

Ryan C Fortenberry

List of Publications by Year in descending order

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172
papers

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176
docs citations

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times ranked

1107
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring different equatorial donors in a series of five-coordinate Cu(II) complexes supported by rigid tetradentate ligands. <i>Polyhedron</i> , 2022, 212, 115558.	1.0	2
2	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
3	Valence-, Dipole- and Quadrupole-Bound Electronically Excited States of Closed-Shell Anions Formed by Deprotonation of Cyano- and Ethynyl-Disubstituted Polycyclic Aromatic Hydrocarbons. <i>Chemistry</i> , 2022, 4, 42-56.	0.9	4
4	Benzvalyne: Real or imaginary?. <i>Journal of Chemical Physics</i> , 2022, 156, 024302.	1.2	1
5	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
6	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
7	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
8	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
9	Spectral Signatures of Hydrogen Thioperoxide (HOSH) and Hydrogen Persulfide (HSSH): Possible Molecular Sulfur Sinks in the Dense ISM. <i>Molecules</i> , 2022, 27, 3200.	1.7	3
10	Polycyclic aliphatic hydrocarbons: is tetrahedrane present in UIR spectra?. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14348-14353.	1.3	4
11	Theoretical Characterization of Carbonic Acid Clusters in the UV. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3739-3744.	1.1	3
12	Vibrational and Rovibrational Spectroscopy Applied to Astrochemistry. , 2022, , 235-295.		14
13	Theoretical Rovibrational Spectroscopy of Magnesium Tricarbide-Multireference Character Thwarts a Full Analysis of All Isomers. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4132-4146.	1.1	5
14	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
15	Determination of vibrational band positions in the E-hook of β -tubulin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 244, 118895.	2.0	1
16	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
17	The First Mid-infrared Detection of HNC in the Interstellar Medium: Probing the Extreme Environment toward the Orion Hot Core. <i>Astrophysical Journal</i> , 2021, 907, 51.	1.6	9
18	Anharmonic vibrational frequencies of ammonia borane (BH ₃ NH ₃). <i>Journal of Chemical Physics</i> , 2021, 154, 041104.	1.2	15

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19	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry C, 2021, 125, 4342-4342.	1.5	0
20	Electronically Excited States of Closed-Shell, Cyano-Functionalized Polycyclic Aromatic Hydrocarbon Anions. Chemistry, 2021, 3, 296-313.	0.9	6
21	Pathways to Detection of Strongly-Bound Inorganic Species: The Vibrational and Rotational Spectral Data of AlH_2OH , HMgOH , AlH_2NH_2 , and HMgNH_2 . Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	16
22	Theoretical rovibrational characterization of HAINP: Weak bonding but strong intensities. Journal of Molecular Spectroscopy, 2021, 377, 111422.	0.4	2
23	Space is the Future: Interdisciplinary Research in Astrochemistry and Planetary Science Leads to Innovations That Impact All of Chemistry. Accounts of Chemical Research, 2021, 54, 1309-1310.	7.6	1
24	A Photoionization Reflectron Time-of-Flight Mass Spectrometric Study on the Detection of Ethynamine (HCCNH_2) and 2HäzAzirine ($\text{cäEH}_2\text{CCHN}$). ChemPhysChem, 2021, 22, 985-994.	1.0	13
25	Accurate determination of the onset wavelength (λ_{onset}) of the photoionization cross section of ethynamine (HCCNH_2) by photoionization mass spectrometry. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 265, 107544.	1.1	30
26	Linear and Helical Carbonic Acid Clusters. Journal of Physical Chemistry A, 2021, 125, 4589-4597.	1.1	3
27	(T)+EOM Quartic Force Fields for Theoretical Vibrational Spectroscopy of Electronically Excited States. Journal of Chemical Theory and Computation, 2021, 17, 4374-4382.	2.3	6
28	Iron Redox Shuttles with Wide Optical Gap Dyes for High-Voltage Dye-Sensitized Solar Cells. ChemSusChem, 2021, 14, 3084-3096.	3.6	8
29	Knowledge Gaps in the Cometary Spectra of Oxygen-bearing Molecular Cations. Astrophysical Journal, Supplement Series, 2021, 256, 6.	3.0	5
30	Tracking the Amide I and δCOO^- Terminal $\nu_2(\text{C=O})$ Raman Bands in a Family of l-Glutamic Acid-Containing Peptide Fragments: A Raman and DFT Study. Molecules, 2021, 26, 4790.	1.7	3
31	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
32	Vibrational and rotational spectral data for possible interstellar detection of AlH_3OH_2 , SiH_3OH , and SiH_3NH_2 . Monthly Notices of the Royal Astronomical Society, 2021, 508, 2613-2619.	1.6	7
33	Anharmonic fundamental vibrational frequencies and spectroscopic constants of the potential HSO_2 radical astromolecule. Journal of Chemical Physics, 2021, 155, 114301.	1.2	2
34	Anharmonic Vibrational Frequencies and Spectroscopic Constants for the Detection of Ethynol in Space. Frontiers in Astronomy and Space Sciences, 2021, 7, .	1.1	2
35	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry A, 2021, 125, 1680-1680.	1.1	0
36	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry B, 2021, 125, 1973-1973.	1.2	0

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37	Rovibrational Quantum Chemical Treatment of Inorganic and Organometallic Astrochemicals. <i>Accounts of Chemical Research</i> , 2021, 54, 271-279.	7.6	8
38	Computational UV spectra for amorphous solids of small molecules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24413-24420.	1.3	4
39	Fundamental Vibrational Frequencies and Spectroscopic Constants of Substituted Cyclopropenylidene ($c\text{-C}_{3\text{H}}\text{X}$, X = F, Cl, CN). <i>Journal of Physical Chemistry A</i> , 2021, 125, 8860-8868.	1.1	8

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55	Spectral characterization for small clusters of silicon and oxygen: SiO ₂ , SiO ₃ , Si ₂ O ₃ , & Si ₂ O ₄ . Planetary and Space Science, 2020, 193, 105076.	0.9	8
56	Coincidence between Bond Strength, Atomic Abundance, and the Composition of Rocky Materials. ACS Earth and Space Chemistry, 2020, 4, 812-817.	1.2	19
57	Highly-excited state properties of cumulenone chlorides in the vacuum-ultraviolet. Physical Chemistry Chemical Physics, 2020, 22, 11838-11849.	1.3	5
58	A Molecular Candle Where Few Molecules Shine: HeHHe ⁺ . Molecules, 2020, 25, 2183.	1.7	9
59	On the Formation of the Popcorn Flavorant 2,3-Butanedione (CH ₃ COCOCH ₃) in Acetaldehyde-Containing Interstellar Ices. ChemPhysChem, 2020, 21, 1531-1540.	1.0	12
60	An Experimental and Theoretical Investigation into the Formation of Ketene (H ₂ CCO) and Ethynol (HCCOH) in Interstellar Analog Ices. Astrophysical Journal, 2020, 896, 88.	1.6	23
61	Theoretical rovibrational characterization of the cis/trans-HCSH and H ₂ SC isomers of the known interstellar molecule thioformaldehyde. Journal of Molecular Spectroscopy, 2020, 369, 111273.	0.4	11
62	Overcoming the out-of-plane bending issue in an aromatic hydrocarbon: the anharmonic vibrational frequencies of c-(CH) ₃ H ₂ ⁺ . Physical Chemistry Chemical Physics, 2020, 22, 12951-12958.	1.3	11
63	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. Journal of Physical Chemistry A, 2020, 124, 3191-3204.	1.1	26
64	On the possibility of electronically excited states in stable amine anions: Dicyanoamine, cyanoethynylamine, and diethynylamine. Molecular Astrophysics, 2020, 19, 100070.	1.7	4
65	An Interstellar Synthesis of Glycerol Phosphates. Astrophysical Journal Letters, 2020, 899, L3.	3.0	9
66	Molecular oxygen generation from the reaction of water cations with oxygen atoms. Journal of Chemical Physics, 2019, 150, 201103.	1.2	6
67	Untangling the Formation of Methoxymethanol (CH ₃ OCH ₂ OH) and Dimethyl Peroxide (CH ₃ OOCH ₃) in Star-forming Regions. Astrophysical Journal, 2019, 881, 156.	1.6	24
68	Computational vibrational spectroscopy for the detection of molecules in space. Annual Reports in Computational Chemistry, 2019, 15, 173-202.	0.9	59
69	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
70	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
71	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
72	The noble gas molecule: Stability, vibrational frequencies, and spectroscopic constants. Journal of Molecular Spectroscopy, 2019, 357, 4-8.	0.4	9

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73	The Oldest Molecular Ancestor Finally Brought into the Light. <i>CheM</i> , 2019, 5, 1028-1030.	5.8	9
74	Quantum Chemical Rovibrational Characterization of CH ₂ ClH ⁺ , a Low-Energy Isomer of Ionized Chloromethane. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1296-1301.	1.2	1
75	A Small Molecule with PAH Vibrational Properties and a Detectable Rotational Spectrum: c-(C) ₃ H ₂ , Cyclopropenylidene Carbene. <i>Astrophysical Journal</i> , 2019, 871, 236.	1.6	37
76	Rovibrational Spectral Analysis of CO ₃ and C ₂ O ₃ : Potential Sources for O ₂ Observed in Comet 67P/Churyumov-Gerasimenko. <i>Astrophysical Journal Letters</i> , 2019, 886, L10.	3.0	10
77	Spectroscopic investigation of [Al,N,C,O] refractory molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 244303.	1.2	25
78	The possibility of :CNH ₂ within Titan's atmosphere: Rovibrational analysis of :CNH ₂ and :CCH ₂ . <i>Icarus</i> , 2019, 321, 321.	1.1	1
79	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
80	Boron-Doped C ₂₄ Fullerenes for Alkyl Functionalization or Potential Polymerization. <i>ACS Omega</i> , 2018, 3, 1001-1006.	1.6	4
81	A high-resolution photoelectron imaging and theoretical study of CP ⁺ and C ₂ P ⁺ . <i>Journal of Chemical Physics</i> , 2018, 148, 044301.	1.2	9
82	Patterns of cation binding to the aromatic amino acid R groups in Trp, Tyr, and Phe. <i>Computational Biology and Chemistry</i> , 2018, 72, 11-15.	1.1	4
83	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
84	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
85	NeON ⁺ : An Atom and a Molecule. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 491-495.	1.2	5
86	Overcoming the Failure of Correlation for Out-of-Plane Motions in a Simple Aromatic: Rovibrational Quantum Chemical Analysis of c-C ₃ H ₂ . <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2155-2164.	2.3	33
87	Hydride: Theoretical rovibrational analysis of CH ₂ and CH ₂ ⁺ . <i>Journal of Chemical Physics</i> , 2018, 148, 044301.	0.4	8
88	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
89	Quantum chemical spectral characterization of CH ₂ NH ₂ for remote sensing of Titan's atmosphere. <i>Icarus</i> , 2018, 299, 187-193.	1.1	7
90	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

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91	Communication: Gas phase vibrational spectroscopy of the azide-water complex. Journal of Chemical Physics, 2018, 149, 191101.	1.2	5
92	Counter Anion Effect on the Photophysical Properties of Emissive Indolizine-Cyanine Dyes in Solution and Solid State. Molecules, 2018, 23, 3051.	1.7	34
93	Identifying Molecular Structural Aromaticity for Hydrocarbon Classification. ACS Omega, 2018, 3, 16035-16039.	1.6	12
94	ArCH ₂ ⁺ : A Detectable Noble Gas Molecule. ChemPhysChem, 2018, 19, 3388-3392.	1.0	5
95	Hydrogen Sulfide as a Scavenger of Sulfur Atomic Cation. Journal of Physical Chemistry A, 2018, 122, 4983-4987.	1.1	16
96	Rovibrational analysis of <i>c</i> -SiC ₂ H ₂ : Further evidence for out-of-plane bending issues in correlated methods. Journal of Chemical Physics, 2018, 149, 024303.	1.2	10
97	Rovibrational Considerations for the Monomers and Dimers of Magnesium Hydride and Magnesium Fluoride. Journal of Physical Chemistry A, 2018, 122, 7079-7088.	1.1	14
98	Quantum astrochemical spectroscopy. International Journal of Quantum Chemistry, 2017, 117, 81-91.	1.0	63
99	Vibrational frequencies and spectroscopic constants of three, stable noble gas molecules: NeCCH ⁺ , ArCCH ⁺ , and ArCN ⁺ . Physical Chemistry Chemical Physics, 2017, 19, 5230-5238.	1.3	16
100	Alkyl-functionalized and methyldiyne-doped boron nitride fullerene polymer precursors. Computational and Theoretical Chemistry, 2017, 1105, 46-51.	1.1	3
101	On the Detectability of the HSS, HSO, and HOS Radicals in the Interstellar Medium. Astrophysical Journal, 2017, 835, 243.	1.6	36
102	On the spectroscopic constants, first electronic state, vibrational frequencies, and isomerization of hydroxymethylene (HCOH) $T_{000} = 10450.302$ cm ⁻¹ . http://www.w3.org/1998/Math/MathML	1.7	4
103	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
104	Quantum Chemical Rovibrational Analysis of the HOSO Radical. Journal of Physical Chemistry A, 2017, 121, 8108-8114.	1.1	14
105	Toward the laboratory identification of the not-so-simple NS ₂ neutral and anion isomers. Journal of Chemical Physics, 2017, 147, 074303.	1.2	5
106	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
107	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11072-E11081.	3.3	13
108	Bridged HPSi and Linear HSiP as Probes of the SiP Radical in Astrophysical/Interstellar Media. Astrophysical Journal, 2017, 843, 124.	1.6	4

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109	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
110	Two small molecular propellers and their rotational potential energy surfaces. <i>Structural Chemistry</i> , 2017, 28, 1653-1662.	1.0	3
111	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
112	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
113	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
114	The rovibrational nature of <i>cis</i> - and <i>trans</i> -HNNS: A possible nitrogen molecule progenitor. <i>Journal of Chemical Physics</i> , 2016, 145, 204302.	1.2	6
115	A spectroscopic case for SPSi detection: The third-row in a single molecule. <i>Journal of Chemical Physics</i> , 2016, 145, 124311.	1.2	41
116	Theoretical rovibrational analysis of the covalent noble gas compound ArNH ⁺ . <i>Journal of Molecular Spectroscopy</i> , 2016, 322, 29-32.	0.4	17
117	Inclusion of ¹³ C and D in protonated acetylene. <i>Chemical Physics Letters</i> , 2016, 650, 126-129.	1.2	13
118	Potential interstellar noble gas molecules: ArOH and NeOH rovibrational analysis from quantum chemical quartic force fields. <i>Molecular Astrophysics</i> , 2016, 2, 1	1.7	39
119	Analysis of a bicyclic, triple disulphide molecular nanopropeller. <i>RSC Advances</i> , 2016, 6, 43509-43517.	1.7	3
120	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
121	Excited State Trends in Bidirectionally Expanded Closed-Shell PAH and PANH Anions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7327-7334.	1.1	8
122	The role of sodium ions in the solubility of peptides. <i>Structural Chemistry</i> , 2016, 27, 1855-1862.	1.0	2
123	Methyldiyne-replaced boron nitride fullerenes and nanotubes: a wave function study. <i>New Journal of Chemistry</i> , 2016, 40, 8149-8157.	1.4	7
124	Quantum Chemical Analysis of the CO ⁺ HNN ⁺ Proton-Bound Complex. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7745-7752.	1.1	12
125	Formation of Potential Interstellar Noble Gas Molecules in Gas and Adsorbed Phases. <i>ACS Omega</i> , 2016, 1, 765-772.	1.6	14
126	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

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127	Communication: Spectroscopic consequences of proton delocalization in OCHCO ⁺ . Journal of Chemical Physics, 2015, 143, 071102.	1.2	42
128	Energetics, structure, and rovibrational spectroscopic properties of the sulfurous anions SNO ⁺ and OSN ⁺ . Journal of Chemical Physics, 2015, 143, 184301.	1.2	13
129	Electronic and rovibrational quantum chemical analysis of C ₃ P ⁺ : the next interstellar anion?. Monthly Notices of the Royal Astronomical Society, 2015, 453, 2825-2830.	1.6	13
130	Optimal cloud use of quartic force fields: The first purely commercial cloud computing based study for rovibrational analysis of SiCH ⁺ . International Journal of Quantum Chemistry, 2015, 115, 1650-1657.	1.0	16
131	The performance of low-cost commercial cloud computing as an alternative in computational chemistry. Journal of Computational Chemistry, 2015, 36, 926-933.	1.5	18
132	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN ⁺ . Journal of Physical Chemistry A, 2015, 119, 11623-11631.	1.1	81
133	Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. Journal of Physical Chemistry A, 2015, 119, 13048-13054.	1.1	13
134	Excited vibrational level rotational constants for SiC ₂ : A sensitive molecular diagnostic for astrophysical conditions. Molecular Astrophysics, 2015, 1, 13-19.	1.7	60
135	ArH ₂ ⁺ and NeH ₂ ⁺ as global minima in the Ar ⁺ /Ne ⁺ +H ₂ reactions: energetic, spectroscopic, and structural data. Monthly Notices of the Royal Astronomical Society, 2015, 446, 195-204.	1.6	31
136	Rovibrational and energetic analysis of the hydroxyethynyl anion (CCOH ⁺). Molecular Physics, 2015, 113, 2012-2017.	0.8	9
137	Factors affecting the solubility of ionic compounds. Computational and Theoretical Chemistry, 2015, 1069, 132-137.	1.1	10
138	Theoretical Rovibronic Treatment of the X ¹ _f ² and ¹ _f ² States of C ₂ H and the X ¹ _f ¹ State of C ₂ H ⁺ from Quartic Force Fields. Journal of Physical Chemistry A, 2015, 119, 7013-7025.	1.1	34
139	Additional diffuse functions in basis sets for dipole-bound excited states of anions. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	26
140	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
141	Electronically excited states of PANH anions. Physical Chemistry Chemical Physics, 2015, 17, 14761-14772.	1.3	23
142	PSI4Education: Computational Chemistry Labs Using Free Software. ACS Symposium Series, 2015, , 85-98.	0.5	17
143	Interstellar Anions: The Role of Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 9941-9953.	1.1	47
144	Quartic force field-derived vibrational frequencies and spectroscopic constants for the isomeric pair SNO and OSN and isotopologues. Journal of Chemical Physics, 2015, 143, 084308.	1.2	21

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145	Force fields for excited electronic states: Rovibronic reference data for the $1 \text{ } ^2\Sigma^+$ and $1 \text{ } ^2\Pi$ states of C_3H^+ . <i>Astrophysical Journal</i> , 2014, 796, 139.	1.6	17
146	QUANTUM CHEMICAL ROVIBRATIONAL DATA FOR THE INTERSTELLAR DETECTION OF C_3H^+ . <i>Astrophysical Journal</i> , 2014, 796, 139.	1.6	17
147	Predictable Valence Excited States of Anions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10763-10769.	1.1	13
148	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
149	Optical spectra of the silicon-terminated carbon chain radicals SiC_nH ($n = 3, 4, 5$). <i>Journal of Chemical Physics</i> , 2014, 141, 044310.	1.2	14
150	Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C_2H_3^+ , and Its Isotopologues. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7034-7043.	1.1	75
151	Novel dihydrate formation in p-nitrophenylglyoxal. <i>Structural Chemistry</i> , 2014, 25, 1513-1520.	1.0	2
152	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
153	On the use of quartic force fields in variational calculations. <i>Chemical Physics Letters</i> , 2013, 574, 1-12.	1.2	66
154	Dipole Surface and Infrared Intensities for the <i>cis</i> - and <i>trans</i> -HOCO and DOCO Radicals. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6932-6939.	1.1	30
155	Vibrational Frequencies and Spectroscopic Constants for $1 \text{ } ^3\Sigma^+$ HNC and $1 \text{ } ^3\Sigma^+$ HOC from High-Accuracy Quartic Force Fields. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11339-11345.	1.1	10
156	Singlet excited states of anions with higher main group elements. <i>Molecular Physics</i> , 2013, 111, 3265-3275.	0.8	26
157	The $1 \text{ } ^3\Sigma^+$ HCN and $1 \text{ } ^3\Sigma^+$ HCO Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9324-9330.	1.1	23
158	SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES FOR <i>l</i> - C_3H^+ AND ISOTOPOLOGUES FROM HIGHLY ACCURATE QUARTIC FORCE FIELDS: THE DETECTION OF <i>l</i> - C_3H^+ IN THE HORSEHEAD NEBULA PDR QUESTIONED. <i>Astrophysical Journal Letters</i> , 2013, 768, L25.	3.0	54
159	HIGH-ACCURACY QUARTIC FORCE FIELD CALCULATIONS FOR THE SPECTROSCOPIC CONSTANTS AND VIBRATIONAL FREQUENCIES OF $1 \text{ } ^1\Sigma^+$ C_3H^+ : A POSSIBLE LINK TO LINES OBSERVED IN THE HORSEHEAD NEBULA PHOTODISSOCIATION REGION. <i>Astrophysical Journal</i> , 2013, 772, 39.	1.6	63
160	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
161	ROVIBRATIONAL SPECTROSCOPIC CONSTANTS AND FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR ISOTOPOLOGUES OF CYCLIC AND BENT SINGLET HC_2N ISOMERS. <i>Astrophysical Journal</i> , 2013, 778, 160.	1.6	13
162	THE POSSIBLE INTERSTELLAR ANION CH_2CN^- : SPECTROSCOPIC CONSTANTS, VIBRATIONAL FREQUENCIES, AND OTHER CONSIDERATIONS. <i>Astrophysical Journal</i> , 2013, 762, 121.	1.6	38

#	ARTICLE	IF	CITATIONS
163	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
164	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
165	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
166	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
167	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
168	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
169	Electronically Excited States in Interstellar Chemistry. <i>Annual Reports in Computational Chemistry</i> , 2011, 7, 195-214.	0.9	9
170	A benchmark study of the vertical electronic spectra of the linear chain radicals C ₂ H and C ₄ H. <i>Journal of Chemical Physics</i> , 2010, 132, 144303.	1.2	40
171	The Thermal Isomerization of Benzvalyne to Benzyne. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
172	PSI4EDUCATION: Free and Open-Source Programming Activities for Chemical Education with Free and Open-Source Software. <i>ACS Symposium Series</i> , 0, , 107-122.	0.5	4