Jacek Koput

List of Publications by Year
in descending order

56 papers	1,054 citations	586496 16 h-index	488211 31 g-index
56 all docs	56 docs citations	56 times ranked	1259 citing authors

#	Article	IF	Citations
1	Ab Initio Potential Energy Surface and Vibrationalâ^'Rotational Energy Levels of X2Î£+CaOH. Journal of Physical Chemistry A, 2002, 106, 9595-9599.	1.1	188
2	Potential Energy Surface and Vibrationalâ^'Rotational Energy Levels of Hydrogen Peroxide. Journal of Physical Chemistry A, 1998, 102, 6325-6330.	1.1	104
3	Ab initio prediction of the vibrational-rotational energy levels of hydrogen peroxide and its isotopomers. Journal of Chemical Physics, 2001, 115, 8345-8350.	1.2	85
4	An ab initio study on the equilibrium structure and torsional potential energy function of hydrogen peroxide. Chemical Physics Letters, 1995, 236, 516-520.	1.2	82
5	Experimental Confirmation of Quantum Monodromy: The Millimeter Wave Spectrum of Cyanogen Isothiocyanate NCNCS. Physical Review Letters, 2005, 95, 243002.	2.9	58
6	Fluorescent H-aggregates of an asymmetrically substituted mono-amino Zn(<scp>ii</scp>) phthalocyanine. Dalton Transactions, 2017, 46, 1914-1926.	1.6	51
7	The ground-state potential energy function of a beryllium dimer determined using the single-reference coupled-cluster approach. Physical Chemistry Chemical Physics, 2011, 13, 20311.	1.3	35
8	Ab initio prediction of the potential energy surface and vibration-rotation energy levels of BeH2. Journal of Chemical Physics, 2006, 125, 044306.	1.2	33
9	Accurate ab initio potential energy surface and vibrationâ€rotation energy levels of hydrogen peroxide. Journal of Computational Chemistry, 2013, 34, 337-345.	1.5	30
10	The Equilibrium Structure and Torsional Potential Energy Function Of Methanol and Silanol. Journal of Physical Chemistry A, 2000, 104, 10017-10022.	1.1	28
11	Hydrogen bond effects in the ground and excited singlet states of 4H-1-benzopyrane-4-thione in waterâ€"theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 8842.	1.3	25
12	An ab Initio Study on the Equilibrium Structure and XCN Bending Energy Levels of Halofulminates:â€‰ ClCNO. Journal of Physical Chemistry A, 1999, 103, 2170-2174.	1.1	20
13	Ab Initio Heat of Formation and Singletâ^'Triplet Splitting for Cyanocarbene (HCCN) and Isocyanocarbene (HCNC). Journal of Physical Chemistry A, 2003, 107, 4717-4723.	1.1	20
14	Theab initiopotential energy surface and vibrationalâ€"rotational energy levels of dilithium monoxide, Li2O. Journal of Chemical Physics, 2002, 116, 9255-9260.	1.2	18
15	Variational Calculation of Highly Excited Rovibrational Energy Levels of H₂O₂. Journal of Physical Chemistry A, 2013, 117, 7367-7377.	1.1	18
16	PM3 study of the proton affinities of 2-, 3-, and 4-monosubstituted pyridines in the gas phase. Journal of Computational Chemistry, 1991, 12, 675-680.	1.5	17
17	Ab Initio Prediction of the Potential Energy Surface and Vibrationalâ^'Rotational Energy Levels of X2Aâ€˜ BeOH. Journal of Physical Chemistry A, 2003, 107, 3981-3986.	1.1	16
18	The ab initio ground-state potential energy function of beryllium monohydride, BeH. Journal of Chemical Physics, 2011, 135, 244308.	1.2	16

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19	Equilibrium Structure and HCC Bending Potential Energy Function of3Aâ€˜â€˜HCCN. Journal of Physical Chemistry A, 2002, 106, 6183-6188.	1.1	15
20	Ab Initio Study on the Equilibrium Structure and XCN Bending Energy Levels of Halofulminates:Â BrCNO. Journal of Physical Chemistry A, 1999, 103, 6017-6022.	1.1	14
21	CaF2 As a Quasilinear Molecule:â€‰ the Vibrationalâ^'Rotational Energy Levels Predicted by Ab Initio Quantum Chemistry Approach. Journal of Physical Chemistry A, 2004, 108, 9267-9273.	1.1	12
22	Ab Initio Prediction of the Potential Energy Surface and Vibrationalâ^'Rotational Energy Levels of Calcium Dihydride, CaH2. Journal of Physical Chemistry A, 2005, 109, 4410-4414.	1.1	11
23	Ab Initio Study on the Equilibrium Structure and CCN Bending Energy Levels of Cyanofulminate (NCCNO). Journal of Physical Chemistry A, 2001, 105, 11347-11350.	1.1	10
24	Ab initio potential energy surface and vibrationâ€rotation energy levels of sulfur dioxide. Journal of Computational Chemistry, 2017, 38, 892-900.	1.5	9
25	Ab initio characterization of the Caâ€“HCl van der Waals complex. Journal of Chemical Physics, 2010, 132, 064307.	1.2	8
26	Ab initio ground-state potential energy functions of beryllium monohydride ions: BeH+ and BeHâ^'. Journal of Chemical Physics, 2013, 139, 104309.	1.2	8
27	Ab initio potential energy surface and vibration-rotation energy levels of disilicon carbide, CSi2. Journal of Molecular Spectroscopy, 2017, 342, 83-91.	0.4	8
28	Ab initio calculations on electronic states of CaOH. Journal of Chemical Physics, 2002, 117, 4810-4819.	1.2	7
29	Ab initio study on the structure and vibration-rotation energy levels of dilithium monofluoride. Journal of Chemical Physics, 2008, 129, 154306.	1.2	7
30	Ab Initio spectroscopic characterization of borane, BH, in its electronic state. Journal of Computational Chemistry, 2015, 36, 2219-2227.	1.5	7
31	Ab initio groundâ€state potential energy function and vibrationâ€rotation energy levels of imidogen, NH. Journal of Computational Chemistry, 2015, 36, 1286-1294.	1.5	7
32	Ab Initio Prediction of the Equilibrium Structure and Vibrationalâ^'Rotational Energy Levels of Fluorofulminate. Journal of Physical Chemistry A, 2002, 106, 12064-12066.	1.1	6
33	Ab initio prediction of the potential energy surface and vibrational-rotational energy levels of dialuminum monoxide, Al[sub 2]O. Journal of Chemical Physics, 2004, 121, 130.	1.2	6
34	Electron transfer in silicon-bridged adjacent chromophores: the source for blue-green emission. Physical Chemistry Chemical Physics, 2017, 19, 11404-11415.	1.3	6
35	Equilibrium Structure and Vibrationalâ^'Rotational Energy Levels of the X2Aâ€˜ SiOH/HSiO Radical System. Journal of Physical Chemistry A, 2002, 106, 12067-12071.	1.1	5
36	Ab Initio Prediction of the Structure and Vibrationâ^'Rotation Spectroscopic Properties of Li2OH and Li2OH+. Journal of Physical Chemistry A, 2008, 112, 3248-3252.	1.1	5

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37	Ab initio potential energy surface and vibrationâ€rotation energy levels of silicon dicarbide, SiC₂. Journal of Computational Chemistry, 2016, 37, 2395-2402.	1.5	5
38	Unusual emission properties of the selected organosilicon compounds containing a styryl-carbazole chromophore: inversion of the singlet excited states. Physical Chemistry Chemical Physics, 2017, 19, 11698-11705.	1.3	5
39	Ab initio potential energy surface and vibrationâ€rotation energy levels of beryllium monohydroxide. Journal of Computational Chemistry, 2017, 38, 37-43.	1.5	5
40	Equilibrium Structure, Spectroscopic Constants, and Gas-Phase Basicity of the Silaformyl Anion, HSiO-. Journal of Physical Chemistry A, 2001, 105, 8248-8253.	1.1	4
41	The equilibrium structure and gas-phase proton affinity of the silanol anion, SiH3Oâ^'. Chemical Physics Letters, 2001, 333, 504-508.	1.2	4
42	Ab Initio Prediction of the Potential Energy Surface and Vibrationâ^'Rotation Energy Levels of CaCl2. Journal of Physical Chemistry A, 2008, 112, 2743-2746.	1.1	4
43	Ab initio potential energy surface and vibration-rotation energy levels of lithium monohydroxide. Journal of Chemical Physics, 2013, 138, 234301.	1.2	4
44	Ground and excited state hydrogen bonding effects of 6-aminocoumarin in water: An ab initio study. Dyes and Pigments, 2015, 112, 335-340.	2.0	4
45	Emission properties of Si-based styryl-carbazole derivatives: Role of meta- and para-vinyl substituents and silicon atom. Journal of Luminescence, 2018, 196, 57-63.	1.5	4
46	Ab initio prediction of the structure and vibrationâ€rotation spectroscopic properties of Na₂OH and K₂OH. Journal of Computational Chemistry, 2010, 31, 1542-1549.	1.5	3
47	Ab Initio Groundâ€State Potential Energy Function and Vibrationâ€Rotation Energy Levels of Aluminum Monohydride. Journal of Computational Chemistry, 2019, 40, 2522-2529.	1.5	3
48	Ab initio structure and vibration-rotation dynamics of the formyl and isoformyl cations, HCO+/HOC+. Journal of Chemical Physics, 2019, 150, 154307.	1.2	3
49	Highly accurate HF dimer ab initio potential energy surface. Journal of Chemical Physics, 2022, 156, 164305.	1.2	3
50	Ab initio characterization of the Mgâ€“HF van der Waals complex. Journal of Chemical Physics, 2010, 133, 164305.	1.2	2
51	Ab initio potential energy surface and vibrationâ€“rotation energy levels of germanium dicarbide, GeC₂. Journal of Computational Chemistry, 2018, 39, 1327-1334.	1.5	2
52	Spectral and photophysical properties of cytisine in acetonitrile â€“ Theory and experiment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 375-382.	2.0	2
53	Ab initio structure and vibrationâ€rotation dynamics of germylene, GeH₂. Journal of Computational Chemistry, 2019, 40, 1911-1918.	1.5	2
54	Why does the presence of silicon atoms improve the emission properties of biphenyl derivatives? â€“ Verification of various hypotheses by experiment and theory. Physical Chemistry Chemical Physics, 2019, 21, 20384-20392.	1.3	0

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55	Groundâ€state potential energy functions and vibrationâ€rotation energy levels of beryllium lithium and its cation. Journal of Computational Chemistry, 2022, 43, 491-498.	1.5	0
56	Ab initio characterization of the aluminum dimer in its X 3Îu$$ {}^3{Pi}_u $$ and A 3Î£gâ^'$$ {}^3{Sigma}_g^{-} $$ electronic states. Journal of Computational Chemistry, 2022, , .	1.5	0