ZdzisÅ‚aw Xl;law Latajka

List of Publications by Year
in descending order

66 papers	1,516 citations	304602 22 h-index	330025 37 g-index
69 all docs	69 docs citations	69 times ranked	1130 citing authors

#	Article	IF	Citations
1	Impact of Deuteration and Temperature on Furan Ring Dynamics. Molecules, 2021, 26, 2889.	1.7	0
2	About the Aromaticity of symm-Triaminotrinitrobenzene. Journal of Physical Chemistry A, 2019, 123, 2244-2251.	1.1	2
3	Introduction: Special issue devoted in memory of Professor Oleg V. Shishkin. Structural Chemistry, 2016, 27, 1-1.	1.0	4
4	Computational Mechanochemistry. , 2016, , 233-243.		0
5	On the multiple BO bonding using the topological analysis of Electron Localisation Function (ELF). Computational and Theoretical Chemistry, 2015, 1053, 130-141.	1.1	13
6	Reaction of atomic hydrogen with formic acid. Physical Chemistry Chemical Physics, 2014, 16, 5993.	1.3	20
7	Effects of Xenon Insertion into Hydrogen Bromide. Comparison of the Electronic Structure of the HBrÂ·Â·CO₂ and HXeBrÂ·Â·CO₂ Complexes Using Quantum Chemical Topology Methods: Electron Localization Function, Atoms in Molecules and Symmetry Adapted Perturbation Theory. Journal of Physical Chemistry A, 2014, 118, 3980-3989.	1.1	5
8	Electron Localization Function Study on the Chemical Bonding in a Real Space for Tetrahedrane, Cubane, Adamantane, and Dodecahedrane and Their Perfluorinated Derivatives and Radical Anions. Journal of Physical Chemistry A, 2014, 118, 4147-4156.	1.1	15
9	Experimental and computational study of the HXeIâ‹¯HY complexes (Y = Br and I). Journal of Chemical Physics, 2013, 138, 104314.	1.2	19
10	Tuning of character of the Nâ€“O bond in HONO from covalent to protocovalent by different types of intramolecular interactions. Journal of Chemical Physics, 2013, 139, 124308.	1.2	3
11	Entropy versus aromaticity in the conformational dynamics of aromatic rings. Journal of Molecular Modeling, 2013, 19, 4073-4077.	0.8	5
12	FONO: A difficult case for theory. The ELF and ELI-D topological studies on the chemical bonding using correlated wavefunctions. Journal of Chemical Physics, 2013, 138, 134313.	1.2	1
13	Spectroscopic and Computational Characterization of the HCOÂ·Â·H2O Complex. Journal of Physical Chemistry A, 2013, 117, 4385-4393.	1.1	22
14	High Kinetic Stability of HXeBr upon Interaction with Carbon Dioxide: HXeBrÂ·Â·CO2 Complex in a Xenon Matrix and HXeBr in a Carbon Dioxide Matrix. Journal of Physical Chemistry A, 2012, 116, 4510-4517.	1.1	32
15	On the multiple Bâ€“N bonding in boron compounds using the topological analysis of electron localization function (ELF). New Journal of Chemistry, 2011, 35, 89-96.	1.4	40
16	Dynamical Nonplanarity of Benzene. Evidences from the Carâ€“Parrinello Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2011, 2, 2881-2884.	2.1	12
17	On the Intramolecular Hydrogen Bond in Solution: Carâ€“Parrinello and Path Integral Molecular Dynamics Perspective. Journal of Chemical Theory and Computation, 2011, 7, 3505-3513.	2.3	32
18	A mechanism of the 1,3â€dipolar cycloaddition between the hydrogen nitryl HNO₂ and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. International Journal of Quantum Chemistry, 2011, 111, 2378-2389.	1.0	9

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19	Electron localization function and electron localizability indicator applied to study the bonding in the peroxynitrous acid HOONO. Journal of Computational Chemistry, 2011, 32, 1528-1540.	1.5	14
20	Oxygen bound iodine (Oâ€“I): The Electron Localization Function (ELF) study on bonding in cis- and trans-IONO. Chemical Physics Letters, 2011, 506, 15-21.	1.2	6
21	Ab Initio and Quantum Chemical Topology studies on the isomerization of HONO to HNO₂. Effect of the basis set in QCT. Journal of Computational Chemistry, 2010, 31, 2555-2567.	1.5	6
22	Rotation around the glycosidic bond as driving force of proton transfer in protonated 2â€²-deoxyriboadenosine monophosphate (dAMP). Chemical Physics Letters, 2010, 490, 221-225.	1.2	6
23	Protocovalent Nâ€“O bonding in methyl nitrite (CH3ONO) and ethyl nitrite (C2H5ONO). Topological analysis of the electron localization function (ELF) and electron localizability indicator (ELI-D) functions. Chemical Physics Letters, 2010, 493, 392-398.	1.2	7
24	Proton-transfer dynamics in the (HCO₃^{â^’})₂dimer of KHCO₃from Carâ€“Parrinello and path-integrals molecular dynamics calculations. Acta Crystallographica Section B: Structural Science, 2010, 66, 222-228.	1.8	13
25	Proton Transfer Dynamics in Crystalline Maleic Acid from Molecular Dynamics Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1455-1461.	2.3	17
26	Quantum chemical topology study on the electronic structure of cis- and trans-FONO. Journal of Chemical Physics, 2010, 133, 034304.	1.2	13
27	Proton distribution in KHCO3 from abinitio molecular dynamics simulation. Chemical Physics Letters, 2009, 476, 223-226.	1.2	11
28	The structure and chemical bonding in the N₂ï£¿CuX and N₂Â·Â·Â·XCu (X = F, Cl, Br) systems studied by means of the molecular orbital and Quantum Chemical Topology methods. Journal of Computational Chemistry, 2008, 29, 2677-2692.	1.5	7
29	The protocovalent NO bond: Quantum chemical topology (QCT of ELF and ELI-D) study on the bonding in the nitrous acid HONO and its relevancy to the experiment. Chemical Physics Letters, 2008, 460, 559-562.	1.2	14
30	Car-Parrinello and path integral molecular dynamics study of the hydrogen bond in the chloroacetic acid dimer system. Journal of Chemical Physics, 2007, 127, 064304.	1.2	22
31	Electron localization function (ELF) study on intramolecular delocalization of the electron density in the H2X, H2CX and XO2 (X=O, S, Se, Te) molecules: Role of the atomic core and lone pair. Journal of Molecular Structure, 2007, 844-845, 278-285.	1.8	7
32	Ab initio characterization of the xenon dihydride dimer â€“ (HXeH)2. Chemical Physics Letters, 2003, 371, 295-303.	1.2	14
33	Structural analysis and sheep pituitary receptor binding of GnRH and its complexes with metal ions. Journal of Inorganic Biochemistry, 2003, 94, 28-35.	1.5	8
34	Density functional studies of hydrogen-bonded systems. Chemical Physics, 2001, 263, 221-230.	0.9	20
35	Quantum chemical calculations on FXeSiF. Chemical Physics Letters, 2001, 348, 147-154.	1.2	25
36	2-(Hydroxyimino)propanohydroxamic acid, a new effective ligand for aluminium. Dalton Transactions RSC, 2000, , 4201-4208.	2.3	31

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37	Dihydrogen-bonded complexes of xenon dihydride with water: Ab initio calculations and topological analysis of electron localisation function (ELF). Physical Chemistry Chemical Physics, 2000, 2, 5521-5527.	1.3	26
38	Density functional study of the Xe2H3+ cation. Chemical Physics, 1999, 247, 215-224.	0.9	11
39	Quantum Chemical Study of the Bimolecular Complex of HONO. Journal of Physical Chemistry A, 1999, 103, 6234-6239.	1.1	25
40	Infrared matrix isolation and theoretical studies of SO2â€“HNO3 and SO2â€“HONO systems. Chemical Physics, 1998, 228, 17-29.	0.9	23
41	Density Functional Study of Hydrogen-Bonded Systems:Â The Waterâ‹¯Carbon Monoxide Complex. Journal of Physical Chemistry A, 1997, 101, 5004-5009.	1.1	84
42	Structure, energetics and vibrational spectra of dimers, trimers, and tetramers of HX (X = Cl, Br, I). Chemical Physics, 1997, 216, 37-52.	0.9	51
43	Direction of Protein Biosynthesis as a Reflection of the Prebiotic Environment. Journal of Theoretical Biology, 1997, 189, 151-158.	0.8	3
44	Spectroscopic and theoretical studies of the OCOâ‹¯HF complex in pressurized gases. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3473-3479.	1.7	9
45	Density functional study of the H3Nî—¸Cl2 systemâ€”the importance of Hartree-Fock exchange in density functional methods. Computational and Theoretical Chemistry, 1996, 371, 11-16.	1.5	16
46	Critical assessment of density functional methods for study of proton transfer processes. (FHF)â‹¯. Chemical Physics Letters, 1995, 234, 159-164.	1.2	82
47	On the structure of the 3B1 excited state of water. Computational and Theoretical Chemistry, 1995, 334, 127-136.	1.5	1
48	Site-site function and successive reaction counterpoise calculation of basis set superposition error for proton transfer. Computational and Theoretical Chemistry, 1995, 342, 153-159.	1.5	6
49	The dimerization shift of the OH-stretching fundamentals of the water dimer. Chemical Physics Letters, 1994, 217, 436-442.	1.2	12
50	Theoretical study of the H2Oî—¸2CO hydrogen-bonded ternary complexes. Chemical Physics Letters, 1994, 222, 33-39.	1.2	10
51	Kinetics and thermochemistry of the reversible gas phase reaction HONO+NH3â‡ŒH3H-HONO studied by infrared diode laser spectroscopy. Chemical Physics Letters, 1994, 227, 6-12.	1.2	16
52	Matrix isolation FTIR and ab initio study of complexes between formic acid and nitrogen. Chemical Physics, 1994, 189, 245-260.	0.9	53
53	Application of density functional methods for the study of hydrogenâ€bonded systems: The hydrogen fluoride dimer. Journal of Chemical Physics, 1994, 101, 9793-9799.	1.2	138
54	Density functional theory applied to proton-transfer systems. A numerical test. Chemical Physics Letters, 1993, 208, 364-368.	1.2	89

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55	Complexes between formic acid and carbon monoxide: an ab initio investigation. The Journal of Physical Chemistry, 1993, 97, 1152-1157.	2.9	19
56	Proton transfer in the ground and first excited triplet states of malonaldehyde. The Journal of Physical Chemistry, 1992, 96, 9764-9767.	2.9	48
57	The proton position in amine-HX (X î—» Br, I) complexes. Chemical Physics, 1992, 166, 85-96.	0.9	19
58	Basis set superposition error in proton transfer potentials. Chemical Physics Letters, 1992, 196, 384-389.	1.2	27
59	Structure, energetics, and vibrational spectrum of ammonia...water. The Journal of Physical Chemistry, 1990, 94, 217-221.	2.9	47
60	Correlation between interaction energy and shift of the carbonyl stretching frequency. Chemical Physics Letters, 1990, 174, 179-184.	1.2	26
61	Basis set superposition errors and counterpoise corrections for some basis sets evaluated for a few X-.cntdot..cntdot..cntdot.M dimers. The Journal of Physical Chemistry, 1990, 94, 2267-2273.	2.9	23
62	Theoretical study of the geometry of GeH3 and electronic structure of SiH3 and GeH3. Computational and Theoretical Chemistry, 1987, 150, 189-197.	1.5	9
63	Kinetics of proton transfer in (H3CH..CH3)-. The Journal of Physical Chemistry, 1987, 91, 724-730.	2.9	25
64	Basis sets for molecular interactions. 1. Construction and tests on (HF)2 and (H2O)2. Journal of Computational Chemistry, 1987, 8, 663-673.	1.5	61
65	Basis sets for molecular interactions. 2. Application to H3N?HF, H3N?HOH, H2O?HF, (NH3)2, and H3CH?OH2. Journal of Computational Chemistry, 1987, 8, 674-682.	1.5	70
66	CNDO/2 molecular orbital calculations of dewar structures of pyridine. Journal of Molecular Structure, 1974, 21, 299-303.	1.8	8