Hubert Cybulski

List of Publications by Year
in descending order

34 papers	629 citations	623734 14 h-index	580821 25 g-index
34 all docs	34 docs citations	34 times ranked	834 citing authors

#	Article	IF	Citations
1	Interaction of NH(XÎ£â¯3) with He: Potential energy surface, bound states, and collisional Zeeman relaxation. Journal of Chemical Physics, 2005, 122, 094307.	3.0	74
2	Characterization of dihydrogen-bonded Dâ€“Hâ‹¯Hâ€“A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104.	3.0	66
3	Triarylamine Substituted Arylene Bisimides as Solution Processable Organic Semiconductors for Field Effect Transistors. Effect of Substituent Position on Their Spectroscopic, Electrochemical, Structural, and Electrical Transport Properties. Journal of Physical Chemistry C, 2011, 115, 15008-15017.	3.1	52
4	Symmetry-Adapted Perturbation-Theory Interaction-Energy Decomposition for Hydrogen-Bonded and Stacking Structures. Journal of Chemical Theory and Computation, 2008, 4, 892-897.	5.3	50
5	Ab Initio Ground- and Excited-State Intermolecular Potential Energy Surfaces for the NOâ€“Ne and NOâ€“Ar van der Waals Complexes. Journal of Physical Chemistry A, 2012, 116, 7319-7328.	2.5	40
6	The Properties of Weak and Strong Dihydrogen-Bonded Dï£¿Hâ‹…â‹…â‹…Hï£¿A Complexes. ChemPhysChem, 2006, 7, 629-639.	2.1	34
7	Strong competition between velocity-changing and phase- or state-changing collisions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>spectra perturbed by Ar. Physical Review A, 2015, 91, .	2.5	27
8	On the calculations of the vibrational Raman spectra of small water clusters. Chemical Physics, 2007, 342, 163-172.	1.9	26
9	Evaluation of different parameterizations of temperature dependences of the line-shape parameters based on ab initio calculations: Case study for the HITRAN database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 240, 106676.	2.3	25
10	Theoretical Studies of Nuclear Magnetic Resonance Parameters for the Proton-Exchange Pathways in Porphyrin and Porphycene. Journal of Physical Chemistry A, 2005, 109, 4162-4171.	2.5	22
11	The water-nitric oxide intermolecular potential-energy surface revisited. Journal of Chemical Physics, 2009, 130, 104303.	3.0	22
12	Arylene bisimides with triarylamine N-substituents as new solution processable organic semiconductors: Synthesis, spectroscopic, electrochemical and electronic properties. Synthetic Metals, 2011, 161, 1600-1610.	3.9	20
13	On the calculations of the nuclear shielding constants in small water clusters. Chemical Physics, 2006, 323, 218-230.	1.9	19
14	On the calculations of the nuclear spinâ€“spin coupling constants in small water clusters. Chemical Physics, 2006, 326, 431-444.	1.9	18
15	Power-law temperature dependence of collision broadening and shift of atomic and molecular rovibronic lines. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 120, 90-103.	2.3	14
16	Ab initio study of the COâ€“N2 complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum. Physical Chemistry Chemical Physics, 2018, 20, 12624-12636.	2.8	14
17	Hyperfine components of all rovibrational quadrupole transitions in the H2 and D2 molecules. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 253, 107186.	2.3	13
18	A computational study of the nuclear magnetic resonance parameters for double proton exchange pathways in the formamideâ€“formic acid and formamideâ€“formamidine complexes. Physical Chemistry Chemical Physics, 2009, 11, 11232.	2.8	12

#	Article	IF	Citations
19	Positions and intensities of hyperfine components of all rovibrational dipole lines in the HD molecule. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 253, 107171.	2.3	11
20	Electrochemical and spectroscopic characterization of poly(1,8-diaminocarbazole): Part I. Electropolymerization and determination of the polymer structure by FTIR studies and DFT calculations. Electrochimica Acta, 2009, 54, 4743-4750.	5.2	10
21	Ab initio ground state phenylacetyleneâ€“argon intermolecular potential energy surface and rovibrational spectrum. Journal of Chemical Physics, 2012, 137, 074305.	3.0	9
22	Subpercent agreement between ab initio and experimental collision-induced line shapes of carbon monoxide perturbed by argon. Physical Review A, 2020, 102, .	2.5	9
23	Ab initio investigation of the COâ€“N2 quantum scattering: The collisional perturbation of the pure rotational R(0) line in CO. Journal of Chemical Physics, 2021, 154, 054314.	3.0	8
24	Small and Efficient Basis Sets for the Evaluation of Accurate Interaction Energies: Aromatic Moleculeâ€“Argon Ground-State Intermolecular Potentials and Rovibrational States. Journal of Physical Chemistry A, 2014, 118, 10288-10297.	2.5	7
25	A high-accuracy theoretical study of the CH_nP Systemsnâ€‰=â€‰1-3. Journal of Computational Chemistry, 2013, 34, 2020-2031.	3.3	6
26	Hyperfine components of rovibrational dipole transitions in HT and DT. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 270, 107662.	2.3	5
27	Hyperfine structure of quadrupole rovibrational transitions in tritium-bearing hydrogen isotopologues. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 256, 107255.	2.3	4
28	Hyperfine structure of rovibrational quadrupole transitions in HD. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 272, 107753.	2.3	4
29	Hyperfine structure of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>E</mml:mi><mml:mi>F</mml:mi><mml:mmultiscripts><mml:mi mathvariant="normal">Î£</mml:mi><mml:mi>g</mml:mi><mml:mo>+</mml:mo><mml:mprescripts /><mml:none /><mml:mn>1</mml:mn></mml:mmultiscripts></mml:mrow></mml:math> state in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review A,	2.5	3
30	Calculated Nuclear Magnetic Resonance Parameters for Multiproton-Exchange and Nonbonded-Hydrogen Rotation Processes in Cyclic Water Clusters. Journal of Physical Chemistry A, 2011, 115, 5774-5784.	2.5	2
31	Theoretical Study of the Pyridineâ€“Helium van der Waals Complexes. Journal of Physical Chemistry A, 2015, 119, 10999-11006.	2.5	2
32	Ab initio studies of the ground and first excited states of the Srâ€“H2 and Ybâ€“H2 complexes. Journal of Chemical Physics, 2019, 150, 064316.	3.0	1
33	Corrigendum to â€œHyperfine structure of quadrupole rovibrational transitions in tritium-bearing hydrogen isotopologuesâ€•[J.ÂQuant.ÂSpectrosc.ÂRadiat.ÂTransf. 256 (2020), 107255]. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 266, 107602.	2.3	0
34	Corrigendum to â€œHyperfine components of all rovibrational quadrupole transitions in the H2 and D2 moleculesâ€•[J.ÂQuant.ÂSpectrosc.ÂRadiat.ÂTransf. 253 (2020), 107186]. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 271, 107750.	2.3	0