David F Bocian

List of Publications by Year
in descending order

113 papers	6,919 citations	87401 40 h-index	68831 81 g-index
113 all docs	113 docs citations	113 times ranked	5769 citing authors

#	ARTICLE	IF	CITATIONS
1	Hidden vibronic and excitonic structure and vibronic coherence transfer in the bacterial reaction center. Science Advances, 2022, 8, eabk0953.	4.7	20
2	De Novo Synthesis of Bacteriochlorins Bearing Four Trideuteriomethyl Groups. Organics, 2022, 3, 22-37.	0.6	3
3	Beyond green with synthetic chlorophylls â€“ Connecting structural features with spectral properties. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2022, 52, 100513.	5.6	12
4	A perspective on the redox properties of tetrapyrrole macrocycles. Physical Chemistry Chemical Physics, 2021, 23, 19130-19140.	1.3	15
5	The fluorescence quantum yield parameter in FÃ¶rster resonance energy transfer (FRET)â€"Meaning, misperception, and molecular design. Chemical Physics Reviews, 2021, 2, 011302.	2.6	20
6	Comprehensive review of photophysical parameters (Îµ, Î¦f, Ï„s) of tetraphenylporphyrin (H2TPP) and zinc tetraphenylporphyrin (ZnTPP) â€“ Critical benchmark molecules in photochemistry and photosynthesis. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 46, 100401.	5.6	90
7	Conjugated-linker dependence of the photophysical properties and electronic structure of chlorin dyads. Journal of Porphyrins and Phthalocyanines, 2021, 25, 639-663.	0.4	4
8	Electronic Structure and Excited-State Dynamics of Ryleneâ€“Tetrapyrrole Panchromatic Absorbers. Journal of Physical Chemistry A, 2021, 125, 7900-7919.	1.1	7
9	Photophysical Properties and Electronic Structure of Zinc(II) Porphyrins Bearing 0â€“4 <i>meso</i>-Phenyl Substituents: Zinc Porphine to Zinc Tetraphenylporphyrin (ZnTPP). Journal of Physical Chemistry A, 2020, 124, 7776-7794.	1.1	28
10	Annulated bacteriochlorins for near-infrared photophysical studies. New Journal of Chemistry, 2019, 43, 7209-7232.	1.4	16
11	New molecular design for blue BODIPYs. New Journal of Chemistry, 2019, 43, 7233-7242.	1.4	7
12	Expanding Covalent Attachment Sites of Nonnative Chromophores to Encompass the Câ€Terminal Hydrophilic Domain in Biohybrid Lightâ€Harvesting Architectures. ChemPhotoChem, 2018, 2, 300-313.	1.5	2
13	Primary processes in the bacterial reaction center probed by two-dimensional electronic spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3563-3568.	3.3	53
14	Origin of Panchromaticity in Multichromophoreâ€“Tetrapyrrole Arrays. Journal of Physical Chemistry A, 2018, 122, 7181-7201.	1.1	20
15	Synthesis of arrays containing porphyrin, chlorin, and perylene-imide constituents for panchromatic light-harvesting and charge separation. RSC Advances, 2018, 8, 23854-23874.	1.7	22
16	Electronic Interactions in the Bacterial Reaction Center Revealed by Two-Color 2D Electronic Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 5219-5225.	2.1	19
17	Synthesis and photophysical characterization of bacteriochlorins equipped with integral swallowtail substituents. New Journal of Chemistry, 2017, 41, 4360-4376.	1.4	10
18	Photophysical Characterization of the Naturally Occurring Dioxobacteriochlorin Tolyporphin A and Synthetic Oxobacteriochlorin Analogues. Photochemistry and Photobiology, 2017, 93, 1204-1215.	1.3	24

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19	Synthesis, photophysics and electronic structure of oxobacteriochlorins. New Journal of Chemistry, 2017, 41, 3732-3744.	1.4	16
20	Characterization of Hydroporphyrins Covalently Attached to Si(100). Journal of Porphyrins and Phthalocyanines, 2017, 21, 453-464.	0.4	4
21	Tailoring Panchromatic Absorption and Excited-State Dynamics of Tetrapyrroleâ€"Chromophore (Bodipy, Rylene) Arraysâ€"Interplay of Orbital Mixing and Configuration Interaction. Journal of the American Chemical Society, 2017, 139, 17547-17564.	6.6	34
22	New insights into the photochemistry of carotenoid spheroidenone in light-harvesting complex 2 from the purple bacterium Rhodobacter sphaeroides. Photosynthesis Research, 2017, 131, 291-304.	1.6	21
23	Photophysical Properties and Electronic Structure of Porphyrins Bearing Zero to Four <i>meso</i>-Phenyl Substituents: New Insights into Seemingly Well Understood Tetrapyrroles. Journal of Physical Chemistry A, 2016, 120, 9719-9731.	1.1	75
24	Integration of Cyanine, Merocyanine and Styryl Dye Motifs with Synthetic Bacteriochlorins. Photochemistry and Photobiology, 2016, 92, 111-125.	1.3	7
25	Photophysical comparisons of PEGylated porphyrins, chlorins and bacteriochlorins in water. New Journal of Chemistry, 2016, 40, 9648-9656.	1.4	23
26	Panchromatic chromophoreâ€"tetrapyrrole light-harvesting arrays constructed from Bodipy, perylene, terrylene, porphyrin, chlorin, and bacteriochlorin building blocks. New Journal of Chemistry, 2016, 40, 8032-8052.	1.4	38
27	Tuning the Electronic Structure and Properties of Peryleneâ€"Porphyrinâ€"Perylene Panchromatic Absorbers. Journal of Physical Chemistry A, 2016, 120, 7434-7450.	1.1	12
28	Bioconjugatable, PEGylated hydroporphyrins for photochemistry and photomedicine. Narrow-band, red-emitting chlorins. New Journal of Chemistry, 2016, 40, 7721-7740.	1.4	29
29	Bioconjugatable, PEGylated hydroporphyrins for photochemistry and photomedicine. Narrow-band, near-infrared-emitting bacteriochlorins. New Journal of Chemistry, 2016, 40, 7750-7767.	1.4	15
30	Quenching Capabilities of Long-Chain Carotenoids in Light-Harvesting-2 Complexes from <i>Rhodobacter sphaeroides</i> with an Engineered Carotenoid Synthesis Pathway. Journal of Physical Chemistry B, 2016, 120, 5429-5443.	1.2	22
31	Synthesis and photophysical characteristics of 2,3,12,13-tetraalkylbacteriochlorins. New Journal of Chemistry, 2016, 40, 5942-5956.	1.4	20
32	Effects of Strong Electronic Coupling in Chlorin and Bacteriochlorin Dyads. Journal of Physical Chemistry A, 2016, 120, 379-395.	1.1	28
33	Synthetic bacteriochlorins bearing polar motifs (carboxylate, phosphonate, ammonium and a short) Tj ETQq1 1 0.784314 rgBT /Overl 2015, 39, 5694-5714.	1.4	25
34	Photophysical Properties and Electronic Structure of Chlorin-Imides: Bridging the Gap between Chlorins and Bacteriochlorins. Journal of Physical Chemistry B, 2015, 119, 7503-7515.	1.2	27
35	Effects of Substituents on Synthetic Analogs of Chlorophylls. Part 4: How Formyl Group Location Dictates the Spectral Properties of Chlorophyllsb,dandf. Photochemistry and Photobiology, 2015, 91, 331-342.	1.3	20
36	Self-Assembled Light-Harvesting System from Chromophores in Lipid Vesicles. Journal of Physical Chemistry B, 2015, 119, 10231-10243.	1.2	35

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37	Functional characteristics of spirilloxanthin and keto-bearing Analogues in light-harvesting LH2 complexes from Rhodobacter sphaeroides with a genetically modified carotenoid synthesis pathway. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 640-655.	0.5	20
38	Extending the Short and Long Wavelength Limits of Bacteriochlorin Near-Infrared Absorption via Dioxo- and Bisimide-Functionalization. Journal of Physical Chemistry B, 2015, 119, 4382-4395.	1.2	55
39	Enhanced Lightâ€Harvesting Capacity by Micellar Assembly of Free Accessory Chromophores and LH1â€like Antennas. Photochemistry and Photobiology, 2014, 90, 1264-1276.	1.3	11
40	Probing Electronic Communication for Efficient Light-Harvesting Functionality: Dyads Containing a Common Perylene and a Porphyrin, Chlorin, or Bacteriochlorin. Journal of Physical Chemistry B, 2014, 118, 1630-1647.	1.2	22
41	Amphiphilic, hydrophilic, or hydrophobic synthetic bacteriochlorins in biohybrid light-harvesting architectures: consideration of molecular designs. Photosynthesis Research, 2014, 122, 187-202.	1.6	11
42	Panchromatic absorbers for solar light-harvesting. Chemical Communications, 2014, 50, 14512-14515.	2.2	34
43	Vibronic Characteristics and Spin-Density Distributions in Bacteriochlorins as Revealed by Spectroscopic Studies of 16 Isotopologues. Implications for Energy- and Electron-Transfer in Natural Photosynthesis and Artificial Solar-Energy Conversion. Journal of Physical Chemistry B, 2014, 118, 7520-7532.	1.2	14
44	Versatile design of biohybrid light-harvesting architectures to tune location, density, and spectral coverage of attached synthetic chromophores for enhanced energy capture. Photosynthesis Research, 2014, 121, 35-48.	1.6	32
45	Distinct Photophysical and Electronic Characteristics of Strongly Coupled Dyads Containing a Perylene Accessory Pigment and a Porphyrin, Chlorin, or Bacteriochlorin. Journal of Physical Chemistry B, 2013, 117, 9288-9304.	1.2	36
46	Palette of lipophilic bioconjugatable bacteriochlorins for construction of biohybrid light-harvesting architectures. Chemical Science, 2013, 4, 2036.	3.7	47
47	Integration of multiple chromophores with native photosynthetic antennas to enhance solar energy capture and delivery. Chemical Science, 2013, 4, 3924.	3.7	37
48	Serendipitous synthetic entrÃ©e to tetradehydro analogues of cobalamins. New Journal of Chemistry, 2013, 37, 3964.	1.4	6
49	Photophysical Properties and Electronic Structure of Bacteriochlorinâ€“Chalcones with Extended Nearâ€Infrared Absorption. Photochemistry and Photobiology, 2013, 89, 586-604.	1.3	21
50	Amphiphilic chlorins and bacteriochlorins in micellar environments. Molecular design, de novo synthesis, and photophysical properties. Chemical Science, 2013, 4, 3459.	3.7	32
51	Biohybrid Photosynthetic Antenna Complexes for Enhanced Light-Harvesting. Journal of the American Chemical Society, 2012, 134, 4589-4599.	6.6	87
52	Synthesis and Physicochemical Properties of Metallobacteriochlorins. Inorganic Chemistry, 2012, 51, 9443-9464.	1.9	89
53	Effects of Substituents on Synthetic Analogs of Chlorophylls. Part 3: The Distinctive Impact of Auxochromes at the 7â€•<i>versus</i> 3â€Positions. Photochemistry and Photobiology, 2012, 88, 651-674.	1.3	34
54	De novo synthesis and properties of analogues of the self-assembling chlorosomal bacteriochlorophylls. New Journal of Chemistry, 2011, 35, 2671.	1.4	17

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55	De novo synthesis and photophysical characterization of annulated bacteriochlorins. Mimicking and extending the properties of bacteriochlorophylls. New Journal of Chemistry, 2011, 35, 587.	1.4	40
56	Photophysical Properties and Electronic Structure of Stable, Tunable Synthetic Bacteriochlorins: Extending the Features of Native Photosynthetic Pigments. Journal of Physical Chemistry B, 2011, 115, 10801-10816.	1.2	93
57	Structural characteristics that make chlorophylls green: interplay of hydrocarbon skeleton and substituents. New Journal of Chemistry, 2011, 35, 76-88.	1.4	40
58	Encoding isotopic watermarks in molecular electronic materials as an anti-counterfeiting strategy: Application to porphyrins for information storage. Journal of Porphyrins and Phthalocyanines, 2011, 15, 505-516.	0.4	8
59	Excited-State Photodynamics of Peryleneâ˘'Porphyrin Dyads. 5. Tuning Light-Harvesting Characteristics via Perylene Substituents, Connection Motif, and Three-Dimensional Architecture. Journal of Physical Chemistry B, 2010, 114, 14249-14264.	1.2	23
60	Photophysical characterization of imidazolium-substituted Pd(II), In(III), and Zn(II) porphyrins as photosensitizers for photodynamic therapy. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 200, 346-355.	2.0	91
61	Accessing the near-infrared spectral region with stable, synthetic, wavelength-tunable bacteriochlorins. New Journal of Chemistry, 2008, 32, 947.	1.4	120
62	Synthesis of porphyrins for metal deposition studies in molecular information storage applications. Journal of Porphyrins and Phthalocyanines, 2007, 11, 699-712.	0.4	7
63	Effects of Substituents on Synthetic Analogs of Chlorophylls. Part 1: Synthesis, Vibrational Properties and Excited-state Decay Characteristics. Photochemistry and Photobiology, 2007, 83, 1110-1124.	1.3	68
64	Diverse porphyrin dimers as candidates for high-density charge-storage molecules. Journal of Porphyrins and Phthalocyanines, 2006, 10, 22-32.	0.4	13
65	Investigation of Stepwise Covalent Synthesis on a Surface Yielding Porphyrin-Based Multicomponent Architectures. Journal of Organic Chemistry, 2006, 71, 3033-3050.	1.7	42
66	Structural Control of the Photodynamics of Boronâ˘'Dipyrrin Complexes. Journal of Physical Chemistry B, 2005, 109, 20433-20443.	1.2	375
67	Solution STM images of porphyrins on HOPG reveal that subtle differences in molecular structure dramatically alter packing geometry. Journal of Porphyrins and Phthalocyanines, 2005, 09, 387-392.	0.4	20
68	Swallowtail Porphyrins:â€‰ Synthesis, Characterization and Incorporation into Porphyrin Dyads. Journal of Organic Chemistry, 2004, 69, 3700-3710.	1.7	38
69	Photophysical Properties of Phenylethyne-Linked Porphyrin and Oxochlorin Dyads. Journal of Physical Chemistry B, 2004, 108, 8190-8200.	1.2	37
70	Structural Control of the Excited-State Dynamics of Bis(dipyrrinato)zinc Complexes:Â Self-Assembling Chromophores for Light-Harvesting Architectures. Journal of the American Chemical Society, 2004, 126, 2664-2665.	6.6	204
71	Excited-State Energy-Transfer Dynamics in Self-Assembled Triads Composed of Two Porphyrins and an Intervening Bis(dipyrrinato)metal Complex. Inorganic Chemistry, 2003, 42, 6629-6647.	1.9	214
72	Comparison of Excited-State Energy Transfer in Arrays of Hydroporphyrins (Chlorins, Oxochlorins) versus Porphyrins:Â Rates, Mechanisms, and Design Criteria. Journal of the American Chemical Society, 2003, 125, 13461-13470.	6.6	37

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73	Electrical characterization of redox-active molecular monolayers on SiO2 for memory applications. Applied Physics Letters, 2003, 83, 198-200.	1.5	59
74	Capacitance and conductance characterization of ferrocene-containing self-assembled monolayers on silicon surfaces for memory applications. Applied Physics Letters, 2002, 81, 1494-1496.	1.5	98
75	Characterization of Charge Storage in Redox-Active Self-Assembled Monolayers. Langmuir, 2002, 18, 4030-4040.	1.6	85
76	Synthesis and properties of weakly coupled dendrimeric multiporphyrin light-harvesting arrays and hole-storage reservoirsElectronic supplementary information (ESI) available: a description of multiphoton effects at high excitation intensities; the complete Experimental section including descriptions of the syntheses of the arrays; SEC data, 1H NMR spectra, and mass spectra for all new porphyrins and multiporphyrin arrays; a description of exploratory studies in the purification of Zn20Fb; data from a compar. Journal of Materials Chemistry, 2002, 12, 65-80.	6.7	90
77	Synthesis and Photophysical Properties of Light-Harvesting Arrays Comprised of a Porphyrin Bearing Multiple Perylene-Monoimide Accessory Pigments. Journal of Organic Chemistry, 2002, 67, 6519-6534.	1.7	134
78	Design, synthesis, and characterization of prototypical multistate counters in three distinct architecturesElectronic supplementary information (ESI) available: 1H NMR and 13C NMR spectra for each dipyrromethane; absorption, LD-MS, and 1H NMR spectra for each porphyrin and each triple decker; absorption and LD-MS spectra for each triple-decker dyad. See http://www.rsc.org/suppdata/jm/b1/b108520d/. Journal of Materials Chemistry, 2002, 12, 808-828.	6.7	56
79	Design and synthesis of light-harvesting rods for intrinsic rectification of the migration of excited-state energy and ground-state holesElectronic supplementary information (ESI) available: 1H and 13C NMR spectra for all new porphyrin precursors; 1H NMR and LD-MS spectra for all new porphyrins and porphyrin arrays (LD-MS only for deprotected arrays 12â€² and 14â€², and pentad 18); analytical SEC data for all porphyrin arrays. See http://www.rsc.org/suppdata/jm/b1/b108168c/. Journal of Materials Chemistry, 2002, 12, 1530-1552.	6.7	43
80	Probing Electronic Communication in Covalently Linked Multiporphyrin Arrays. A Guide to the Rational Design of Molecular Photonic Devices. Accounts of Chemical Research, 2002, 35, 57-69.	7.6	834
81	Studies related to the design and synthesis of a molecular octal counter. Journal of Materials Chemistry, 2001, 11, 1162-1180.	6.7	95
82	Synthesis and Excited-State Photodynamics of Peryleneâ^'Porphyrin Dyads. 1. Parallel Energy and Charge Transfer via a Diphenylethyne Linker. Journal of Physical Chemistry B, 2001, 105, 8237-8248.	1.2	110
83	Synthesis and excited-state photodynamics of peryleneâ€"porphyrin dyads Part 3. Effects of perylene, linker, and connectivity on ultrafast energy transfer. Journal of Materials Chemistry, 2001, 11, 2420-2430.	6.7	63
84	Mechanisms of Excited-State Energy-Transfer Gating in Linear versus Branched Multiporphyrin Arrays. Journal of Physical Chemistry B, 2001, 105, 5341-5352.	1.2	85
85	Characterization of Carotenoid and Chlorophyll Photooxidation in Photosystem II. Biochemistry, 2001, 40, 193-203.	1.2	114
86	Raman signatures of ligand binding and allosteric conformation change in hexameric insulin. Biopolymers, 2001, 62, 249-260.	1.2	23
87	Molecular approach toward information storage based on the redox properties of porphyrins in self-assembled monolayers. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2000, 18, 2359.	1.6	105
88	Structural Control of Photoinduced Energy Transfer between Adjacent and Distant Sites in Multiporphyrin Arrays. Journal of the American Chemical Society, 2000, 122, 7579-7591.	6.6	141
89	Synthesis and excitedâ€state photodynamics of phenylethyneâ€linked porphyrinâ€"phthalocyanine dyads. Journal of Materials Chemistry, 2000, 10, 283-296.	6.7	87
90	Ground and Excited State Electronic Properties of Halogenated Tetraarylporphyrins: Tuning the Building Blocks for Porphyrin-based Photonic Devices. Journal of Porphyrins and Phthalocyanines, 1999, 03, 117-147.	0.4	112

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91	Relationship between altered structure and photochemistry in mutant reaction centers in which bacteriochlorophyll replaces the photoactive bacteriopheophytin. , 1999, 5, 346-357.		5
92	Synthesis and Characterization of Tetrachlorodiarylethyne-Linked Porphyrin Dimers. Effects of Linker Architecture on Intradimer Electronic Communication. Inorganic Chemistry, 1998, 37, 1191-1201.	1.9	59
93	Identification of Histidine 118 in the D1 Polypeptide of Photosystem II as the Axial Ligand to Chlorophyll Z. Biochemistry, 1998, 37, 10040-10046.	1.2	75
94	Selective Resonance Raman Scattering from Chlorophyll Z in Photosystem II via Excitation into the Near-Infrared Absorption Band of the Cation. Journal of the American Chemical Society, 1998, 120, 4532-4533.	6.6	17
95	Design, Synthesis, and Photodynamics of Light-Harvesting Arrays Comprised of a Porphyrin and One, Two, or Eight Boron-Dipyrrin Accessory Pigments. Journal of the American Chemical Society, 1998, 120, 10001-10017.	6.6	428
96	Excited-State Energy Transfer and Ground-State Hole/Electron Hopping inp-Phenylene-Linked Porphyrin Dimers. Journal of Physical Chemistry B, 1998, 102, 9426-9436.	1.2	107
97	Qy-Excitation Resonance Raman Spectra of Chlorophyllaand Related Complexes. Normal Mode Characteristics of the Low-Frequency Vibrations. Journal of Physical Chemistry B, 1997, 101, 9635-9644.	1.2	28
98	Identification of the Magnesiumâ˘'Histidine Stretching Vibration of the Bacteriochlorophyll Cofactors in Photosynthetic Reaction Centers via 15N-Labeling of the Histidines. Journal of the American Chemical Society, 1997, 119, 2594-2595.	6.6	20
99	Effects of Orbital Ordering on Electronic Communication in Multiporphyrin Arrays. Journal of the American Chemical Society, 1997, 119, 11191-11201.	6.6	224
100	Effects of central metal ion (Mg, Zn) and solvent on singlet excited-state energy flow in porphyrin-based nanostructures. Journal of Materials Chemistry, 1997, 7, 1245-1262.	6.7	105
101	Acid-induced transformations of myoglobin. II. Effect of ionic strength on the free energy and formation rate of the 426-nm absorbing deoxyheme intermediate. Biospectroscopy, 1997, 3, 17-29.	0.4	10
102	Soluble Synthetic Multiporphyrin Arrays. 2. Photodynamics of Energy-Transfer Processes. Journal of the American Chemical Society, 1996, 118, 11181-11193.	6.6	310
103	Evidence for Porphyrin (Ï€)â˘'Chlorine (p) Orbital Overlap in the Ï€-Cation Radicals of Zinc(II) and Magnesium(II) Tetrakis(o-dichlorophenyl)porphyrin. Inorganic Chemistry, 1996, 35, 7935-7937.	1.9	21
104	Carbonyl Tilting and Bending Potential Energy Surface of Carbon Monoxyhemes. The Journal of Physical Chemistry, 1996, 100, 6363-6367.	2.9	123
105	Calculation of molecular polarizabilities using a semiclassical Slaterâ€type orbitalâ€point dipole interaction (STOPDI) model. Journal of Chemical Physics, 1983, 79, 2256-2264.	1.2	29
106	Low temperature spectroscopy of internally hydrogenâ€bonded 2â€(2â€²â€hydroxyâ€5â€²â€methylphenyl)â€benzotriazole in a mixed crystal. Journal of Chemical Physics, 1983, 79, 5802-5807.	1.2	21
107	Calculation of Raman intensities for the torsional vibrations of ethyl halides. Journal of Chemical Physics, 1982, 76, 4828-4833.	1.2	8
108	Calculation of Raman intensities for the torsional vibrations of methylcyclopropane and propylene oxide. Journal of Chemical Physics, 1982, 76, 6454-6456.	1.2	3

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109	Raman intensity de-enhancement in nontotally symmetric vibrations of copper(II) acetate by forbidden ligand-field transitions. Journal of Raman Spectroscopy, 1981, 11, 27-31.	1.2	8
110	Calculation of Raman intensities for the ringâ€puckering vibrations of 2,5â€dihydropyrrole and trimethyleneimine. Electrical versus mechanical anharmonicity in asymmetric potential wells. Journal of Chemical Physics, 1981, 75, 2626-2634.	1.2	19
111	Calculation of Raman intensities for the ringâ€puckering vibrations of cyclopentene and 2,5â€dihydrofuran. Journal of Chemical Physics, 1981, 75, 3215-3219.	1.2	14
112	Calculation of Raman intensities for the ringâ€puckering vibrations of trimethylene oxide and cyclobutane. The importance of electrical anharmonicity. Journal of Chemical Physics, 1981, 74, 3660-3667.	1.2	29
113	Vibrational spectra, potential functions, and conformations of cycloheptanone. Journal of Chemical Physics, 1977, 67, 1071.	1.2	24