Zoltan Varga

List of Publications by Citations

60 papers	1,120 citations	17 h-index	31 g-index
72 ext. papers	1,404 ext. citations	3.9 avg, IF	4.72 L-index

#	Paper	IF	Citations
60	Halogen acceptors in hydrogen bonding. *Coordination Chemistry Reviews*, **2006**, 250, 710-727	23.2	160
59	Global ab initio ground-state potential energy surface of N4. *Journal of Chemical Physics*, **2013**, 139, 044309	3.9	128
58	An improved potential energy surface and multi-temperature quasiclassical trajectory calculations of N2 + N2 dissociation reactions. *Journal of Chemical Physics*, **2015**, 143, 054304	3.9	124
57	Assessment of electronic structure methods for the determination of the ground spin states of Fe(ii), Fe(iii) and Fe(iv) complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 13049-13069	3.6	72
56	Potential energy surface of triplet N2O2. *Journal of Chemical Physics*, **2016**, 144, 024310	3.9	44
55	Potential energy surfaces for O + O collisions. *Journal of Chemical Physics*, **2017**, 147, 154312	3.9	41
54	Potential energy surfaces of quintet and singlet O. *Journal of Chemical Physics*, **2017**, 147, 034301	3.9	35
53	Vibrational Energy Transfer and Collision-Induced Dissociation in O+O2 Collisions. *Journal of Thermophysics and Heat Transfer*, **2019**, 33, 797-807	1.3	28
52	Global triplet potential energy surfaces for the N2(X(1)Σ+g) + O((3)P) -NO(X(2)Π) + N((4)S) reaction. *Journal of Chemical Physics*, **2016**, 144, 024309	3.9	28
51	Potential energy surface of triplet O. *Journal of Chemical Physics*, **2018**, 148, 124314	3.9	27
50	Theoretical study of the structure and bonding in ThC2 and UC2. *Journal of Physical Chemistry A*, **2012**, 116, 747-55	2.8	24
49	Quasilinear molecule par excellence, SrCl2: structure from high-temperature gas-phase electron diffraction and quantum-chemical calculations--computed structures of SrCl2.argon complexes. *Chemistry - A European Journal*, **2006**, 12, 8345-57	4.8	23
48	Long-Range Effects in Oligopeptides. A Theoretical Study of the β-Sheet Structure of Glyn (n = 2−10). *Journal of Physical Chemistry A*, **2004**, 108, 6869-6873	2.8	23
47	On the effect of 4f electrons on the structural characteristics of lanthanide trihalides: computational and electron diffraction study of dysprosium trichloride. *Journal of Chemical Physics*, **2008**, 128, 074301	3.9	22
46	Many-Body Permutationally Invariant Polynomial Neural Network Potential Energy Surface for N. *Journal of Chemical Theory and Computation*, **2020**, 16, 4822-4832	6.4	18
45	The elusive structure of CrCl(2): a combined computational and gas-phase electron-diffraction study. *Chemistry - A European Journal*, **2008**, 14, 5130-43	4.8	17
44	Does the 4f electron configuration affect molecular geometries? A joint computational, vibrational spectroscopic, and electron diffraction study of dysprosium tribromide. *Inorganic Chemistry*, **2009**, 48, 4143-53	5.1	15

43	Multi-state pair-density functional theory. *Faraday Discussions*, **2020**, 224, 348-372	3.6	14
42	Substituent effects on long-range interactions in the β-sheet structure of oligopeptides. *Computational and Theoretical Chemistry*, **2005**, 755, 247-251		14
41	Gas-phase structures of iron trihalides: a computational study of all iron trihalides and an electron diffraction study of iron trichloride. *Inorganic Chemistry*, **2010**, 49, 1039-45	5.1	12
40	Molecular constants of aluminum monohalides: caveats for computations of simple inorganic molecules. *Journal of Physical Chemistry A*, **2007**, 111, 6-8	2.8	12
39	A quasiclassical trajectory study of the N2(X(1)Σ+g) + O((3)P) -> NO(X(2)Π) + N((4)S) reaction. *Journal of Chemical Physics*, **2016**, 144, 234314	3.9	12
38	Structure and other molecular properties of actinide trichlorides AnCl3 (An = Th-Cm). *Journal of Physical Chemistry A*, **2013**, 117, 11357-63	2.8	11
37	Quasiclassical Trajectory Analysis of the N2 + N2 Reaction Using a New Ab Initio Potential Energy Surface **2014**,		10
36	Hydrogen bonding in peptide secondary structures. *International Journal of Quantum Chemistry*, **2005**, 105, 302-312	2.1	10
35	On the thermal expansion of molecules. *Structural Chemistry*, **2011**, 22, 111-121	1.8	9
34	Conservation of Angular Momentum in Direct Nonadiabatic Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 1135-1140	6.4	8
33	Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF, FeF-Ethane, and FeF-Ethylene. *Journal of Physical Chemistry A*, **2018**, 122, 2563-2579	2.8	8
32	Hyper Open-Shell States: The Lowest Excited Spin States of O Atom, Fe Ion, and FeF. *Journal of the American Chemical Society*, **2017**, 139, 12569-12578	16.4	8
31	Comprehensive study of the structure of aluminum trihalides from electron diffraction and computation. *Structural Chemistry*, **2012**, 23, 879-893	1.8	8
30	Iron dihalides: structures and thermodynamic properties from computation and an electron diffraction study of iron diiodide. *Structural Chemistry*, **2011**, 22, 327-336	1.8	8
29	Is the Inversion of Phosphorus Trihalides (PF, PCl, PBr, and PI) a Diradical Process?. *Journal of Physical Chemistry A*, **2019**, 123, 301-312	2.8	8
28	Direct diabatization based on nonadiabatic couplings: the N/D method. *Physical Chemistry Chemical Physics*, **2018**, 20, 26643-26659	3.6	8
27	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. *Angewandte Chemie - International Edition*, **2020**, 59, 10826-10830	16.4	7
26	Molecular geometry of vanadium dichloride and vanadium trichloride: a gas-phase electron diffraction and computational study. *Inorganic Chemistry*, **2010**, 49, 2816-21	5.1	7

25	Oviposition preferences of Maculinea alcon as influenced by aphid (Aphis gentianae) and fungal (Puccinia gentianae) infestation of larval host plants. *Ecological Entomology*, **2009**, 34, 90-97	2.1	7
24	Vapor phase tin diiodide: its structure and thermodynamics, a computational study. *Structural Chemistry*, **2007**, 18, 641-648	1.8	7
23	The NaDyBr4 complex; its molecular structure and thermodynamic properties. *Structural Chemistry*, **2006**, 17, 225-233	1.8	6
22	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. *Angewandte Chemie*, **2020**, 132, 10918-10922	3.6	5
21	On the thermal expansion of molecules: a sequel. *Structural Chemistry*, **2011**, 22, 1065-1066	1.8	5
20	Curious matrix effects: a computational, electron diffraction, and vibrational spectroscopic study of dysprosium triiodide. *Dalton Transactions*, **2010**, 39, 6221-30	4.3	5
19	Structures and thermodynamic properties of aluminum oxyhalides: a computational study. *Structural Chemistry*, **2008**, 19, 595-602	1.8	5
18	Modification of Jet Structure in High-Multiplicity pp Collisions due to Multiple-Parton Interactions and Observing a Multiplicity-Independent Characteristic Jet Size. *Advances in High Energy Physics*, **2019**, 2019, 1-12	1	5
17	Group 14 structural variations: perhalo derivatives of the dimetallenes dicarbenes, disilenes, digermenes, distannenes, and diplumbenes. *Structural Chemistry*, **2013**, 24, 837-850	1.8	4
16	Permutationally Restrained Diabatization by Machine Intelligence. *Journal of Chemical Theory and Computation*, **2021**, 17, 1106-1116	6.4	4
15	Potential energy surfaces for high-energy N + O collisions. *Journal of Chemical Physics*, **2021**, 154, 084304	3.9	4
14	About the structure of CH5 + and structural variations in related systems. *Structural Chemistry*, **2017**, 28, 297-301	1.8	3
13	Molecular structure and vibrational spectra of mixed MDyX4 (M = Li, Na, K, Rb, Cs; X = F, Cl, Br, I) vapor complexes: a computational and matrix-isolation infrared spectroscopic study. *Inorganic Chemistry*, **2012**, 51, 543-56	5.1	3
12	Chemistry, commentary and community: Discussion of The NaDyBr4 complex: its molecular structure and thermodynamic properties by Varga and Hargittai. *Structural Chemistry*, **2007**, 18, 269-271	1.8	3
11	Significant stacking effect between 2,4,6-triphenyl-1-phosphabenzenes. *Structural Chemistry*, **2017**, 28, 1243-1253	1.8	2
10	Jet Structure Studies in Small Systems. *Universe*, **2019**, 5, 132	2.5	2
9	Multiplicity Dependence of the Jet Structures in pp Collisions at LHC Energies. *Proceedings (mdpi)*, **2019**, 10, 3	0.3	2
8	Singlet riplet competition in the low-lying energy states of C4O4 S n (n = 1) molecules. *Structural Chemistry*, **2015**, 26, 1229-1240	1.8	2

7	Paradigms and paradoxes: the conformation of the fundamental unit of hyaluronic acid. *Structural Chemistry*, **2010**, 21, 1211-1214	1.8	2
6	Production of pions, kaons, (anti-)protons and (phi) mesons in XeXe collisions at (sqrt{s_{mathrm{NN}}}) = 5.44 TeV. *European Physical Journal C*, **2021**, 81, 1	4.2	2
5	B2N2O4: Prediction of a Magnetic Ground State for a Light Main-Group Molecule. *Inorganic Chemistry*, **2015**, 54, 8552-9	5.1	1
4	Potential energy surface for high-energy N + N collisions. *Physical Chemistry Chemical Physics*, **2021**, 23, 26273-26284	3.6	1
3	H2O coordination in macropa complexes of f elements (Ac, La, Lu): feasibility of the 11th coordination site. *Structural Chemistry*, **2021**, 32, 643-653	1.8	1
2	Prompt D0, D+, and D*+ production in PbPb collisions at $$ sqrt{s_{mathrm{NN}}} $$ = 5.02 TeV. *Journal of High Energy Physics*, **2022**, 2022, 1	5.4	1
1	Metal–ligand interactions in complexes of cyclen-based ligands with Bi and Ac. *Structural Chemistry*, **2021**, 32, 1719-1731	1.8	0