

# Gary E Douberly

## List of Publications by Year in descending order

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73  
papers

1,559  
citations

257450

24  
h-index

330143

37  
g-index

74  
all docs

74  
docs citations

74  
times ranked

1238  
citing authors

#	ARTICLE	IF	CITATIONS
1	How to VPT2: Accurate and Intuitive Simulations of CH Stretching Infrared Spectra Using VPT2+K with Large Effective Hamiltonian Resonance Treatments. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1301-1324.	2.5	72
2	Four isomers of In <sub>2</sub> H <sub>2</sub> : a careful comparison between theory and experiment. <i>Molecular Physics</i> , 2021, 119, .	1.7	5
3	Kinetic Stability of Pentazole. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9092-9098.	2.5	5
4	Potential energy profile for the Cl + (H <sub>2</sub> O) <sub>3</sub> → HCl + (H <sub>2</sub> O) <sub>2</sub> OH reaction. A CCSD(T) study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26837-26842.	2.8	2
5	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. <i>Journal of Chemical Physics</i> , 2020, 152, 024302.	3.0	8
6	Infrared spectroscopy of H+(CO) <sub>2</sub> in the gas phase and in para-hydrogen matrices. <i>Journal of Chemical Physics</i> , 2020, 153, 084305.	3.0	4
7	Infrared photodissociation spectroscopy and anharmonic vibrational study of the HO <sub>4</sub> <sup>+</sup> molecular ion. <i>Journal of Chemical Physics</i> , 2020, 152, 174309.	3.0	3
8	The 75th International Symposium on Molecular Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4873-4874.	2.5	0
9	Infrared spectroscopy of the n-propyl and i-propyl radicals in solid para-hydrogen. <i>Journal of Molecular Spectroscopy</i> , 2019, 363, 111170.	1.2	8
10	Characterization of the 2-methylvinoxy radical + O <sub>2</sub> reaction: A focal point analysis and composite multireference study. <i>Journal of Chemical Physics</i> , 2019, 151, 124302.	3.0	11
11	<i>tert</i> -Butyl peroxy radical: ground and first excited state energetics and fundamental frequencies. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9747-9758.	2.8	7
12	Convergent energies and anharmonic vibrational spectra of Ca <sub>2</sub> H <sub>2</sub> and Ca <sub>2</sub> H <sub>4</sub> constitutional isomers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10914-10922.	2.8	4
13	Ethyl + O <sub>2</sub> in Helium Nanodroplets: Infrared Spectroscopy of the Ethylperoxy Radical. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3558-3568.	2.5	16
14	Infrared Spectrum of Fulvenallene and Fulvenallenyl in Helium Droplets. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3782-3792.	2.5	5
15	Rotamers of Isoprene: Infrared Spectroscopy in Helium Droplets and Ab Initio Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2018, 122, 148-158.	2.5	17
16	Infrared spectroscopy of propene in solid para-hydrogen and helium droplets: The role of matrix shifts in the analysis of anharmonic resonances. <i>Journal of Molecular Spectroscopy</i> , 2018, 354, 7-14.	1.2	10
17	Formation of Exotic Networks of Water Clusters in Helium Droplets Facilitated by the Presence of Neon Atoms. <i>Journal of the American Chemical Society</i> , 2017, 139, 4152-4156.	13.7	20
18	Infrared Spectroscopy of the Entrance Channel Complex Formed Between the Hydroxyl Radical and Methane in Helium Nanodroplets. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7597-7602.	2.5	6

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19	Helium Nanodroplet Isolation of the Cyclobutyl, 1-Methylallyl, and Allylcarbinyl Radicals: Infrared Spectroscopy and Ab Initio Computations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7576-7587.	2.5	12
20	Sequential Capture of O(3P) and HCN by Helium Nanodroplets: Infrared Spectroscopy and ab Initio Computations of the $3\Sigma^- \text{O} \cdots \text{HCN}$ Complex. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9466-9473.	2.5	4
21	Infrared laser spectroscopy of the <i>n</i> -propyl and <i>i</i> -propyl radicals: Stretch-bend Fermi coupling in the alkyl CH stretch region. <i>Journal of Chemical Physics</i> , 2016, 145, 224304.	3.0	19
22	Infrared Stark and Zeeman spectroscopy of OH $\cdots$ CO: The entrance channel complex along the OH + CO $\hat{\rightarrow}$ trans-HOCO reaction pathway. <i>Journal of Chemical Physics</i> , 2016, 145, 124310.	3.0	6
23	Two-center three-electron bonding in ClNH <sub>3</sub> revealed via helium droplet infrared laser Stark spectroscopy: Entrance channel complex along the Cl + NH <sub>3</sub> $\hat{\rightarrow}$ ClNH <sub>2</sub> + H reaction. <i>Journal of Chemical Physics</i> , 2016, 144, 164301.	3.0	13
24	Infrared Spectroscopy of the Tropyli Radical in Helium Droplets. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6768-6773.	2.5	6
25	Mid-infrared signatures of hydroxyl containing water clusters: Infrared laser Stark spectroscopy of OH $\cdots$ H <sub>2</sub> O and OH(D <sub>2</sub> O) ( <i>n</i> = 1-3). <i>Journal of Chemical Physics</i> , 2015, 143, 164304.	3.0	23
26	On the Stark effect in open shell complexes exhibiting partially quenched electronic angular momentum: Infrared laser Stark spectroscopy of OH $\cdots$ C <sub>2</sub> H <sub>2</sub> , OH $\cdots$ C <sub>2</sub> H <sub>4</sub> , and OH $\cdots$ H <sub>2</sub> O. <i>Journal of Molecular Spectroscopy</i> , 2015, 314, 54-62.	1.2	2
27	Infrared rovibrational spectroscopy of OH $\cdots$ C <sub>2</sub> H <sub>2</sub> in 4He nanodroplets: Parity splitting due to partially quenched electronic angular momentum. <i>Journal of Chemical Physics</i> , 2015, 142, 134306.	3.0	9
28	Infrared Spectroscopy of OH $\cdots$ CH <sub>3</sub> OH: Hydrogen-Bonded Intermediate Along the Hydrogen Abstraction Reaction Path. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8125-8132.	2.5	26
29	Reactive intermediates in 4He nanodroplets: Infrared laser Stark spectroscopy of dihydroxycarbene. <i>Journal of Chemical Physics</i> , 2015, 142, 144309.	3.0	6
30	Infrared Laser Spectroscopy of the L-Shaped Cl $\cdots$ HCl Complex Formed in Superfluid <sup>4</sup> He Nanodroplets. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12028-12035.	2.5	8
31	Infrared laser Stark spectroscopy of hydroxymethoxycarbene in 4He nanodroplets. <i>Chemical Physics Letters</i> , 2015, 639, 99-104.	2.6	2
32	Single and double resonance spectroscopy of methanol embedded in superfluid helium nanodroplets. <i>Journal of Chemical Physics</i> , 2014, 141, 044301.	3.0	13
33	Communication: Helium nanodroplet isolation and rovibrational spectroscopy of hydroxymethylene. <i>Journal of Chemical Physics</i> , 2014, 140, 171102.	3.0	9
34	Observation of the <i>Q</i> ( <sup>3</sup> / <sub>2</sub> ) $\hat{\rightarrow}$ doublet transitions for <i>X</i> ( <sup>2</sup> / <sub>2</sub> ) $\hat{\rightarrow}$ <sup>3</sup> / <sub>2</sub> OD in helium nanodroplets. <i>Molecular Physics</i> , 2014, 112, 301-303.	1.7	4
35	Liquid Hot NAGMA Cooled to 0.4 K: Benchmark Thermochemistry of a Gas-Phase Peptide. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9692-9700.	2.5	14
36	Helium Nanodroplet Isolation and Infrared Spectroscopy of the Isolated Ion-Pair 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9047-9056.	2.5	34

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37	Infrared Spectra in the 3 $\hat{1}/4$ m Region of Ethane and Ethane Clusters in Helium Droplets. Journal of Physical Chemistry A, 2013, 117, 13648-13653.	2.5	16
38	Rovibrational spectroscopy of formaldehyde in helium nanodroplets. Journal of Molecular Spectroscopy, 2013, 292, 15-19.	1.2	11
39	Automation of an $\hat{e}$ continuous-wave optical parametric oscillator. Review of Scientific Instruments, 2013, 84, 013102.	1.3	49
40	The ethyl radical in superfluid helium nanodroplets: Rovibrational spectroscopy and <i>ab initio</i> computations. Journal of Chemical Physics, 2013, 138, 194303.	3.0	26
41	Infrared spectroscopy and tunneling dynamics of the vinyl radical in 4He nanodroplets. Journal of Chemical Physics, 2013, 138, 174302.	3.0	12
42	Dipole Moment of the HOOO Radical: Resolution of a Structural Enigma. Journal of Physical Chemistry Letters, 2013, 4, 3584-3589.	4.6	23
43	Rotational Dynamics of the Methyl Radical in Superfluid <sup>4</sup> He Nanodroplets. Journal of Physical Chemistry A, 2013, 117, 11640-11647.	2.5	27
44	Propargyl + O <sub>2</sub> Reaction in Helium Droplets: Entrance Channel Barrier or Not?. Journal of Physical Chemistry A, 2013, 117, 13626-13635.	2.5	39
45	Anomalous $\hat{b}$ -Doubling in the Infrared Spectrum of the Hydroxyl Radical in Helium Nanodroplets. Journal of Physical Chemistry A, 2013, 117, 8103-8110.	2.5	24
46	Infrared laser spectroscopy of the helium-solvated allyl and allyl peroxy radicals. Journal of Chemical Physics, 2013, 139, 234301.	3.0	16
47	Helium Nanodroplet Isolation Spectroscopy and <i>ab Initio</i> Calculations of HO <sub>3</sub> $\hat{z}$ (O <sub>2</sub> ) <sub>n</sub> Clusters. ChemPhysChem, 2013, 14, 764-770.	2.1	6
48	Infrared spectroscopy of HOOO and DOOO in 4He nanodroplets. Journal of Chemical Physics, 2012, 137, 184302.	3.0	30
49	On the Al+HCN reaction in helium nanodroplets. Chemical Physics Letters, 2012, 551, 54-59.	2.6	6
50	Infrared Laser Spectroscopy of the CH <sub>3</sub> OO Radical Formed from the Reaction of CH <sub>3</sub> and O <sub>2</sub> within a Helium Nanodroplet. Journal of Physical Chemistry A, 2012, 116, 5299-5304.	2.5	28
51	Quantum Cascade Laser Spectroscopy and Photoinduced Chemistry of Al $\hat{e}$ (CO) <sub>n</sub> Clusters in Helium Nanodroplets. Journal of Physical Chemistry A, 2011, 115, 7437-7447.	2.5	26
52	Infrared Spectra of HCl $\hat{h}$ H <sub>2</sub> O Clusters in Helium Nanodroplets. Journal of Physical Chemistry Letters, 2010, 1, 2233-2238.	4.6	75
53	Infrared Spectroscopy of (HCl) <sub>m</sub> (H <sub>2</sub> O) <sub>n</sub> Clusters in Helium Nanodroplets: Definitive Assignments in the HCl Stretch Region. Journal of Physical Chemistry A, 2010, 114, 8090-8098.	2.5	56
54	(HCN) <sub>m</sub> $\hat{h}$ M <sub>n</sub> (M = K, Ca, Sr): Vibrational Excitation Induced Solvation and Desolvation of Dopants in and on Helium Nanodroplets. Journal of Physical Chemistry A, 2010, 114, 3391-3402.	2.5	18

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55	THE INFRARED SPECTRUM OF PROTONATED NAPHTHALENE AND ITS RELEVANCE FOR THE UNIDENTIFIED INFRARED BANDS. <i>Astrophysical Journal</i> , 2009, 702, 301-306.	4.5	137
56	Infrared spectroscopy of the protonated nitrogen dimer: The complexity of shared proton vibrations. <i>Journal of Chemical Physics</i> , 2009, 131, 104312.	3.0	32
57	High-resolution infrared spectroscopy of Mg <sup>+</sup> HF and Mg <sup>+</sup> (HF) <sub>2</sub> solvated in helium nanodroplets. <i>Journal of Chemical Physics</i> , 2009, 130, 184313.	3.0	4
58	Vibrational dynamics of the linear and bent isomers of HF <sup>+</sup> N <sub>2</sub> O trapped in 0.4K helium nanodroplets. <i>Chemical Physics</i> , 2009, 361, 118-124.	1.9	3
59	Infrared spectroscopy of protonated ethylene: The nature of proton binding in the non-classical structure. <i>Chemical Physics Letters</i> , 2009, 480, 17-20.	2.6	36
60	Infrared Spectroscopy of Perdeuterated Protonated Water Clusters in the Vicinity of the Clathrate Cage. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8449-8453.	2.5	43
61	Infrared spectroscopy of gas phase C <sub>3</sub> H <sub>5</sub> <sup>+</sup> : The allyl and 2-propenyl cations. <i>Journal of Chemical Physics</i> , 2008, 128, 021102.	3.0	42
62	The structure of protonated acetone and its dimer: infrared photodissociation spectroscopy from 800 to 4000 cm <sup>-1</sup> . <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 77-79.	2.8	41
63	Infrared Spectroscopy of the tert-Butyl Cation in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2007, 129, 13782-13783.	13.7	48
64	Infrared <sup>+</sup> Infrared Double Resonance Spectroscopy of the Isomers of Acetylene <sup>+</sup> HCN and Cyanoacetylene <sup>+</sup> HCN in Helium Nanodroplets <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2007, 111, 7282-7291.	2.5	13
65	Rotational Dynamics of HCN <sup>+</sup> M (M = Na, K, Rb, Cs) van der Waals Complexes Formed on the Surface of Helium Nanodroplets <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2007, 111, 7292-7302.	2.5	15
66	Rovibrational Spectra for the HCCCN <sup>+</sup> HCN and HCN <sup>+</sup> HCCCN Binary Complexes in 4He Droplets <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2007, 111, 7516-7528.	2.5	8
67	Infrared Spectroscopy of Prereactive Aluminum <sup>+</sup> , Gallium <sup>+</sup> , and Indium <sup>+</sup> HCN Entrance Channel Complexes Solvated in Helium Nanodroplets. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12304-12316.	2.5	12
68	IR <sup>+</sup> IR double resonance spectroscopy in helium nanodroplets: Photo-induced isomerization. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 463-468.	2.8	33
69	Organization of Peptide Nanotubes into Macroscopic Bundles. <i>Langmuir</i> , 2001, 17, 7918-7922.	3.5	39
70	Fabrication of Nanocrystal Tube Using Peptide Tubule as Template and Its Application as Signal-Enhancing Cuvette. <i>Journal of Physical Chemistry B</i> , 2001, 105, 1683-1686.	2.6	45
71	Fabrication of Protein Tubules: Immobilization of Proteins on Peptide Tubules. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7612-7618.	2.6	52
72	Protein Tubule Immobilization on Self-Assembled Monolayers on Au Substrates. <i>Nano Letters</i> , 2001, 1, 461-464.	9.1	55

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73	The noncovalent interaction between water and the $3P$ ground state of the oxygen atom*. Molecular Physics, 0, , .	1.7	0