
84	Quantum Chemical Analysis of the CO ⁺ HNN ⁺ Proton-Bound Complex. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7745-7752.	1.1	12
85	Binding of the atomic cations hydrogen through argon to water and hydrogen sulfide. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25967-25973.	1.3	12
86	Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. <i>ACS Omega</i> , 2018, 3, 16035-16039.	1.6	12
87	Anharmonic Frequencies and Spectroscopic Constants of OAlOH and AlOH: Strong Bonding but Unhindered Motion. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8834-8841.	1.1	12
88	Full Visible Spectrum Panchromatic Triple Donor Dye for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2020, 124, 25211-25220.	1.5	12
89	On the Formation of the Popcorn Flavorant 2,3-Butanedione (CH ₃ COCOCH ₃) in Acetaldehyde-Containing Interstellar Ices. <i>ChemPhysChem</i> , 2020, 21, 1531-1540.	1.0	12
90	The unsolved issue with out-of-plane bending frequencies for C C multiply bonded systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 248, 119148.	2.0	12

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109	Iron Redox Shuttles with Wide Optical Gap Dyes for High-Voltage Dye-Sensitized Solar Cells. <i>ChemSusChem</i> , 2021, 14, 3084-3096.	3.6	8
110	Rovibrational Quantum Chemical Treatment of Inorganic and Organometallic Astrochemicals. <i>Accounts of Chemical Research</i> , 2021, 54, 271-279.	7.6	8
111	Fundamental Vibrational Frequencies and Spectroscopic Constants of Substituted Cyclopropenylidene ($c\text{-C}_3\text{HX}$, X = F, Cl, CN). <i>Journal of Physical Chemistry A</i> , 2021, 125, 8860-8868.	1.1	8
112	Spectroscopic Characterization of HSO_2^+ and HOSO^+ Intermediates Involved in SO_2 Geoengineering. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10615-10621.	1.1	8
113	Probing halogen bonding interactions between heptafluoro-2-iodopropane and three azabenzenes with Raman spectroscopy and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11713-11720.	1.3	8
114	Methylidyne-replaced boron nitride fullerenes and nanotubes: a wave function study. <i>New Journal of Chemistry</i> , 2016, 40, 8149-8157.	1.4	7
115	A Possible Progenitor of the Interstellar Sulfide Bond: Rovibrational Characterization of the Hydrogen Disulfide Cation HSSH^+ . <i>Astrophysical Journal</i> , 2018, 856, 30.	1.6	7
116	Quantum chemical spectral characterization of CH_2NH_2 for remote sensing of Titan's atmosphere. <i>Icarus</i> , 2018, 299, 187-193.	1.1	7
117	Vibrational analysis of the ubiquitous interstellar molecule cyclopropenylidene ($c\text{-C}_3\text{H}_2$): the importance of numerical stability. <i>Molecular Physics</i> , 2020, 118, e1589007.	0.8	7
118	Vibrational and rotational spectral data for possible interstellar detection of AlH_3OH_2 , SiH_3OH , and SiH_3NH_2 . <i>Monthly Notices of the Royal Astronomical Society</i> , 2021, 508, 2613-2619.	1.6	7
119	Formation of Magnesium and Aluminum Oxides from Water and Metal Hydrides: Creation of the Smallest Ruby. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 18-24.	1.2	7
120	The rovibrational nature of cis- and trans-HNNS: A possible nitrogen molecule progenitor. <i>Journal of Chemical Physics</i> , 2016, 145, 204302.	1.2	6
121	Molecular oxygen generation from the reaction of water cations with oxygen atoms. <i>Journal of Chemical Physics</i> , 2019, 150, 201103.	1.2	6
122	Electronically Excited States of Closed-Shell, Cyano-Functionalized Polycyclic Aromatic Hydrocarbon Anions. <i>Chemistry</i> , 2021, 3, 296-313.	0.9	6
123	(T)+EOM Quartic Force Fields for Theoretical Vibrational Spectroscopy of Electronically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4374-4382.	2.3	6
124	Lewis Acid-Lewis Base Interactions Promote Fast Interfacial Electron Transfers with a Pyridine-Based Donor Dye in Dye-Sensitized Solar Cells. <i>ACS Applied Energy Materials</i> , 2022, 5, 1516-1527.	2.5	6
125	Toward the laboratory identification of the not-so-simple NS_2 neutral and anion isomers. <i>Journal of Chemical Physics</i> , 2017, 147, 074303.	1.2	5
126	NeON^+ : An Atom and a Molecule. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 491-495.	1.2	5

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127	Communication: Gas phase vibrational spectroscopy of the azide-water complex. Journal of Chemical Physics, 2018, 149, 191101.	1.2	5
128	ArCH ₂ ⁺ : A Detectable Noble Gas Molecule. ChemPhysChem, 2018, 19, 3388-3392.	1.0	5
129	The Fundamental Vibrational Frequencies and Spectroscopic Constants of the Dicyanoamine Anion, NCNCN ⁻ (C ₂ N ₃ ⁻): Quantum Chemical Analysis for Astrophysical and Planetary Environments. Astrophysical Journal, 2019, 883, 109.	1.6	5
130	Highly-excited state properties of cumulenone chlorides in the vacuum-ultraviolet. Physical Chemistry Chemical Physics, 2020, 22, 11838-11849.	1.3	5
131	Knowledge Gaps in the Cometary Spectra of Oxygen-bearing Molecular Cations. Astrophysical Journal, Supplement Series, 2021, 256, 6.	3.0	5
132	Theoretical Rovibrational Spectroscopy of Magnesium Tricarbide ⁻ “Multireference Character Thwarts a Full Analysis of All Isomers. Journal of Physical Chemistry A, 2022, 126, 4132-4146.	1.1	5
133	On the spectroscopic constants, first electronic state, vibrational frequencies, and isomerization of hydroxymethylene (HCOH) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.7	4
134	Towards completing the cyclopropenylidene cycle: rovibrational analysis of cyclic N ₃ ⁺ , CNN, HCNN ⁺ , and CNC ⁺ . Physical Chemistry Chemical Physics, 2017, 19, 22860-22869.	1.3	4
135	Bridged HPSi and Linear HSIP as Probes of the SiP Radical in Astrophysical/Interstellar Media. Astrophysical Journal, 2017, 843, 124.	1.6	4
136	Boron-Doped C ₂₄ Fullerenes for Alkyl Functionalization or Potential Polymerization. ACS Omega, 2018, 3, 1001-1006.	1.6	4
137	Patterns of cation binding to the aromatic amino acid R groups in Trp, Tyr, and Phe. Computational Biology and Chemistry, 2018, 72, 11-15.	1.1	4
138	Spectroscopic study of magnesium dinitrogen and sodium dinitrogen cation. Monthly Notices of the Royal Astronomical Society, 2020, 498, 5417-5423.	1.6	4
139	On the possibility of electronically excited states in stable amine anions: Dicyanoamine, cyanoethylamine, and diethylamine. Molecular Astrophysics, 2020, 19, 100070.	1.7	4
140	Computational UV spectra for amorphous solids of small molecules. Physical Chemistry Chemical Physics, 2021, 23, 24413-24420.	1.3	4
141	Valence-, Dipole- and Quadrupole-Bound Electronically Excited States of Closed-Shell Anions Formed by Deprotonation of Cyano- and Ethynyl-Disubstituted Polycyclic Aromatic Hydrocarbons. Chemistry, 2022, 4, 42-56.	0.9	4
142	Anharmonic Vibrational Frequencies of Water Borane and Associated Molecules. Molecules, 2021, 26, 7348.	1.7	4
143	Polycyclic aliphatic hydrocarbons: is tetrahedrane present in UIR spectra?. Physical Chemistry Chemical Physics, 2022, 24, 14348-14353.	1.3	4
144	PSI4EDUCATION: Free and Open-Source Programing Activities for Chemical Education with Free and Open-Source Software. ACS Symposium Series, 0, , 107-122.	0.5	4

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145	Analysis of a bicyclic, triple disulphide molecular nanopropeller. RSC Advances, 2016, 6, 43509-43517.	1.7	3
146	Alkyl-functionalized and methyldiyne-doped boron nitride fullerene polymer precursors. Computational and Theoretical Chemistry, 2017, 1105, 46-51.	1.1	3
147	Two small molecular propellers and their rotational potential energy surfaces. Structural Chemistry, 2017, 28, 1653-1662.	1.0	3
148	Rotational and vibrational fingerprints of the oxywater cation (H ₂ OO ⁺), a possible precursor to abiotic O ₂ . Journal of Molecular Spectroscopy, 2019, 364, 111183.	0.4	3
149	Solvation of HeH ⁺ in neon atoms: Proton-bound complexes of mixed He and Ne. Chemical Physics, 2020, 539, 110927.	0.9	3
150	Infrared spectroscopy and anharmonic theory of H ₃ +Ar _{2,3} complexes: The role of symmetry in solvation. Journal of Chemical Physics, 2020, 153, 134305.	1.2	3
151	Linear and Helical Carbonic Acid Clusters. Journal of Physical Chemistry A, 2021, 125, 4589-4597.	1.1	3
152	Tracking the Amide I and $\hat{\nu}_{\pm}\text{COO}^{\hat{\nu}}$ Terminal $\hat{\nu}_{1/2}(\text{C}=\text{O})$ Raman Bands in a Family of l-Glutamic Acid-Containing Peptide Fragments: A Raman and DFT Study. Molecules, 2021, 26, 4790.	1.7	3
153	Spectral Signatures of Hydrogen Thioperoxide (HOSH) and Hydrogen Persulfide (HSSH): Possible Molecular Sulfur Sinks in the Dense ISM. Molecules, 2022, 27, 3200.	1.7	3
154	Theoretical Characterization of Carbonic Acid Clusters in the UV. Journal of Physical Chemistry A, 2022, 126, 3739-3744.	1.1	3
155	Novel dihydrate formation in p-nitrophenylglyoxal. Structural Chemistry, 2014, 25, 1513-1520.	1.0	2
156	The role of sodium ions in the solubility of peptides. Structural Chemistry, 2016, 27, 1855-1862.	1.0	2
157	Theoretical rovibrational characterization of HAlNP: Weak bonding but strong intensities. Journal of Molecular Spectroscopy, 2021, 377, 111422.	0.4	2
158	Further Astrochemical Insights From Bond Strengths of Small Molecules Containing Atoms From the First Three Rows of the Periodic Table. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	2
159	Anharmonic fundamental vibrational frequencies and spectroscopic constants of the potential HSO ₂ radical astromolecule. Journal of Chemical Physics, 2021, 155, 114301.	1.2	2
160	Anharmonic Vibrational Frequencies and Spectroscopic Constants for the Detection of Ethynol in Space. Frontiers in Astronomy and Space Sciences, 2021, 7, .	1.1	2
161	Exploring different equatorial donors in a series of five-coordinate Cu(II) complexes supported by rigid tetradentate ligands. Polyhedron, 2022, 212, 115558.	1.0	2
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