Per Jensen

List of Publications by Year in descending order

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232 papers	6,829 citations	66234 42 h-index	85405 71 g-index
236 all docs	236 docs citations	236 times ranked	2221 citing authors

#	Article	IF	Citations
1	The potential surface and stretching frequencies of XÌƒâ€‰3B1 methylene (CH2) determined from experiment using the Morse oscillatorâ€rigid bender internal dynamics Hamiltonian. Journal of Chemical Physics, 1988, 89, 1327-1332.	1.2	290
2	Theoretical ROVibrational Energies (TROVE): A robust numerical approach to the calculation of rovibrational energies for polyatomic molecules. Journal of Molecular Spectroscopy, 2007, 245, 126-140.	0.4	248
3	A new morse oscillator-rigid bender internal dynamics (MORBID) Hamiltonian for triatomic molecules. Journal of Molecular Spectroscopy, 1988, 128, 478-501.	0.4	241
4	The potential energy surface for the electronic ground state of the water molecule determined from experimental data using a variational approach. Journal of Molecular Spectroscopy, 1989, 133, 438-460.	0.4	196
5	The potential energy surface of H2â€‰16O. Journal of Chemical Physics, 1996, 105, 6490-6497.	1.2	161
6	The potential surface of XÌƒâ€‰3B1 methylene (CH2) and the singletâ€“triplet splitting. Journal of Chemical Physics, 1986, 85, 3724-3731.	1.2	159
7	A Variationally Computed T = 300 K Line List for NH₃. Journal of Physical Chemistry A, 2009, 113, 11845-11855.	1.1	159
8	The nonrigid bender Hamiltonian for calculating the rotation-vibration energy levels of a triatomic molecule. Computer Physics Reports, 1983, 1, 1-55.	2.3	140
9	Determination of the Effective Ground State Potential Energy Function of Ozone from High-Resolution Infrared Spectra. Journal of Molecular Spectroscopy, 1999, 198, 57-76.	0.4	137
10	An introduction to the theory of local mode vibrations. Molecular Physics, 2000, 98, 1253-1285.	0.8	126
11	A spectroscopically determined potential energy surface for the ground state of H216O: A new level of accuracy. Journal of Chemical Physics, 1994, 101, 7651-7657.	1.2	118
12	A refined potential surface for the XÌƒâ€‰3B1 electronic state of methylene CH2. Journal of Chemical Physics, 1983, 79, 1224-1228.	1.2	117
13	Anabinitiodetermination of the potentialâ€energy surfaces and rotationâ€“vibration energy levels of methylene in the lowest triplet and singlet states and the singletâ€“triplet splitting. Journal of Chemical Physics, 1989, 90, 6491-6500.	1.2	107
14	Determination of A0 for CH335Cl and CH337Cl from the Î½4 infrared and Raman bands. Journal of Molecular Spectroscopy, 1981, 88, 378-393.	0.4	104
15	Hamiltonians for the internal dynamics of triatomic molecules. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1315.	1.1	100
16	The development of a new Morse-oscillator based rotation-vibration Hamiltonian for H3+. Journal of Molecular Spectroscopy, 1985, 112, 183-202.	0.4	84
17	The geometry and the inversion potential function of formaldehyde in the and electronic states. Journal of Molecular Spectroscopy, 1982, 94, 114-125.	0.4	80
18	A Treatment of the Renner Effect Using the MORBID Hamiltonian. Journal of Molecular Spectroscopy, 1995, 171, 31-57.	0.4	78

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19	Calculation of rotation-vibration linestrengths for triatomic molecules using a variational approach. Journal of Molecular Spectroscopy, 1988, 132, 429-457.	0.4	77
20	Towards efficient refinement of molecular potential energy surfaces: Ammonia as a case study. Journal of Molecular Spectroscopy, 2011, 268, 123-129.	0.4	77
21	A Refined Potential Energy Surface for the Electronic Ground State of the Water Molecule. Journal of Molecular Spectroscopy, 1994, 168, 271-289.	0.4	73
22	The equilibrium geometry, potential function, and rotationâ€vibration energies of CH2 in the XÌƒâ€‰3B1 ground state. Journal of Chemical Physics, 1982, 77, 5370-5374.	1.2	71
23	Fourfold Clusters of Rovibrational Energy Levels for H2S Studied with a Potential Energy Surface Derived from Experiment. Journal of Molecular Spectroscopy, 1994, 163, 483-509.	0.4	71
24	An ab initio calculation of the intramolecular stretching spectra for the HF dimer and its Dâ€substituted isotopic species. Journal of Chemical Physics, 1990, 93, 6266-6280.	1.2	68
25	Vibrational energies for NH3 based on high level ab initio potential energy surfaces. Journal of Chemical Physics, 2002, 117, 11265-11276.	1.2	68
26	Potential-energy surface for the electronic ground state of NH3 up to 20000cmâ^'1 above equilibrium. Journal of Chemical Physics, 2005, 123, 134308.	1.2	68
27	The infrared spectrum of carbon suboxide in the Î½6 fundamental region: Experimental observation and semirigid bender analysis. Journal of Molecular Spectroscopy, 1986, 118, 248-266.	0.4	63
28	An ab initio calculation of the stretching energies for the HF dimer. Journal of Chemical Physics, 1990, 92, 7432-7440.	1.2	62
29	An ab initio study of the hydrogen chloride dimer: The potential energy surface and the characterization of the stationary points. Chemical Physics, 1991, 149, 299-309.	0.9	57
30	Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378.	0.8	55
31	An analytical ab initio potential surface and the calculated tunneling energies for the HCl dimer. Journal of Molecular Spectroscopy, 1991, 146, 200-219.	0.4	51
32	Potential parameters of PH3 obtained by simultaneous fitting of ab initio data and experimental vibrational band origins. Chemical Physics, 2003, 290, 59-67.	0.9	51
33	An ab initio calculation of Î½1 and Î½3 for triplet methylene (XÌƒâ€‰3B1â€‰CH2) and the determination of the vibrationless singletâ€“triplet splitting Te(aÌƒâ€‰1A1). Journal of Chemical Physics, 1987, 87, 2166-2169.	1.2	49
34	Calculation of the completeâ€activeâ€space selfâ€consistentâ€field potentialâ€energy surface, the dipole moment surfaces, the rotationâ€“vibration energies, and the vibrational transition moments for C3(XÌƒâ€‰1Î£+g). Journal of Chemical Physics, 1992, 97, 3399-3411.	1.2	49
35	The Dipole Moment Surface and the Vibrational Transition Moments of H2O. Journal of Molecular Spectroscopy, 1993, 161, 219-242.	0.4	48
36	A theoretical calculation of the absorption spectrum of CH2+. Chemical Physics, 1997, 225, 33-54.	0.9	48

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37	A new â€œspectroscopicâ€•potential energy surface for formaldehyde in its ground electronic state. Journal of Chemical Physics, 2011, 134, 244307.	1.2	48
38	The Potential Energy Surface for the Electronic Ground State of H2Se Derived from Experiment. Journal of Molecular Spectroscopy, 1993, 160, 39-57.	0.4	47
39	Ab initio dipole moment and theoretical rovibrational intensities in the electronic ground state of PH3. Journal of Molecular Spectroscopy, 2006, 239, 71-87.	0.4	47
40	Rotation-vibration energy levels of H2O and C3 calculated using the nonrigid bender Hamiltonian. Journal of Molecular Spectroscopy, 1986, 118, 50-63.	0.4	45
41	The Renner effect in triatomic molecules with application to CH2+, MgNC and NH2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 763-794.	2.0	45
42	Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317.	1.2	43
43	An ab initio calculation of the rotation-vibration energies of the state of CCH using the nonrigid bender Hamiltonian. Journal of Molecular Spectroscopy, 1986, 120, 236-238.	0.4	42
44	The Far-Infrared Fourier Transform Spectrum of H2Se. Journal of Molecular Spectroscopy, 1993, 158, 409-422.	0.4	42
45	On the Spectroscopically Determined Potential Energy Surfaces for the Electronic Ground States of NO2and H2O. Journal of Molecular Spectroscopy, 1997, 185, 234-243.	0.4	42
46	An ab initio calculation of the rovibronic energies of the BH2 molecule. Molecular Physics, 1996, 88, 105-124.	0.8	42
47	An ab initio study of the rotationâ€”vibration energy levels of GeH2 in the Ä3B1 state. Chemical Physics Letters, 1985, 118, 60-63.	1.2	40
48	An ab initio close-coupling calculation of the lower vibrational energies of the HF dimer. Chemical Physics Letters, 1991, 176, 255-260.	1.2	39
49	An ab Initio Calculation of the Low Rotation-Vibration Energies of the CO Dimer. Journal of Molecular Spectroscopy, 1993, 157, 208-219.	0.4	39
50	Fourfold Clusters of Rovibrational Energy Levels in the Fundamental Vibrational States of H2Se. Journal of Molecular Spectroscopy, 1993, 161, 186-207.	0.4	39
51	The nonrigid bender Hamiltonian using an alternative perturbation technique. Journal of Molecular Spectroscopy, 1986, 118, 18-39.	0.4	37
52	The Low-Energy Part of the Potential Function for the Electronic Ground State of NO2 Derived from Experiment. Journal of Molecular Spectroscopy, 1994, 165, 173-184.	0.4	37
53	A Theoretical Study of the Stark Effect in Triatomic Molecules: Application to H2O. Journal of Molecular Spectroscopy, 1995, 169, 73-91.	0.4	37
54	Rotationâ€“Vibration Motion of Pyramidal XY3 Molecules Described in the Eckart Frame: The Calculation of Intensities with Application to NH3. Advances in Quantum Chemistry, 2005, 48, 209-238.	0.4	37

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55	HCNO as a semirigid bender: The degenerate Î½4 state. Journal of Molecular Spectroscopy, 1983, 101, 422-439.	0.4	35
56	A theoretical study of FeNC in the 6Î” electronic ground state. Journal of Molecular Spectroscopy, 2006, 236, 234-247.	0.4	35
57	The geometry and the out-of-plane bending potential function of thioformaldehyde in the and electronic states. Journal of Molecular Spectroscopy, 1982, 95, 92-100.	0.4	34
58	A Theoretical Investigation of the Renner Interactions and Magnetic Dipole Transitions in the Ãƒâ€“XÌƒ Electronic Band System of HO2. Journal of Molecular Spectroscopy, 1999, 197, 262-274.	0.4	34
59	Theoretical evidence for the formation of rotational energy level clusters in the vibrational ground state of PH3. Physical Chemistry Chemical Physics, 2005, 7, 573.	1.3	34
60	The application of the nonrigid bender Hamiltonian to a quasilinear molecule. Journal of Molecular Spectroscopy, 1983, 99, 348-356.	0.4	33
61	Toluene internal-rotation: Measurement and simulation of the high-resolution S1â€“S0 fluorescence excitation spectrum at 0.5 K. Journal of Chemical Physics, 2000, 112, 167-175.	1.2	33
62	Thermal averaging of the indirect nuclear spin-spin coupling constants of ammonia: The importance of the large amplitude inversion mode. Journal of Chemical Physics, 2010, 132, 114305.	1.2	33
63	A new Morse-oscillator based Hamiltonian for H3+: Calculation of line strengths. Journal of Molecular Spectroscopy, 1986, 118, 208-231.	0.4	32
64	An ab initio calculation of the rotation-vibration energies of singlet and triplet NH2+ using the morbid Hamiltonian. Chemical Physics Letters, 1987, 141, 53-57.	1.2	32
65	Rotation-vibration energies for the HO2 molecule. Journal of Molecular Spectroscopy, 1992, 155, 44-54.	0.4	32
66	New rovibrational data for MgOH and MgOD and the internuclear potential function of the ground electronic state. Chemical Physics Letters, 1995, 239, 217-222.	1.2	32
67	The Potential Energy Surface of Hydrogen Sulfide. Journal of Molecular Spectroscopy, 1996, 178, 184-188.	0.4	32
68	An ab initio calculation of the vibrational energies and transition moments of HSOH. Journal of Molecular Spectroscopy, 2009, 257, 57-65.	0.4	32
69	A comparison of perturbative and variational rotation-vibration energies calculated for HOC+ and C3 using the nonrigid bender and MORBID Hamiltonians. Journal of Molecular Spectroscopy, 1988, 129, 172-185.	0.4	31
70	Vibrational levels for the lowestâ€lying triplet and singlet states of CH2 and NH+2. Journal of Chemical Physics, 1993, 99, 9709-9719.	1.2	31
71	An ab Initio Calculation of the Rovibronic Energies of the Ch+2 Molecule. Journal of Molecular Spectroscopy, 1995, 172, 194-204.	0.4	31
72	A variational calculation of the rotation-vibration energies for CNC+ and CCN+. Journal of Molecular Spectroscopy, 1988, 129, 216-222.	0.4	30

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73	The infrared spectrum of fulminic acid, HCNO, in the Î½4 fundamental region. Journal of Molecular Spectroscopy, 1983, 101, 408-421.	0.4	29
74	Anab InitioStudy of the NH2+Absorption Spectrum. Journal of Molecular Spectroscopy, 1997, 186, 319-334.	0.4	28
75	Vibrational energies of PH3 calculated variationally at the complete basis set limit. Journal of Chemical Physics, 2008, 129, 044309.	1.2	28
76	Symmetry of extremely floppy molecules: Molecular states beyond rotation-vibration separation. Journal of Chemical Physics, 2015, 143, 154302.	1.2	26
77	Determination of the B0 constant of C6H6. Journal of Molecular Spectroscopy, 1980, 83, 161-174.	0.4	25
78	Determination of the skeletal bending potential function for SiH3NCO from the microwave spectrum. Journal of Molecular Spectroscopy, 1984, 103, 312-320.	0.4	25
79	Vibro-rotational analysis of Si2C from an ab initio potential energy surface. A comparison between perturbative and variational methods. Journal of Molecular Spectroscopy, 1992, 154, 252-264.	0.4	25
80	An ab initio calculation of the vibronic energies of the CH₂⁺ molecule. Canadian Journal of Physics, 1994, 72, 871-878.	0.4	25
81	A new Morse-oscillator based Hamiltonian for H3+: Extension to H2D+ and D2H+. Journal of Molecular Spectroscopy, 1986, 115, 269-293.	0.4	24
82	Experimental Evidence for the Formation of Fourfold Rovibrational Energy Clusters in the Î½1/Î½3 Vibrational States of H280Se. Journal of Molecular Spectroscopy, 1995, 172, 126-134.	0.4	24
83	High-Resolution Spectroscopy of C₃ around 3 Î¼m. Journal of Physical Chemistry A, 2013, 117, 3332-3339.	1.1	23
84	C3O2 as a semirigid bender: The degenerate Î½5 state. Journal of Molecular Spectroscopy, 1984, 104, 59-71.	0.4	22
85	Anab initiocalculation of the rotational-vibrational energies in the electronic ground state of NH2. Molecular Physics, 1990, 70, 443-454.	0.8	22
86	A Theoretical Study of MgNC and MgCN in the XÌƒ2Î£+ Electronic State. Journal of Molecular Spectroscopy, 2002, 215, 42-57.	0.4	22
87	Internal rotation tunnelling in HSOH. Journal of Molecular Structure, 2004, 695-696, 323-337.	1.8	21
88	PH3 revisited: Theoretical transition moments for the vibrational transitions below. Journal of Molecular Spectroscopy, 2008, 252, 121-128.	0.4	21
89	Collective Molecular Superrotation: A Model for Extremely Flexible Molecules Applied to Protonated Methane. Physical Review Letters, 2016, 117, 223002.	2.9	21
90	Bending wavefunctions for linear molecules. Journal of Molecular Spectroscopy, 2018, 343, 54-61.	0.4	21

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91	Calculation of Molecular Rotation-Vibration Energies Directly from the Potential Energy Function. NATO ASI Series Series B: Physics, 1992, , 423-469.	0.2	21
92	An ab initio close-coupling calculation of the lower vibrational energies of the HCl dimer. Chemical Physics Letters, 1991, 180, 594-600.	1.2	20
93	A theoretical study of FeCN in the 6Î” electronic ground state. Journal of Molecular Spectroscopy, 2007, 243, 267-279.	0.4	20
94	Computational molecular spectroscopy for NiCN: Large-amplitude bending motion. Journal of Molecular Spectroscopy, 2008, 250, 33-43.	0.4	20
95	A study of the electronic, optical and thermal properties for ZnAl₂Se₄ using the FPâ€ŁAPW method. Physica Status Solidi (B): Basic Research, 2011, 248, 1682-1689.	0.7	20
96	Refined potential-energy surfaces for the <img src="/cisti/journals/rp/gifs/Xtilde.gif" BORDER=0> ²<I>A</I>" and Ã ²A' electronic states of the HO₂ molecule. Canadian Journal of Physics, 2001, 79, 641-652.	0.4	19
97	The Rotational Spectrum of H2Te. Journal of Molecular Spectroscopy, 1996, 180, 402-413.	0.4	18
98	Calculation of Rotationâ€“Vibration Energy Levels in Ground State C3by a Bornâ€“Oppenheimer-Type Separation of the Vibrational Motions. Journal of Molecular Spectroscopy, 1997, 183, 129-138.	0.4	18
99	Transition moments and NH2cometary spectra. Molecular Physics, 2003, 101, 613-622.	0.8	18
100	A theoretical study of CoCN in the3Î¦ electronic ground state. Molecular Physics, 2007, 105, 599-611.	0.8	18
101	Ab initio studies of structural, electronic, optical and thermal properties of CuAlS2 chalcopyrite. Computational and Theoretical Chemistry, 2011, 975, 122-127.	1.1	18
102	Rotational spectrum of SO3 and theoretical evidence for the formation of sixfold rotational energy-level clusters in its vibrational ground state. Journal of Chemical Physics, 2014, 140, 244316.	1.2	18
103	Ab initio rotation-vibration energies of HOC+ calculated using the nonrigid bender Hamiltonian. Journal of Molecular Spectroscopy, 1986, 118, 40-49.	0.4	17
104	Diode laser infrared spectra and potential energy curve for SH+. Journal of Molecular Spectroscopy, 1989, 138, 69-78.	0.4	17
105	Theoretical vibrational and rotational energies and intensities of the HNSi and DNSi molecules. Journal of Chemical Physics, 1993, 98, 1352-1357.	1.2	17
106	Spherical top molecules and the molecular symmetry group. Molecular Physics, 1999, 97, 255-264.	0.8	17
107	An ab Initio Study of the Ãƒ2Î â†Ìƒ2Σ+ Electronic Transition of MgNC. Journal of Molecular Spectroscopy, 2002, 211, 147-161.	0.4	17
108	Rotational energy cluster formation in XY3 molecules: Excited vibrational states of BiH3 and SbH3. Journal of Molecular Spectroscopy, 2006, 240, 174-187.	0.4	17

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109	Rotation-vibration motion of extremely flexible molecules â€“ The molecular superrotor. Chemical Physics Letters, 2017, 672, 34-46.	1.2	17
110	A theoretical calculation of the rotation-vibration energies for lithium hydroxide, LiOH. Journal of Molecular Spectroscopy, 1989, 135, 89-104.	0.4	16
111	Coulomb explosion imaging and the CH2+ molecule. Chemical Physics Letters, 1999, 309, 299-306.	1.2	16
112	High-resolution terahertz spectrum of CH2 Â— Low J rotational transitions near 2 THz. Canadian Journal of Chemistry, 2004, 82, 676-683.	0.6	16
113	The double Renner effect in the XÌƒAâ€³2 and AÌƒAâ€²2 electronic states of HO2. Journal of Chemical Physics, 2008, 128, 114316.	1.2	16
114	Local modes in vibrationâ€“rotation spectroscopy. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 494-512.	6.2	16
115	Theoretical rotation-torsion energies of HSOH. Journal of Chemical Physics, 2008, 129, 154314.	1.2	15
116	An ab initio calculation of the fundamental and overtone HCl stretching vibrations for the HCl dimer. Journal of Molecular Spectroscopy, 1992, 151, 384-395.	0.4	14
117	High-Levelab InitioCalculation of the Rotationâ^'Vibration Energies in the cÌƒ1A1State of Methylene, CH2. The Journal of Physical Chemistry, 1996, 100, 18088-18092.	2.9	14
118	The Rovibrational Energy Levels of Quasilinearc1A1Methylene. Journal of Molecular Spectroscopy, 1996, 179, 263-268.	0.4	14
119	Theoretical study of the double Renner effect for AÌƒÎ2 MgNCâ•MgCN: Higher excited rovibrational states. Journal of Chemical Physics, 2007, 126, 094301.	1.2	14
120	Electronic and optical properties of defect chalcopyrite HgAl2Se4. Journal of Physics and Chemistry of Solids, 2011, 72, 1414-1418.	1.9	14
121	Variationally Computed IR Line List for the Methyl Radical CH₃. Journal of Physical Chemistry A, 2019, 123, 4755-4763.	1.1	14
122	The calculation of the bound and quasibound vibrational states for ozone in its 1B2 electronic state. Molecular Physics, 1997, 91, 653-661.	0.8	14
123	Ab initio rotation-vibration energies and intensities for the H2F+ molecule. Journal of Molecular Spectroscopy, 1990, 144, 310-322.	0.4	13
124	The v1 + v2 = 4 stretching overtones of the HF dimer, and H-atom exchange. Journal of Molecular Spectroscopy, 1991, 149, 512-518.	0.4	13
125	The H2O++ Ground State Potential Energy Surface. Journal of Molecular Spectroscopy, 1999, 198, 371-375.	0.4	13
126	Vibronic transition moments and line intensities for H2O+. Journal of Molecular Spectroscopy, 2004, 225, 96-106.	0.4	13

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127	A theoretical study of the MgNC/MgCN isomerization in the electronic ground state. Journal of Molecular Structure, 2004, 695-696, 219-226.	1.8	13
128	Ab initio potential energy surface, electric-dipole moment, polarizability tensor, and theoretical rovibrational spectra in the electronic ground state of. Chemical Physics, 2008, 346, 146-159.	0.9	13
129	Computational molecular spectroscopy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:mi>X</mml:mi></mml:mrow><mml:mrow><mml:mo>Ìƒ</mml:mo></mml:mrow></mml:mover><mml:mspace width="0.25em" /><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup><mml:mi mathvariant="normal">Î</mml:mi>	0.4	13
130	The Molecular Symmetry Group for Molecules in High Angular Momentum States. Journal of Molecular Spectroscopy, 1994, 164, 315-317.	0.4	12
131	Fourfold clusters of rovibrational energies in H2Te studied with an ab initio potential energy function. Chemical Physics, 1995, 190, 179-189.	0.9	12
132	The calculation of the bound and quasibound vibrational states for ozone in its B 1 electronic state. Molecular Physics, 1997, 91, 653-662.	0.8	12
133	A dispersed fluorescence andab initioinvestigation of the XÌƒB12 and AÌƒA12 electronic states of the PH2 molecule. Journal of Chemical Physics, 2006, 124, 094306.	1.2	12
134	The predicted spectrum of FeOH in its Renner-degenerate and electronic states. Journal of Molecular Spectroscopy, 2009, 256, 45-52.	0.4	12
135	The predicted infrared spectrum of the hyperberyllium molecule BeOBe in its and electronic states. Journal of Molecular Spectroscopy, 2010, 263, 21-26.	0.4	12
136	Ab initiostudies of structural, electronic, magnetic and mechanical properties of alkali earth metal silicides. Semiconductor Science and Technology, 2010, 25, 105002.	1.0	12
137	Ro-vibrational averaging of the isotropic hyperfine coupling constant for the methyl radical. Journal of Chemical Physics, 2015, 143, 244306.	1.2	12
138	Geometric dependence of the mean excitation energy and spectral moments of water. Physical Review A, 1991, 43, 4040-4043.	1.0	11
139	The Î½6 Band System of C3O2 Near 540 cmâ^'11. Journal of Molecular Spectroscopy, 1994, 163, 529-540.	0.4	11
140	The Potential Energy Function of CS2 Derived from Rovibrational Data. Journal of Molecular Spectroscopy, 1995, 170, 158-165.	0.4	11
141	Coulomb explosion imaging: the CH2+, H2O+ and NH2+ ions as benchmarks. Chemical Physics Letters, 2000, 318, 597-606.	1.2	11
142	The Near Ultraviolet Band System of Singlet Methylene. Journal of Molecular Spectroscopy, 2001, 208, 136-143.	0.4	11
143	The spectrum of singlet SiH2. Canadian Journal of Chemistry, 2004, 82, 694-708.	0.6	11
144	A theoretical study of BrCN+ in the 2Î electronic ground state: Large amplitude bending motion. Journal of Molecular Spectroscopy, 2007, 243, 202-218.	0.4	11

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145	Ro-vibrationally averaged dipole moments of linear triatomic molecules. Journal of Molecular Spectroscopy, 2019, 362, 29-36.	0.4	11
146	The CO2 molecule is never linear. Journal of Molecular Structure, 2020, 1212, 128087.	1.8	11
147	Calculated rotation-vibration energies for HOC+. Journal of Molecular Spectroscopy, 1987, 121, 450-452.	0.4	10
148	A variational calculation of the rotationâ€"vibration energies for H2O from AB initio data. Journal of Molecular Structure, 1988, 190, 149-161.	1.8	10
149	An ab initio calculation of the nonadiabatic effect on the tunneling splitting in vibrationally excited (HF)2. Journal of Molecular Spectroscopy, 1991, 148, 385-390.	0.4	10
150	Theoretical Rotationâ€"Vibration Energies ofX3B1NH2+. Journal of Molecular Spectroscopy, 1997, 181, 207-214.	0.4	10
151	A Potential Energy Surface for the Electronic Ground State of H2Te Derived from Experiment. Journal of Molecular Spectroscopy, 1997, 185, 282-289.	0.4	10
152	A refined potential energy function for the electronic ground state of H2Se. Journal of Molecular Spectroscopy, 2004, 227, 1-12.	0.4	10
153	The double Renner effect: A theoretical study of the MgNC/MgCN isomerization in the 2Î electronic state. Journal of Molecular Structure, 2006, 795, 14-41.	1.8	10
154	Ab initio molecular orbital study of ground and low-lying electronic states of NiCN. Chemical Physics, 2008, 346, 13-22.	0.9	10
155	A theoretical-spectroscopy, ab initio-based study of the electronic ground state of 121SbH3. Journal of Quantitative Spectroscopy and Radiative Transfer, 2010, 111, 2279-2290.	1.1	10
156	Large amplitude bending motion in CsOH, studied through ab initio-based three-dimensional potential energy functions. Journal of Molecular Spectroscopy, 2010, 263, 150-159.	0.4	10
157	Electronic structures and rovibronically averaged geometries of the XÌƒâ€‰A6iâ€² and AÌƒâ€‰A6iâ€³ states of FeOH. Journal of Chemical Physics, 2010, 132, 094303.	1.2	10
158	Symmetry Adaptation of the Rotation-Vibration Theory for Linear Molecules. Symmetry, 2018, 10, 137.	1.1	10
159	A new Morse-oscillator based Hamiltonian for H3+: Explicit expressions for some vibrational matrix elements. Journal of Molecular Spectroscopy, 1987, 124, 430-436.	0.4	9
160	Predicted rovibronic spectra of CH2+ and CD2+. Chemical Physics Letters, 2001, 341, 358-362.	1.2	9
161	A Theoretical Study of Atilde2Î MgCN. Journal of Molecular Spectroscopy, 2002, 216, 379-396.	0.4	9
162	The Matrix Isolation Spectrum of the CH2+ Ion. Journal of Molecular Spectroscopy, 2002, 216, 419-423.	0.4	9

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163	Rotationâ€“vibration energy level clustering in the ground electronic state of PH2. Journal of Molecular Spectroscopy, 2006, 239, 160-173.	0.4	9
164	Ab initio molecular orbital study of ground and low-lying electronic states of CoCN. Journal of Chemical Physics, 2007, 127, 014303.	1.2	9
165	New potential energy surfaces for the and states of CH. Molecular Physics, 2007, 105, 1369-1376.	0.8	9
166	Pressure effects on energy gaps and phase transitions in ZnAl2Se4. Zeitschrift FÃ¼r Kristallographie, 2010, 225, .	1.1	9
167	Theoretical rotationâ€“torsion spectra of HSOH. Physical Chemistry Chemical Physics, 2010, 12, 8387.	1.3	9
168	Geometries and electronic structures of the ground and low-lying excited states of FeCO: An ab initio study. Journal of Chemical Physics, 2012, 137, 244303.	1.2	9
169	Electronic structure and rovibrational properties of ZnOH in the XÌƒ2Aâ€² electronic state: A computational molecular spectroscopy study. Journal of Chemical Physics, 2014, 141, 094308.	1.2	9
170	Ab initio rotation-vibration energies and intensities for the HNC+ molecule. Journal of Molecular Spectroscopy, 1992, 153, 240-254.	0.4	8
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